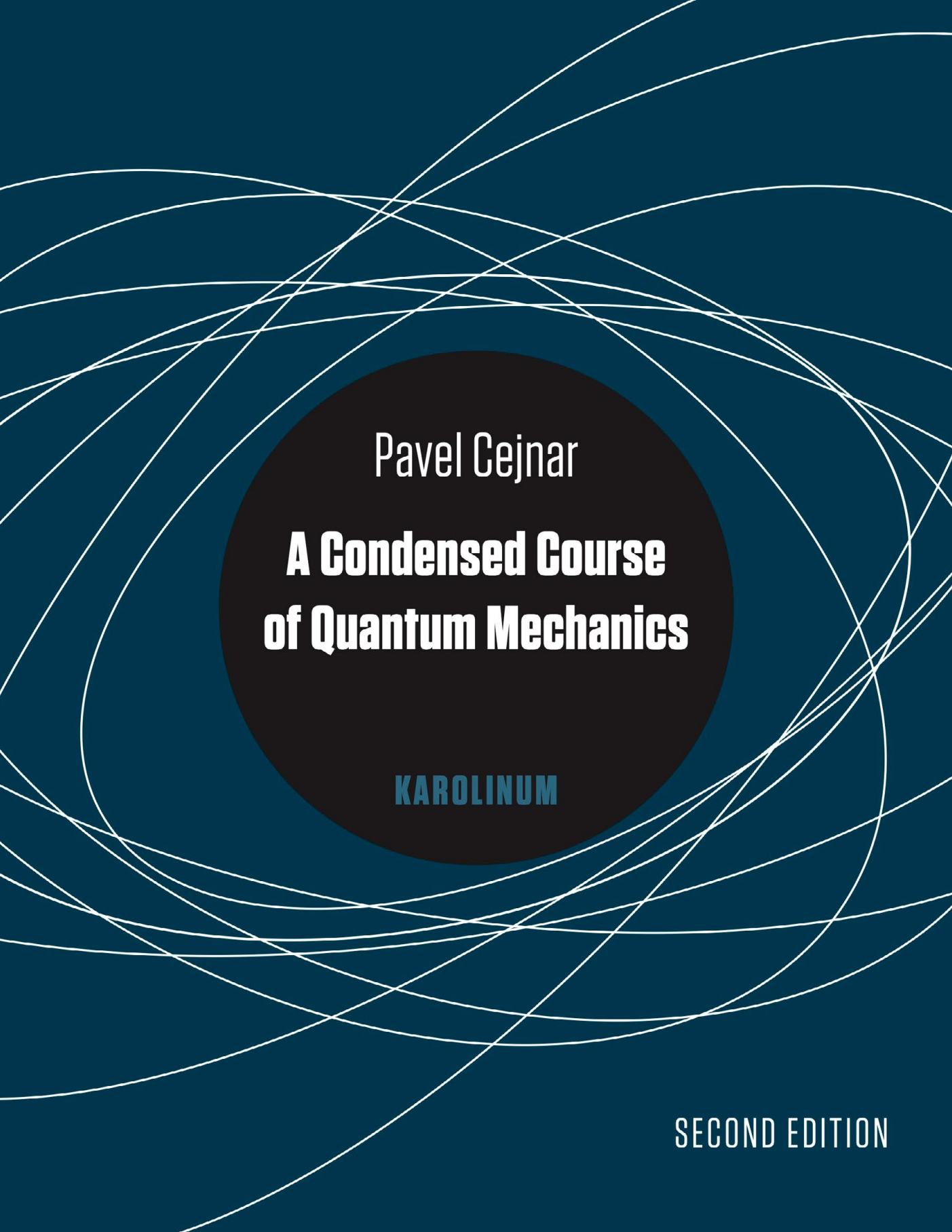
Pavel Cejnar
A Condensed Course of Quantum Mechanics
KAROLINUM
SECOND EDITION

A Condensed Course of Quantum Mechanics (2nd ed.)

Pavel Cejnar

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Preface to the first edition

This book was conceived as a collection of notes to my two-semester lecture on quantum mechanics for third-year students of physics at the Faculty of Mathematics and Physics of the Charles University in Prague. It was created in 2011-12.

At first, I just wanted to write down the most important facts, formulas and derivations in a compact form. The information flew in a succinct, "staccato" style, organized in larger and smaller bits (the ■ and ▶ items), rarely interrupted by wordy explanations. I enjoyed the thick, homogeneous mathematical form of the notes. Calculations, calculations, calculations... I thought of a horrified historian or sociologist who finds no oasis of words. This is how we, tough guys, speak!

However, I discovered that the dense form of the notes was hardly digestible even for tough guys. I had to add some words. To create a "storyteller" who wraps the bare formulas into some minimal amount of phrases. His voice, though still rather laconic, may help to provide the proper motivation and clarify the relevant context. I also formed a system of specific "environments" to facilitate the navigation. In particular: Among crowds of calculations there appears a hierarchy of highlighted formulas:*

important essential 1 essential 2 crucial

Assumptions or foundational concepts, irreducible to other statements/concepts, appear in boxes:† Answer to ultimate question of life, universe & everything = 42
Here and there come some historical notes:‡ ◀ 2013: *Condensed Course* issued
Handmade schemes (drawn on a whiteboard) illustrate some basic notions.

In this way, the notes have turned into a more serious thing. They almost became a *textbook*! The one distinguished from many others by expanded mathematical derivations (they are mostly given really step by step) and reduced verbal stuffing (just necessary comments in between calculations). This makes the book particularly well suited for conservation purposes—acquired knowledge needs to be stored in a *condensed,* dense enough form, having a compact, nearly tabular structure.

However, as follows from what has been said, this book *cannot* be considered a standard textbook. It may hardly be read with ease and fluency of some more epic treatises. One rather needs to proceed cautiously as a detective, who has to precisely fix all objects on the stage (all symbols, relations etc.) before making any small step forward. This book can be used as a teaching tool, but preferably together with an

*Such formulas are highly recommended to memorize! Although all students of physics & mathematics seem to share a deep contempt for any kind of memorization, I have to stress that all results cannot be rederived in reasonable time limits. There is no escape from saving the key formulas to the memory and using them as quickly reachable starting points for further calculations.

†However, these assumptions do not constitute a closed system of axioms in the strict mathematical sense.

‡I believe that knowledge of history is an important part of understanding. The concepts do not levitate in vacuum but grow from the roots formed by concrete circumstances of their creation. If overlooking these roots, one may misunderstand the concepts.

oral course or a more talkative textbook on quantum mechanics. Below I list some of my favorite candidates for additional guiding texts [1–10].

I have to stress that the notes cover only some parts of *non-relativistic* quantum mechanics. The selection of topics is partly fixed by the settled presentation of the field, and partly results from my personal orientation. The strategy is to introduce the complete general formalism along with its exemplary applications to simple systems (this takes approx. one semester) and then (in the second semester) to proceed to some more specialized problems. Relativistic quantum mechanics is totally absent here; it is postponed as a prelude for the quantum field theory course.

Quantum mechanics is a complex subject. It obligates one to have the skills of a mathematician as well as the thinking of a philosopher. Indeed, the mathematical basis of quantum physics is rather abstract and it is not obvious how to connect it with the observed "reality". No physical theory but quantum mechanics needs such a sophisticated PR department. We will touch the interpretation issues here, but only very slightly. Those who want to cultivate their opinion (but not to disappear from the intelligible world) are forwarded to the classic [11]. The life saving trick in this *terra incognita* is to tune mind to the joy of thinking rather than to the demand of final answers. The concluding part of the theory may still be missing.

Before we start I should not forget to thank all the brave testers—the first men, mostly students, who have been subject to the influence of this book at its various stages of preparation. They were clever enough to discover a lot of mistakes. Be sure that the remaining mistakes are due to their generous decision to leave some fish for the successors.

In Prague, January 2013

Comments on the second edition

Welcome to the new edition of the *Condensed course*.

While using the first edition for more than a decade of my teaching, I found many items that needed to be fixed, many explanations that should be improved, and many topics that would be worth adding. I have tried to make these important changes in this new edition. In particular, I have made most of the explanations a bit more wordy, I have added several new themes, I have drawn many new figures, I have partly rearranged the content and created a detailed index, and I have corrected numerous misprints.

I hope that the new edition will be much more user-friendly and also more complete than the first one. Though the telegraphic style is deliberately preserved to keep all explications condensed, the book is more viable for all readers, including those with limited initial knowledge. Extensions and new topics make the book more robust, providing necessary initial knowledge for most of the main presently active directions of nonrelativistic quantum theory. I believe that the *Condensed*

course in the present form offers a balanced concise introduction to the traditional topics, related to the general formalism and natural quantum systems, as well as to modern topics, focused on artificial quantum systems and quantum information.

And the last but not least: I pay off my big debt from the first edition by adding the following "essential historical remark":

◀ Essential historical remark ☺

1902: Jára Cimrman anticipates quantum uncertainty by studying his rat trap bait-box mechanism & answering naughty teenager's questions of E. Schrödinger

In Prague, August 2025

Recommended textbooks:

[1] J.J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, 1985, 1994)
[2] J.J. Sakurai, J.J. Napolitano, *Modern Quantum Mechanics* (Addison-Wesley, 2011)
(a modified edition of [1])
[3] G. Auletta, M. Fortunato, G. Parisi, *Quantum Mechanics* (Cambridge University Press, 2009)
[4] L.E. Ballantine, *Quantum Mechanics. A Modern Development* (World Scientific, Singapore, 1998)
[5] A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer, 1995)
[6] A. Bohm, *Quantum Mechanics: Foundations and Applications* (Springer, 1979, 1993)
[7] W. Greiner, *Quantum Mechanics: An Introduction* (Springer, 1989)
W. Greiner, *Quantum Mechanics: Special Chapters* (Springer, 1998)
W. Greiner, B Müller, *Quantum Mechanics: Symmetries* (Springer, 1989)
[8] E. Merzbacher, *Quantum Mechanics* (Wiley, 1998)
[9] V. Zelevinsky, *Quantum Physics*, Volume 1 & 2 (Wiley-VCH, 2011)
[10] A. Messiah, *Quantum Mechanics* (Dover, 1999)
(living classic, first published in 1958)

Further reading:

[11] J.S. Bell, *Speakable and Unspeakable in Quantum Mechanics* (Cambridge University Press, 1987)
(a collection on brilliant essays on the interpretation of quantum theory)
[12] R. Omnés, *The Interpretation of Quantum Mechanics* (Princeton University Press, 1994)
(a more systematic treatment of the interpretation questions)
[13] T. Lancaster, S.J. Blundell, *Quantum Field Theory for a Gifted Amateur* (Oxford Univ. Press, 2014)
(a readable introduction to the world behind nonrelativistic QM)
[14] D. Griffiths, *Introduction to Elementary Particles* (Wiley-VCH, 2008)
(an accessible overview of the standard model of fundamental particles and interactions)
[15] C. Gardiner, P. Zoller *The quantum world of ultracold atoms and light*
Book I: *Foundations of quantum optics* (Imperial College Press, 2014)
Book II: *The physics of quantum-optical devices* (Imperial College Press, 2015)
Book III: *Ultra-cold atoms* (World Scientific, 2017)
(an introduction to controllable quantum systems)
[16] A. Pais, *Inward Bound of Matter and Forces in the Physical World* (Clarendon Press, 1986)
(an exciting treatise on the history of the physics of microworld)

Rough guide to notation (no notation is perfect!)

	Hilbert spaces, vectors & wavefunctions, scalar products
$\alpha\|\psi\rangle+\beta\|\psi'\rangle$	superposition ≡ linear combination of state vectors ($\alpha,\beta\in\mathbb{C}$)
$\{\|\phi_i\rangle\}_{i=1}^{d_\mathcal{H}}$, $d_\mathcal{H}$	general set of basis vectors in Hilbert space $\mathcal{H}$, dimension of $\mathcal{H}$
$\|\psi\rangle$, $\langle\psi'\|$, $\langle\psi'\|\psi\rangle$	ket & bra forms of state vectors, scalar product
$\|\|\psi\|\|=\sqrt{\langle\psi\|\psi\rangle}=1/\mathcal{N}$	norm of vector = 1/normalization coefficient
$\underline{\mathcal{H}}$, $\mathcal{H}$, $\overline{\mathcal{H}}$	Gelfand's hierarchy of spaces (rigged Hilbert space)
ℓ^2, $\mathcal{L}^2(\mathbb{R}^3)$, $\mathbb{C}^d$	specific separable or finite Hilbert spaces
$\mathrm{Span}\{\|\psi_1\rangle...\|\psi_n\rangle\}$	linear space spanned by the given vectors
$\mathcal{H}^{(N)}$, $\mathcal{H}_\pm^{(N)}$	N-particle Hilbert space, its exchange symmetric/antisym.subspaces
$\mathcal{H}_1\otimes\mathcal{H}_2$, $\bigotimes_{i=1}^{n}\mathcal{H}_i$, $\mathcal{H}_1\oplus\mathcal{H}_2$, $\bigoplus_{i=1}^{n}\mathcal{H}_i$	direct product & sum of Hilbert spaces
$\|\psi\rangle_1\|\psi'\rangle_2$, $\|\Phi_{ij}\rangle\equiv\|\phi_{1i}\rangle_1\|\phi_{2j}\rangle_2$	general factorized state vector, factorized basis in $\mathcal{H}_1\otimes\mathcal{H}_2$
$\psi(\vec{x})\equiv\langle\vec{x}\|\psi\rangle$, $\widetilde{\psi}(\vec{p})\equiv\langle\vec{p}\|\psi\rangle$	wavefunction of spinless particle in coordinate & momentum repres.
$\psi(\vec{x},m_s)\equiv\boldsymbol{\psi}(\vec{x})$	single-particle wavefunction in single/multicomponent forms
$\Psi(\boldsymbol{\xi}_1\dots\boldsymbol{\xi}_N)$	N-particle wavefunction with $\boldsymbol{\xi}_1\equiv(\vec{x}_i,m_i)$
$\|a\rangle$, $\|a^{(k)}\rangle$ $\|a_i\rangle$, $\|a_i^{(k)}\rangle$	eigenvector of operator $\hat{A}$ with eigenvalue a or a_i (degeneracy index k)
$\|E_i\rangle$, $\|E_i^{(k)}\rangle$, $\|E\rangle$	eigenvectors of Hamiltonian (discrete or continuous energy)
$\|\uparrow\rangle$, $\|\downarrow\rangle$	up & down projection states of spin $s=\frac{1}{2}$
$\|lm\rangle$, $\|sm_s\rangle$, $\|jm_j\rangle$	states with orbital, spin & total ang. momentum l, s & j, projection $m_\bullet$
$R_{nl}(r)=u_{nl}(r)/r$, $R_{kl}(r)$	radial wavefunction (n≡princ.q.num., l≡orb.ang.mom., k≡|wave vec.|)
$C^{jm}_{j_1m_1j_2m_2}\equiv\langle j_1j_2jm\|j_1m_1j_2m_2\rangle$	Clebsch-Gordan coefficient for the coupling of 2 angular momenta
$\|\psi_{ni}\rangle$, $\|\psi_i^{(n)}(\lambda)\rangle$	nth-order perturbation correction & approx. of ith energy eigenstate
$\|0\rangle$, $\|n_1,n_2,...\rangle$	vacuum state, basis states of $\mathcal{H}_\pm^{(N)}$ in occupation-number repres.
$\|\Psi_{\mathrm{HF}}\rangle$, $\|\Psi_{\mathrm{HB}}\rangle$, $\|\Psi_{\mathrm{BCS}}\rangle$	Hartree-Fock/Bose & BCS approx. of many-body ground state
	Operators: observables, transformations & evolution
$\hat{O}$, $\hat{O}^\dagger$, $\hat{O}^{-1}$	linear operator, its Hermitian conjugate & inverse
$O_{ij}=\langle\phi_i\|\hat{O}\|\phi_j\rangle$	matrix element of operator $\hat{O}$
$\|\|\hat{O}\|\|$, $\mathrm{Def}(\hat{O})$	norm & definition domain of operator
$\hat{A}$, $\hat{U}$, $\hat{I}$, $\hat{I}_\mathcal{H}$	general Hermitian & unitary operator, identity operator (in space $\mathcal{H}$)
$\hat{A}_{\mathrm{S}}$, $\hat{A}_{\mathrm{H}}(t)$, $\hat{A}_{\mathrm{D}}(t)$	Schrödinger, Heisenberg, Dirac representations of observable
$\dot{\hat{A}}$	operator expressing time derivative of observable
$\hat{A}_1\otimes\hat{A}_2$	tensor product of operators acting in $\mathcal{H}_1\otimes\mathcal{H}_2$
$\mathcal{S}(\hat{A})$, $\mathcal{D}(\hat{A})$, $\mathcal{C}(\hat{A})$	full spectrum of observable $\hat{A}$, its discrete & continuous parts
$\hat{P}_0$, $\hat{P}_\pm^{(N)}$	projector to a general subspace $\mathcal{H}_0\subset\mathcal{H}$, projector to $\mathcal{H}_\pm^{(N)}$
$\hat{P}_a$, $\hat{\Pi}_a$, $\hat{\mathbf{\Pi}}_{(a_1,a_2)}$	projectors to discrete & continuous eigenvalue subspaces
$\vec{\nabla}$, Δ	gradient & Laplace operator (if not an interval or gap)
$\hat{\vec{x}}$, $\hat{\vec{p}}$, $\hat{\vec{\pi}}$	coordinate operator, canonical & mechanical momentum operator
$\hat{H}$, $\hat{K}$, $\hat{V}$, $\hat{H}'$	Hamiltonian, its kinetic & potential terms, Hamiltonian perturbation
$\hat{\vec{L}}$, $\hat{\vec{S}}$, $\hat{\vec{J}}$	orbital, spin & total angular momentum operators
$\hat{J}_0\equiv\hat{J}_z$, $\hat{J}_\pm\equiv\hat{J}_x\pm i\hat{J}_y$	spherical components of $\hat{\vec{J}}$, shift operators for $\|jm\rangle$ eigenstates
$\hat{\vec{\sigma}}\equiv(\hat{\sigma}_x,\hat{\sigma}_y,\hat{\sigma}_z)$	the triplet of Pauli matrices
$\hat{\vec{D}}$, $\hat{\vec{\mu}}$	operators of electric & magnetic dipole moments
$\hat{b}_k,\hat{b}_k^\dagger$; $\hat{a}_k,\hat{a}_k^\dagger$; $\hat{c}_k,\hat{c}_k^\dagger$	annih. & creation operator of boson, fermion or gen.particle in state $\|\phi_k\rangle$
$\hat{N}$, $\hat{N}_k$	total number of particles & number of particles in basis state $\|\phi_k\rangle$
$\hat{O}^{(n)}$	n-body operator
$\hat{T}_{\vec{a}}$, $\hat{T}_{\Delta o}$	space translation or general eigenstate shift operator $\|o\rangle\to\|o+\Delta o\rangle$
$\hat{R}_{\vec{n}\phi}\equiv\hat{R}_{\mathbf{R}}$, $\mathbf{R}(\alpha\beta\gamma)$	rotation operator in $\mathcal{H}$ (axis,angle) & rot.matrix in 3D (Euler angles)
$\hat{\mathcal{P}}$, $\hat{\mathcal{T}}$	space inversion operator (parity) & time reversal operator
$\hat{G}_i$, $\hat{C}_\mathcal{G}$	generator & Casimir operator of a group $\mathcal{G}$

$\hat{U}(t)$, $\hat{U}(t_1,t_0)$	evolution operator for times $t_0 \overset{t}{\to} t_1$
$\hat{G}^{\pm}(t,t_0)$, $G^{+}(\vec{x}t\vert\vec{x}_0t_0)$	retarded & advanced Green operators, propagator
$\hat{G}^{\pm}(E)$, $\hat{T}^{\pm}(E)$	energy image of Green operators, T-operator in scattering theory
$\langle\Phi_{E'n'}\vert\hat{S}\vert\Phi_{En}\rangle$,$\langle\phi_{\vec{k}'}\vert\hat{S}\vert\phi_{\vec{k}}\rangle$	S-matrix elements
$\mathfrak{T}$	time ordering of operator product
$[\hat{A}^{\lambda_1}\times\hat{B}^{\lambda_1}]^{\lambda}_{\mu}$	tensor coupling of spherical tensor operators $\hat{A}^{\lambda_1}_{\mu_1}$, $\hat{B}^{\lambda_1}_{\mu_2}$
$[\hat{A},\hat{B}]$,$\{\hat{A},\hat{B}\}$	commutator & anticommutator of operators
$\{A,B\}$	Poisson bracket of classical observables
$\mathrm{Tr}\,\hat{O}$, $\mathrm{Tr}_1\hat{O}$, $\mathrm{Det}\,\hat{O}$	trace of operator/matrix, partial trace over $\mathcal{H}_1$ in $\mathcal{H}_1\otimes\mathcal{H}_2$, determinant
	Statistics, probabilities & densities
$\mathfrak{a}_{\psi}(\psi')$, $\mathfrak{a}_{\psi}(x)$	amplitude to identify $\vert\psi\rangle$ with $\vert\psi'\rangle$ or to measure value x of an observable
$\mathfrak{p}_{\psi}(\psi')$, $\mathfrak{p}_{\psi}(\mathcal{H}_0)$	probability to identify $\vert\psi\rangle$ with $\vert\psi'\rangle$ or with an arbitrary state from $\mathcal{H}_0\subset\mathcal{H}$
$\mathfrak{p}_{\psi}(x)$	probability to measure values x of some observables in state $\vert\psi\rangle$
$\mathfrak{a}_0(t)$, $\mathfrak{p}_0(t)$	survival amplitude & probability of $t=0$ initial state at time t
$\mathfrak{p}_c(a\vert b)$	conditional probability of a given b (depending on parameter c)
$\mathfrak{a}_{ji}(t),\mathfrak{p}_{ji}(t),\mathcal{R}_{ji}(t),\mathcal{R}_{\mathrm{X}}$	$\vert\phi_i\rangle \overset{t}{\to} \vert\phi_j\rangle$ transition amplitude, probability & rate, rate of event X
$\langle A\rangle_{\psi}$, $\langle a\rangle_c$	average value of observable A in $\vert\psi\rangle$, average of a for a fixed parameter c
$\langle\!\langle A^2\rangle\!\rangle_{\psi}\equiv\Delta^2_{\psi}A$	variance of the distribution $\mathfrak{p}_{\psi}(a)$ (squared uncertainty of observable A)
$\rho(\vec{x},t)$, $\vec{j}(\vec{x},t)$	single-particle probability density & flow at point $\vec{x}$, time t
$\hat{\rho}(t)$, $\hat{\rho}_1(t)=\mathrm{Tr}_2\hat{\rho}(t)$	general density operator, density operator of a subsystem (partial trace)
$W_{\rho}(\vec{x},\vec{p},t)$	Wigner quasiprobability distribution in phase space for a given $\hat{\rho}$
$\rho(\vec{x},\vec{p},t)$	classical probability distribution in phase space
$\varrho(E)$, $\varrho_{\mathrm{f}}(E)$, $\varrho(\boldsymbol{\xi})$	level density, density of final states, particle density at $\boldsymbol{\xi}\equiv(\vec{x},m_s)$
	Physical constants & parameters, various physical quantities
$\hbar=h/2\pi$	reduced & unreduced Planck constant
c, e, ϵ_0, α	speed of light, elementary charge, vacuum permitivity, fine-structure const.
λ_{C}, λ_{C}, λ_{B}, λ_{B}, a_{B}	reduced & unreduced Compton & de Broglie wavelengths, Bohr radius
$\vec{k}$, ω	wavevector, angular frequency
$M,\mathcal{M}$, q	particle mass, two-particle reduced mass, particle charge
E, E_i, E_{ni}, $E_i^{(n)}(\lambda)$	continuous & discrete energy, its n^{th}order perturb.correction & approximation
ε_k, n_k	energies & occupation numbers of single-particle states
V, $\vec{A}$, $\vec{\mathcal{E}}$, $\vec{B}$	scalar & vector electromagnetic potentials, el. intensity & mag. induction
$\frac{d\sigma}{d\Omega}$, σ^{el}, σ^{inel}, σ^{tot}	differential cross section, integral elastic, inelastic & total cross sections
$f_{\vec{k}}(\vec{k}')$, $f_{n\vec{k}}(\vec{k}')$, $f^{(n)}_{\vec{k}}(\vec{k}')$	scattering amplitude, its n^{th}order Born correction & approximation
$F_l(k)$, $S_l(k)$, $\delta_l(k)$, $\eta_l(k)$	partial wave amplitude, S-matrix, phase shift & inelastic suppression factor
R, $l_{\max}$	range of potential, maximal orbital angular momentum
S_{ρ}	von Neumann entropy of density operator $\hat{\rho}$
$Z(\beta)$, $Z(\beta,\mu)$	(grand)canonical partition function ($\beta\equiv$ inverse temp., $\mu\equiv$ chem. pot.)
$S[\vec{x}(t)]$, $S(\vec{x},t)$, $\mathcal{L}(\vec{x},\dot{\vec{x}})$	classical action (functional & function forms), Lagrangian
	Special functions & miscellaneous mathematical symbols
$j_l, n_l, h_l^{\pm}(kr)$	Bessel, Neumann & Hankel functions
$L_i^j(\rho)$, $H_n(\xi)$	associated or generalized Laguerre polynomials & Hermite polynomials
$P_{lm}(\cos\vartheta)$,$Y_{lm}(\vartheta,\varphi)$	associated Legendre polynomial, spherical harmonics ($\vartheta,\varphi\equiv$sph.angles)
$D^j_{m'm}(\alpha\beta\gamma)\equiv D^j_{m'm}(\mathbf{R})$	Wigner matrix/function (Euler angles of rotation matrix)
$\delta(x)$, $\delta_{\epsilon}(x)$, $\Theta(x)$	Dirac δ-function, imperfect δ functions, step function
δ_{ij}, ε_{ijk}	Kronecker & Levi-Civita symbols
$(1,2,3)\equiv(x,y,z)$	indices of Cartesian components
$\vec{n}$, $\left\{\begin{smallmatrix}(\vec{n}_x,\vec{n}_y,\vec{n}_z)\\(\vec{n}_r,\vec{n}_\vartheta,\vec{n}_\varphi)\end{smallmatrix}\right\}$	unit vector, $\left\{\begin{smallmatrix}\text{Cartesian}\\\text{spherical}\end{smallmatrix}\right\}$ orthonormal coordinate vectors
$\{X_i\}_{i=1}^n$,$\{X_i\}_{i\in\mathcal{D}}$,$\{X(c)\}_{c\in\mathcal{C}}$	discrete/continuous set of objects
Min, Max, Sup$\{X_i\}_i$	minimum, maximum, supremum of a set of numbers
iff, l.h.s., r.h.s	"if and only if", the left- / right-hand side (of an equation)

Distant outline of quantum physics

Historical origins: Quantum mechanics was born in the 1900s in analyses of (i) electromagnetic radiation emitted by matter in thermal equilibrium and (ii) specific heats of solids at low absolute temperatures. A few years later, the discovery of the structure of atom implied a more fundamental problem: (iii) the question of stability of matter. A solution of all these problems was found in a modification of the laws of classical (Newtonian) physics by assuming some particular rules of quantization for certain physical quantities like energy. These principles (which invited the word "quantum") moreover explained an older mystery of discrete spectra of light radiated by single elements. However, it turned out that a much more radical modification of the physics paradigm was needed. The consistent theory of quantum phenomena was build in the piece by piece manner during the 1920s and 1930s. This development explains why quantum theory (in contrast to Einstein's relativity) carries traces of rather different approaches and ways of thinking. Discussions on the interpretation of quantum theory continue up to the present days.

Probabilistic character: Quantum physics is ultimately indeterministic. It does not generally predict precise outcomes of individual experiments but only probabilities of various alternative results. It is the only theory in which randomness represents a really fundamental concept (its use in the classical context is just a tool to overcome a lack of information). Quantum physics may be considered as a simultaneous description of multiple alternatives of physical reality with no possibility to predict which of the alternatives will be finally actualized for a particular observer.

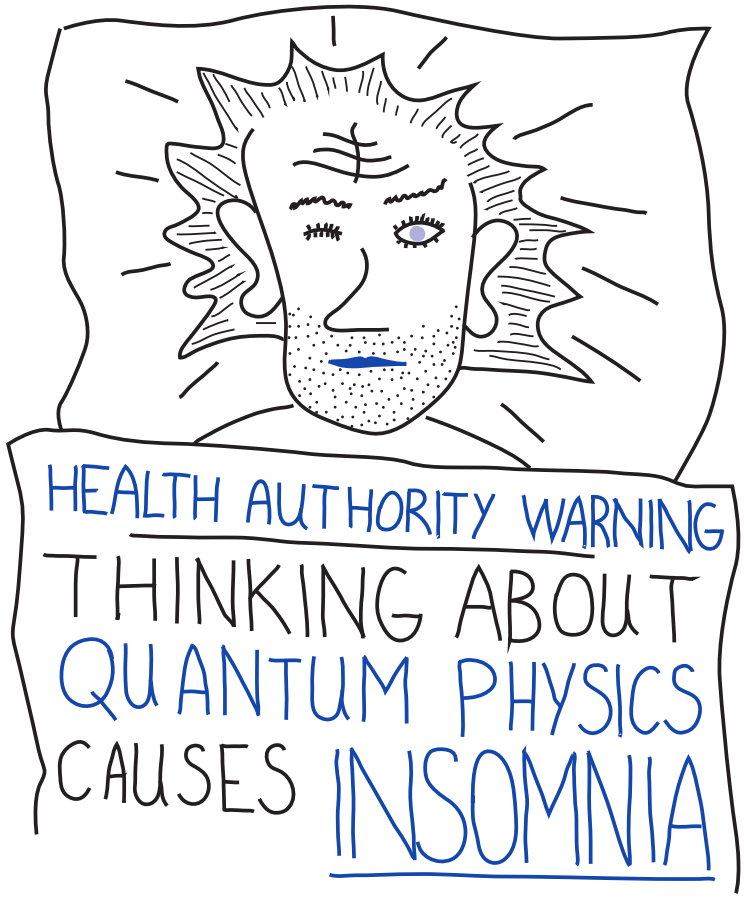
Linearity: Underlying the dynamics of quantum probabilities, there is a rather simple linear theory which makes use of so-called quantum amplitudes. An amplitude $\mathfrak{a}=|\mathfrak{a}|e^{i\varphi}$ of a certain physical event is a number inside the unit circle of the $\mathbb{C}$ plane such that the probability of the event is $\mathfrak{p}=|\mathfrak{a}|^2$. Though the observable output (probability $\mathfrak{p}$) is contained only in $|\mathfrak{a}|$, the phase angle φ is irreducible. Manifestation of linearity is twofold: (i) If a given system can be prepared in two particular initial states, denoted as $|\psi_1\rangle$ and $|\psi_2\rangle$ (generalization to more states is obvious), quantum theory requires that it can also be prepared in a state $\alpha_1|\psi_1\rangle+\alpha_2|\psi_2\rangle$, which corresponds to a linear combination (quantum superposition) of the above two states with arbitrary complex coefficients α_1 and α_2. The meaning of quantum superpositions is highly counterintuitive — e.g., they may represent states in which a particle simultaneously takes several positions. (ii) If the quantum amplitudes of a given measurement outcome for the two initial states are $\mathfrak{a}_1$ and $\mathfrak{a}_2$, the corresponding amplitude for the above superposition is $\mathfrak{a}=\mathcal{N}(\alpha_1\mathfrak{a}_1+\alpha_2\mathfrak{a}_2)$, where the normalization coefficient $\mathcal{N}\in\mathbb{R}$ ensures that an integral of $\mathfrak{p}=|\mathfrak{a}|^2$ over all possible outcomes is equal to 1. Linearity of amplitudes implies nonlinearity of probabilities, which is the key for explanation of various quantum interference effects.

Complementarity: In quantum theory, all conceivable quantities that can be measured on a given system are sorted according to their mutual compatibility. Any observable is compatible only with a subset of the remaining observables and incompatible with the others. Any set of compatible observables can be simultaneously known with certainty, but this knowledge excludes a precise determination of any incompatible observable. Joint probabilities of simultaneous measurement outcomes can be consistently determined only for sets of compatible observables; for sets of incompatible observables they depend on details of the measurement procedure.

Nonseparability: Evolution of a given quantum system S often includes interaction with an external environment and/or other degrees of freedom E. Linearity of quantum theory leads to creation of superpositions of the composite system $\mathrm{S}+\mathrm{E}$ that have a form $\sum_i \alpha_i |\psi_i\rangle_\mathrm{S} |\psi'_i\rangle_\mathrm{E}$. Here $|\psi_i\rangle_\mathrm{S}$ and $|\psi'_i\rangle_\mathrm{E}$ are mutually correlated states of S and E, joint into a separable state $|\psi_i\rangle_\mathrm{S}|\psi'_i\rangle_\mathrm{E}$ of the $\mathrm{S}+\mathrm{E}$ system, and α_i are some coefficients. The whole superposition (unlike its individual terms) cannot in general be factorized to a single product of S and E states. Hence in these so-called entangled states the subsystems S and E are not separable. An ensemble of interacting quantum subsystems can become a strongly holistic object in which correlations between distant parts are stronger than allowed in classical physics.

Quantum measurement: The entanglement process takes place also during the act of a general measurement. Unfactorizable superpositions resulting from this process correlate various states of the measuring apparatus (different measurement outputs) with the associated states of the measured system. Identifying the actual reality with only a single output, we select only a part of the superposition. This is often treated as an irreducible influence of quantum measurement (or of an observer, who may be considered as the "selector" of reality) on the measured object.

Links to other branches of physics: Quantum physics is a continuation of classical physics to the world of small objects and/or tiny actions. It is treated in two parts: the nonrelativistic and relativistic quantum theory. Since the combination of relativistic and quantum laws implies new phenomena, the general formalism of quantum theory is first applied to nonrelativistic mechanics, which is sufficient in the description of a large class of objects. The same formalism is subsequently recalled in the context of special relativity, leading to the quantum field theory, which provides so far the deepest description of elementary particles of matter and their mutual interactions. Unification of quantum theory with general relativity (theory of gravity) is not available yet. Quantum theory is a basis for great majority of contemporary "applied" physics, like molecular, atomic, nuclear and subnuclear physics, condensed matter and solid-state physics, optics, astrophysics etc. Recently, some particular applications of quantum laws gave rise to a special branch of physics called "quantum information".


HEALTH AUTHORITY WARNING
THINKING ABOUT
QUANTUM PHYSICS
CAUSES INSOMNIA

INTRODUCTION

Before sailing out, we encourage the crew to get ready for adventures. Quantum mechanics deals with phenomena, which are rather unusual from the viewpoint of our common macroscopic experience. Description of these phenomena makes us sacrifice some principles which we used to consider self-evident.

■ Quantum level

Quantum theory describes objects on the atomic and subatomic scales, but also larger objects if they are observed with an extremely **high resolution**.

▶ Planck constant

The domain of applicability of quantum mechanics is determined by constant

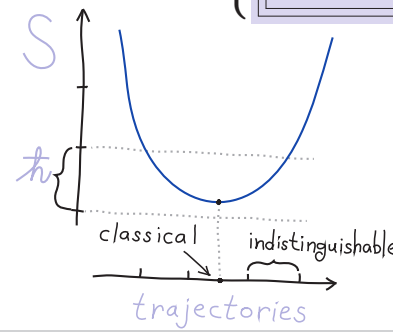
$$\boxed{\hbar \doteq 1.05 \cdot 10^{-34}\ \mathrm{J{\cdot}s} \doteq 0.66\ \mathrm{eV{\cdot}fs}}$$

which defines a **quantum unit of action**

▶ Phenomena whose actions are on/below the scale of $\hbar$ belong to the quantum jurisdiction. However, even phenomena with larger absolute actions can get to the quantum domain if the difference of actions between distinguishable alternatives reaches the $\hbar$ scale. Consider two trajectories $\mathbf{q}_1(t)$ & $\mathbf{q}_2(t)$ in the configuration space of the system ($\mathbf{q}$ is a multidimensional vector of generalized coordinates depending on time t) which, in the given experimental situation, are on the limit of mutual distinguishability (so these and similar trajectories can still be experimentally distinguished from each other, but the trajectories which are closer than these cannot). The classical action of each trajectory is $S[\mathbf{q}_\bullet(t)]$. The difference $\Delta S = |S[\mathbf{q}_1(t)] - S[\mathbf{q}_2(t)]|$ determines whether the situation can be described in the classical or quantum way:

Classical mechanics
Quantum mechanics
} applies if the difference satisfies $\begin{cases} \Delta S \gg \hbar \\ \Delta S \lesssim \hbar \end{cases}$

In particular, if the minimum of the action functional S expressed on the level of resolution $\Delta S \sim \hbar$ extends across several distinguishable trajectories, all these trajectories must be *somehow* taken into account *simultaneously*. Quantum description is then unavoidable.



◀ Historical remark

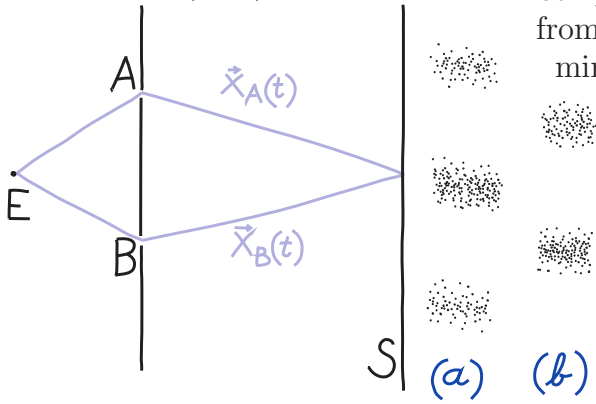
1900: Max Planck introduced $\hbar$ along with the quanta of electromagnetic radiation to explain the blackbody radiation law
1905: Albert Einstein confirmed elmag. quanta in the explanation of photoeffect
1913: Niels Bohr introduces a quantum model of atoms (“old quantum mechanics”)

■ Double-slit experiment

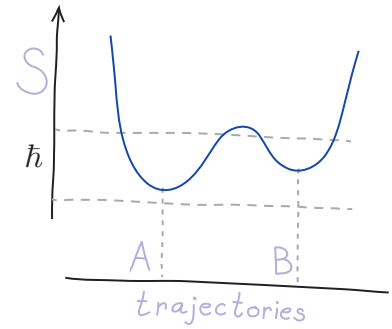
According to Richard Feynman and many others, this is the most crucial quantum experiment that allows one to realize how unusual the quantum world is. There exist numerous variations and improvements of this experiment.

▸ Arrangement

Components: Emitter E which emits particles (in the one by one mode), the plate with open slits A and B, the screen S where positions of arriving particles are detected (dots)



Both particle trajectories $\vec{x}_{\rm A}(t)$ and $\vec{x}_{\rm B}(t)$ from the emitter ($\vec{x}_{\rm E}$) to the screen ($\vec{x}_{\rm S}$) minimize the action functional $S[\vec{x}(t)]$. Suppose $|S_{\rm A} - S_{\rm B}| \lesssim \hbar$



▸ Regimes and results of measurements

(a) Interference setup: position of the particle is measured only at the screen ⇒ individual particle hits are randomly scattered within strips that form a wave-like interference pattern

(b) Which-path setup: prior the screen measurement, the particle position is measured—either explicitly (with the results observed), or implicitly (results hidden)—immediately after the slits ⇒ individual particle hits at the screen cumulate straight behind the slits, no interference behavior is observed

Delayed choice: The choice of setup (a)/(b) is made *after* the particle passed the slits. The outcome is the same as if the decision was made before.

Quantum eraser: The unobserved which-path information from setup (b) is erased before the particle hits the screen. The interference pattern appears.

▸ Some conceptual implications

Indeterminism: It is not possible to predict the positions of individual particle hits, but only their overall distribution. Quantum physics invites randomness and probabilistic description into the fundamental theory.

Particle-wave duality: Particles show either wave or corpuscular properties, in accord with the specific experimental arrangement. In particular, the existence of the which-path information invariably leads to the corpuscular behavior, while its actual nonexistence implies a wave-like behavior.

Contextuality etc.: The actual result of a physical observation depends on a wider "context" of the process investigated. The observed "reality" emerges only during the act of observation. And many more sentences like these.

◂ Historical remark
1805 (approx.): Thomas Young performed double-slit experiment with light
1927: C. Davisson & L. Germer demonstrate interference of electrons on crystals
1961: first double-slit experiment with massive particles (electrons)
1970's: double-slit experiments with individual electrons
1990's-present: progress in realizations of which-path setup & delayed-choice exp.

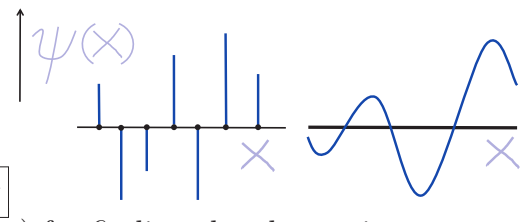
■ Wavefunction and superposition principle

To explain the outcome of the interference setup of the double-slit experiment (interference pattern formed by individual dots), we will assume that the undisturbed particle inside the interferometer represents a wave-like object comprising a variety of potential particle localizations and that the position measurement on the screen makes one of these potential localizations actual.

▸ Concept of wavefunction

Quantum physics deals not with one, but with **several alternative versions of reality**—with many potential outcomes of any conceivable measurement performed on a given system. Complete determination of the physical state of the system must somehow include all these alternatives and to quantify their probabilities. If variable x denotes possible outcomes of a complete set of measurements (specifying all degrees of freedom of a given system), the quantum state of the system is determined by a complex wavefunction $\psi(x)$:

Wavefunction value $\boxed{\psi(x) \equiv \textbf{amplitude}}$ of probability (or density of amplitude of probability if x is continuous) for finding the particular alternative x.



Squared modulus $\boxed{|\psi(x)|^2 \equiv \textbf{probability}}$ (or density of probability for x continuous) for finding the alternative x.
Although the detectable probabilities are given by $|\psi(x)|^2 \in \mathbb{R}$, their amplitudes $\boxed{\psi(x) \in \mathbb{C}}$ play a substantial role in the quantum description of reality!

The wavefunction evolves in time t, so: $\psi(x) \to \psi(x,t)$

▸ Wavefunction of a single **structureless particle**: $\boxed{\psi(\vec{x},t) \equiv \sqrt{\rho(\vec{x},t)}\; e^{i\varphi(\vec{x},t)}}$
where $\vec{x} \equiv$ alternative positions of the particle in the real 3D space
$|\psi(\vec{x},t)|^2 = \rho(\vec{x},t) \geq 0$ is the probability density to detect the particle at position $\vec{x}$. Normalization: $\int \rho(\vec{x},t)\, d\vec{x} = 1\ \forall t$. Phase $\varphi(\vec{x},t) \in \mathbb{R}$ has no "classical" interpretation, but plays an important role in interference phenomena

▶ Superposition of wavefunctions

The outcome of the interference setup depends on the fact that waves can be summed up. Consider two normalizable wavefunctions $\psi_{\mathrm{A}}(\vec{x},t)$ and $\psi_{\mathrm{B}}(\vec{x},t)$:

$$\int |\psi_{\mathrm{A}}|^2 d\vec{x} < \infty, \int |\psi_{\mathrm{B}}|^2 d\vec{x} < \infty \Rightarrow \boxed{\int |\alpha\psi_{\mathrm{A}} + \beta\psi_{\mathrm{B}}|^2 d\vec{x} < \infty} \; \forall \alpha, \beta \in \mathbb{C}$$

$\Rightarrow$ any linear combination of normalizable wavefunctions is a normalizable wavefunction $\Rightarrow$ these functions form a linear vector space $\mathcal{L}^2(\mathbb{R}^3)$

▶ Interference phenomenon

Probability density for a superposition of waves is not the sum of densities for individual waves. Choose arbitrary $\alpha = |\alpha| e^{i\varphi_\alpha}$ and $\beta = |\beta| e^{i\varphi_\beta}$ such that $\int |\alpha\psi_{\mathrm{A}} + \beta\psi_{\mathrm{B}}|^2 \, d\vec{x} = 1$ with both ψ_{A} and ψ_{B} normalized ($\int |\psi_\bullet|^2 \, d\vec{x} = 1$)

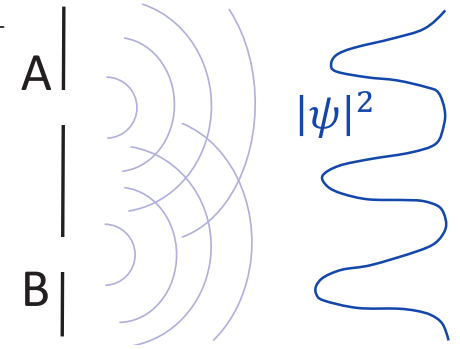
$$\Rightarrow \boxed{\underbrace{|\alpha\psi_{\mathrm{A}} + \beta\psi_{\mathrm{B}}|^2}_{\rho_{\alpha\mathrm{A}+\beta\mathrm{B}}} = \underbrace{|\alpha\psi_{\mathrm{A}}|^2}_{|\alpha|^2\rho_{\mathrm{A}}} + \underbrace{|\beta\psi_{\mathrm{B}}|^2}_{|\beta|^2\rho_{\mathrm{B}}} + \underbrace{2|\alpha\beta\psi_{\mathrm{A}}\psi_{\mathrm{B}}| \cos(\varphi_{\mathrm{A}} + \varphi_\alpha - \varphi_{\mathrm{B}} - \varphi_\beta)}_{\text{interference terms}}}$$

▶ Description of the interference setup in the double-slit experiment

Despite generally delocalized nature of wavefunctions we assume an approximate assignment of times: at $t \approx t_0$ the particle passes the double-slit plate and at $t \approx t_1$ it reaches the detection screen. At the plate we have

$$\psi(\vec{x}, t_0) \approx \alpha\delta_{\mathrm{A}}(\vec{x} - \vec{x}_{\mathrm{A}}) + \beta\delta_{\mathrm{B}}(\vec{x} - \vec{x}_{\mathrm{B}})$$

with $\delta_\bullet(\vec{x} - \vec{x}_\bullet)$ denoting the wavefunction localized at the respective slit ($\delta_\bullet = 0$ away from it) and α, β some coefficients depending on the emitted state and experimental details. If $\psi_\bullet(\vec{x}, \Delta t)$ is the wavefunction developed in time $\Delta t = t_1 - t_0$ from $\delta_\bullet(\vec{x} - \vec{x}_\bullet)$, the wavefunction on the screen reads as:



$$\psi(\vec{x}, t_1) \approx \alpha\psi_{\mathrm{A}}(\vec{x}, \Delta t) + \beta\psi_{\mathrm{B}}(\vec{x}, \Delta t) \quad \Rightarrow \quad \boxed{\rho(\vec{x}) \approx |\alpha\psi_{\mathrm{A}}(\vec{x}, \Delta t) + \beta\psi_{\mathrm{B}}(\vec{x}, \Delta t)|^2}$$

Thus the probability distribution on the screen shows the interference pattern.

▶ Dirac delta function (mathematical intermezzo)

To deal with arbitrary wavefunctions, it is convenient to introduce a generalized function (more precisely, a so-called distribution) describing a perfectly localized particle. Consider first the 1D case. In a vague sense, the δ-function can be seen as a "limit" of a series of ordinary functions whose support contracts to a single point but the integral remains constant, equal to unity:

$$\delta(x) = \lim_{\epsilon \to 0} \delta_\epsilon(x) \qquad \mathrm{Support}\,[\delta(x)] \equiv \{x = 0\} \quad \text{and} \quad \int_{-\infty}^{+\infty} \delta(x)\, dx = 1$$

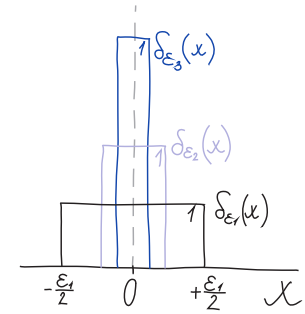
For instance, we can choose the following sequences:

(a) $\delta_\epsilon(x) \equiv \begin{cases} \frac{1}{\epsilon} & \text{for } x \in [-\frac{\epsilon}{2}, +\frac{\epsilon}{2}] \\ 0 & \text{otherwise} \end{cases}$

(b) $\delta_\epsilon(x) = \frac{1}{\pi} \frac{\epsilon}{\epsilon^2 + x^2}$ (Cauchy or Breit-Wigner form)

(c) $\delta_\epsilon(x) = \frac{1}{\sqrt{2\pi\epsilon^2}} e^{-\frac{x^2}{2\epsilon^2}}$ (Gaussian form)

(d) $\boxed{\delta_\epsilon(x) = \frac{1}{\pi} \frac{\sin(x\epsilon^{-1})}{x} = \frac{1}{2\pi} \int_{-\epsilon^{-1}}^{+\epsilon^{-1}} e^{iqx} dq}$ (Fourier transform of unity)



In 3D space: $\overbrace{\delta_{\epsilon_1}(x_1 - x_1')\delta_{\epsilon_2}(x_2 - x_2')\delta_{\epsilon_3}(x_3 - x_3')}^{\delta_{\vec{\epsilon}}(\vec{x} - \vec{x}')} \xrightarrow{\vec{\epsilon} \to 0} \overbrace{\delta(x_1 - x_1')\delta(x_2 - x_2')\delta(x_3 - x_3')}^{\delta(\vec{x} - \vec{x}')}$

Defining property of δ-function in terms of distribution theory: $\boxed{\int f(\vec{x})\delta(\vec{x} - \vec{x}')\, d\vec{x} = f(\vec{x}')}$

► Delocalized wavefunctions

Any wavefunction can be expressed as: $\boxed{\psi(\vec{x}, t) = \int \psi(\vec{x}', t)\delta(\vec{x} - \vec{x}')\, d\vec{x}'}$

General state given by a wavefunction $\psi(\vec{x}, t) \equiv$ **superposition of localized states** $\delta(\vec{x} - \vec{x}')$ with coefficients equal to the respective values $\psi(\vec{x}', t)$

However, note that $\delta(\vec{x} - \vec{x}') \notin \mathcal{L}^2(\mathbb{R}^3)$ (it is not even a function). This anticipates problems with incorporating some physically plausible states (like the localized states in coordinate or momentum space) into the mathematical formalism of quantum theory

◄ Historical remark

1800-10: Thomas Young formulates the superposition principle for waves
1924: Louis de Broglie introduces the concept of particle wavefunction
1926: Erwin Schrödinger formulates wave mechanics
1926: Max Born provides the probabilistic interpretation of wavefunction
1926-32: John von Neumann formulates QM through linear vector spaces
1927-30: Paul Dirac includes into the formulation the δ-function

■ Quantum measurement

To explain the which-path version of the double-slit experiment, we assume that the measurement has a dramatic effect on a quantum system: "**reduction**" or "**collapse**" of its wavefunction to the single alternative that was observed.

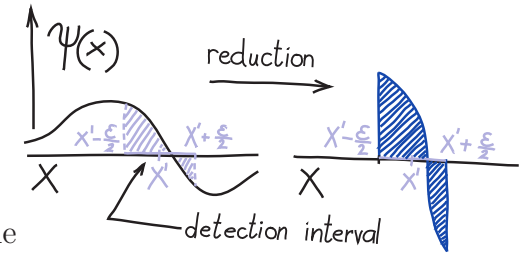
► Change of wavefunction in measurement

Example: position measurement detecting the particle (in time t_0) within the box $(x_1' \pm \frac{\epsilon_1}{2}, x_2' \pm \frac{\epsilon_2}{2}, x_3' \pm \frac{\epsilon_3}{2}) \Rightarrow$ the wavefunction changes as:

$\psi(\vec{x}, t_0)$ delocalized $\xrightarrow{\text{reduction}}$ $\psi(\vec{x}, t_0 + dt) \propto \delta_{\vec{\epsilon}}(\vec{x} - \vec{x}')\psi(\vec{x}, t_0)$ localized

In an *ideal* ($\epsilon \to 0$) measurement that detects the particle at $\vec{x}'$:

$$\boxed{\psi(\vec{x},t) \xrightarrow{\text{reduction}} \delta(\vec{x}-\vec{x}')}$$



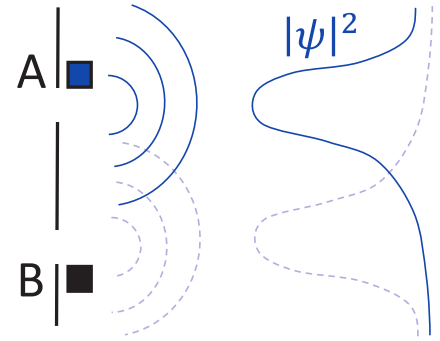
After the position measurement, the wavefunction evolves from a localized one

► **Description of the which-path setup in the double-slit experiment**

At the double-slit plate:
$\psi(\vec{x},t_0) \approx \alpha\delta_{\rm A}(\vec{x}-\vec{x}_{\rm A}) + \beta\delta_{\rm B}(\vec{x}-\vec{x}_{\rm B})$

After which-path measurement ($\delta t \ll \Delta t$):
$\psi(\vec{x},t_0+\delta t) \approx \begin{cases} \delta_{\rm A}(\vec{x}-\vec{x}_{\rm A}) & \text{probability } \approx|\alpha|^2 \\ \delta_{\rm B}(\vec{x}-\vec{x}_{\rm B}) & \text{probability } \approx|\beta|^2 \end{cases}$

At the screen:
$\psi(\vec{x},t_0+\Delta t) \approx \begin{cases} \psi_{\rm A}(\vec{x},\Delta t) & \text{probability } \approx|\alpha|^2 \\ \psi_{\rm B}(\vec{x},\Delta t) & \text{probability } \approx|\beta|^2 \end{cases}$



$\Rightarrow \boxed{\rho(\vec{x}) \approx |\alpha\psi_{\rm A}(\vec{x},\Delta t)|^2 + |\beta\psi_{\rm B}(\vec{x},\Delta t)|^2}$ probability distribution on the screen

So the interference pattern is destroyed! This is a direct consequence of the wavefunction collapse caused by the which-path measurement.

Note: Disappearance of the interference pattern can be also induced by the presence of an additional quantum system (an "atom") that interacts with the particle inside the two-slit device so that it records the which-path information—without any observer actually reading it! The composite particle–atom system is described by an extended wavefunction with both particle & atom degrees of freedom. The measurement-like effect then follows from a continuous, collapse-free evolution of the extended wavefunction reflecting the particle–atom interaction. The collapse assumption is nevertheless useful if we want to describe the measured system autonomously, irrespective of the "measuring agents".

► **Summing amplitudes versus summing probabilities**: For a general branching processes with disjunct alternative paths A & B (real or symbolic), the probability to pass the branching while the path is not *explicitly* measured depends on whether the paths can/cannot, *in principle*, be distinguished:

For **indistinguishable paths** we sum amplitudes: $\boxed{\mathfrak{a} \propto \mathfrak{a}_{\rm A} + \mathfrak{a}_{\rm B}}$
$\Rightarrow$ interference effects occur in $\mathfrak{p} = |\mathfrak{a}|^2$

For **distinguishable paths** we sum probabilities: $\boxed{\mathfrak{p} \propto \mathfrak{p}_{\rm A} + \mathfrak{p}_{\rm B}}$
$\Rightarrow$ interference effects do not occur

► **Quantum logic**: An attempt was made to assign the strange properties of the quantum world to a non-classical underlying logic. In the double-slit experiment it can be introduced via the following "propositions":

$A, B \equiv$ passage through slit A,B $\quad S \equiv$ detection at given place of screen
Different outcomes of interference & which-path setups indicate that:

$$\underbrace{(A \vee B) \wedge S}_{\textbf{interference setup}} \neq \underbrace{(A \wedge S) \vee (B \wedge S)}_{\textbf{which-path setup}}$$

(where $\vee \equiv$ "or" and $\wedge \equiv$ "and")
$\Rightarrow$ violation of a common logic axiom

◀ Historical remark
1924-35: Bohr (Copenhagen) versus Einstein debate. Niels Bohr defends a "subjective" approach (with the observer playing a role in the "creation" of reality)
1927: the first explicit note of wavefunction collapse by Werner Heisenberg
1932: inclusion of collapse into the mathematical formulation of QM by John von Neumann (discussions about its physical meaning continue up to now)
1936: Garrett Birkhoff and J. von Neumann formally introduce quantum logic

1a. SPACE OF QUANTUM STATES

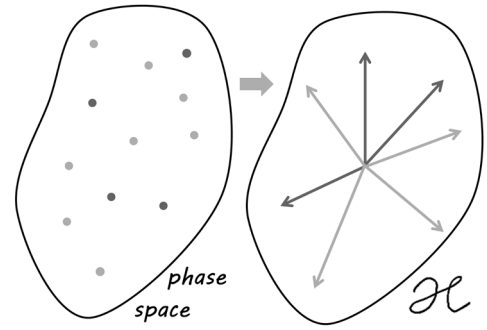
Quantum theory has rather sophisticated formalism based on the mathematics matured at the beginning of the 20th century. Its interpretation in terms of "common sense" becomes a nontrivial issue rising questions about the link of physical theory to reality. The problem starts already on the deepest level—with the definition of states of quantum systems, i.e., sets of attributes sufficient for a unique description of the system's evolution. While the mathematical representation of states in classical physics is rather intuitive and comprehensible (using the notion of phase space), quantum physics resorts to much more abstract ideas.

Roughly the first half of this book attempts to give a complete overview of the quantum formalism. The chapters that contain letter "a" in the numbering outline, step by step, the basic elements of the mathematical description. The chapters with letter "b" give some simple concrete examples (mostly in single-particle systems) of the respective ideas. To keep immediate link between the *Geist* and *Substanz*, we present the "a" and "b" chapters in an alternating, entangled way.

■ Hilbert space

To capture the quantum uncertainty, i.e., the possibility of different outcomes of various measurements performed on systems in the same state, we will assume that *distinct states of the system are not always perfectly distinguishable*. The states may show some "overlaps", which allow one to identify a given state with another state—e.g., the state of a particle described by a delocalized wavefunction $\psi(\vec{x})$ with a state localized at a single place $\vec{x}\,'$. This means that the states are not represented by isolated points *à la* points in the classical phase space. Instead, they can be associated with **vectors** in linear vector spaces. If two vectors are not perpendicular to each other, they have a common component

whose size sets limits to their mutual distinguishability.



▶ State of a physical system

The state represents a complete set of parameters characterizing a physical system in the sense of an autonomous determinism: The knowledge of state at a *single time* (t=0) suffices to determine the state at *any time* in past or future ($t \gtrless 0$). Let $|\psi\rangle$ denote a mathematical entity describing an arbitrary physical state of a given quantum system (shortcut: $|\psi\rangle \equiv$ "a state"). Let $\mathcal{H}$ be a system-specific space containing all such entities (**state space**). We make our first fundamental assumption:

The space of states $\mathcal{H}$ of an arbitrary quantum system is a **Hilbert space**, in which individual states are represented by rays of vectors.

The Hilbert space is defined by the following 3 requirements:

▶ Requirement 1: The space $\mathcal{H}$ supports the **superposition principle**

$$\left.\begin{array}{r} |\psi_1\rangle, |\psi_2\rangle \in \mathcal{H} \\ \alpha, \beta \in \mathbb{C} \end{array}\right\} \Rightarrow \boxed{|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle \quad \in \mathcal{H}}$$

superposition of states $|\psi_1\rangle$ and $|\psi_2\rangle$

$\Rightarrow \mathcal{H}$ is a **complex vector space**

Why we need superpositions: To describe the single-particle interference in the double-slit experiment (Intro.), we must add the waves from both slits.

▶ Requirement 2: The space $\mathcal{H}$ supports a **scalar product** $\boxed{\langle\psi_1|\psi_2\rangle \in \mathbb{C}}$

Properties: $\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle^*$, $\langle\psi_1|\alpha\psi_2 + \beta\psi_3\rangle = \alpha\langle\psi_1|\psi_2\rangle + \beta\langle\psi_1|\psi_3\rangle$, $\langle\psi|\psi\rangle \geq 0$

Normalization of state vectors: Real number $\boxed{||\psi|| \equiv \sqrt{\langle\psi|\psi\rangle} \geq 0}$ is a norm of $|\psi\rangle$. Scaling of state vectors, i.e. multiplication $|\psi'\rangle = a|\psi\rangle$ by any constant $a \in \mathbb{C}$, does not change their physical content (so both $|\psi'\rangle$, $|\psi\rangle$ describe the same state). Hence any state vector can be scaled so that it becomes normalized: $\boxed{\langle\psi|\psi\rangle = 1}$. In QM we use normalized vectors, but this cannot be set as a constraint in $\mathcal{H}$ because of the superposition principle (if linearly combining two normalized states, the resulting superposition is generally not normalized).

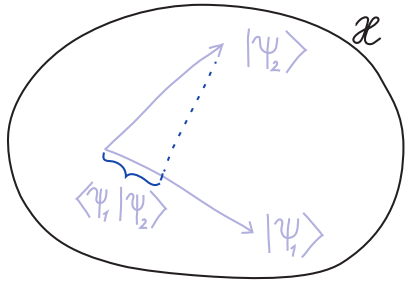
Distance of 2 vectors: $d^2(\psi_1, \psi_2) \equiv ||\psi_1 - \psi_2||^2 = \langle\psi_1|\psi_1\rangle + \langle\psi_2|\psi_2\rangle - 2\mathrm{Re}\langle\psi_1|\psi_2\rangle$

Schwarz inequality for normalized vectors: $\boxed{|\langle\psi_1|\psi_2\rangle|^2 \leq \underbrace{\langle\psi_1|\psi_1\rangle}_{1}\underbrace{\langle\psi_2|\psi_2\rangle}_{1} = 1}$

Why we need scalar product:

Results of quantum measurements are generally indeterministic (described in the probabilistic way, see Intro. & Sec. 2a.). A single measurement does not allow one to uniquely determine the state. The possibility to identify state $|\psi_2\rangle$

with $|\psi_1\rangle$ or vice versa in an "optimal" single measurement is determined by the overlap of the corresponding vectors. For $||\psi_1||=||\psi_2||=1$ we have:



$$\underbrace{\mathfrak{a}_{\psi_2}(\psi_1) \equiv \langle\psi_1|\psi_2\rangle}_{\text{amplitude}} \qquad \underbrace{\mathfrak{p}_{\psi_2}(\psi_1) \equiv |\langle\psi_1|\psi_2\rangle|^2}_{\text{probability}}$$

Number $\mathfrak{a}_{\psi_2}(\psi_1) \in \mathbb{C}$ satisfying $|\mathfrak{a}_{\psi_2}(\psi_1)| \in [0,1]$ represents **amplitude** for finding $|\psi_1\rangle$ in $|\psi_2\rangle$

The corresponding **probability** $\mathfrak{p}_{\psi_2}(\psi_1) \in [0,1]$ is obtained by squaring the amplitude's modulus

Consequence:

States $|\psi_1\rangle$,$|\psi_2\rangle$ are perfectly **distinguishable** *iff* orthogonal: $\langle\psi_1|\psi_2\rangle = 0$

▶ **Requirement 3**: $\mathcal{H}$ is **complete**, i.e. $\forall$ converging sequence (in the Cauchy sense with distance d) of vectors $\{|\psi_i\rangle\}_i$ the limit $\lim_{i\to\infty}|\psi_i\rangle \equiv |\psi_\infty\rangle \in \mathcal{H}$. This shall avoid problems with missing limits (unfortunately, it does not apply to the δ-function, see Intro., as the "convergence" to δ is not of the Cauchy type).

▶ **Separable Hilbert spaces**

$\mathcal{H}$ is separable if it has a **countable** (possibly finite) **set of basis vectors**

We can choose an **orthonormal basis** $\{|\phi_i\rangle\}_{i=1}^{d_\mathcal{H}}$ satisfying $\langle\phi_i|\phi_j\rangle = \delta_{ij}$

The number of basis vectors $d_\mathcal{H}$ is called dimension of $\mathcal{H}$

⇒ Each state $|\psi\rangle$ can be expressed as a unique complex superposition of basis vectors:

$$|\psi\rangle = \sum_{i=1}^{d_\mathcal{H}} \underbrace{\langle\phi_i|\psi\rangle}_{\alpha_i} |\phi_i\rangle$$

Normalization:

$$\langle\psi|\psi\rangle = \sum_{i=1}^{d_\mathcal{H}}\sum_{j=1}^{d_\mathcal{H}} \alpha_i^*\alpha_j \overbrace{\langle\phi_i|\phi_j\rangle}^{\delta_{ij}} = \sum_{i=1}^{d_\mathcal{H}} |\alpha_i|^2 = 1$$

Applicability: Systems with finite numbers of particles, systems with finite numbers of degrees of freedom (possibly selected subsets of degrees of freedom)

Isomorphism of separable Hilbert spaces

Any separable $\mathcal{H}$ with an infinite basis set is isomorphic with the **space ℓ^2** formed by infinite "columns" of complex numbers $\begin{pmatrix}\alpha_1\\ \alpha_2\\ \vdots\end{pmatrix}$ satisfying $\sum_{i=1}^{\infty}|\alpha_i|^2 < \infty$

Mapping $\mathcal{H} \to \ell^2$: Expansion coefficients $\langle\phi_i|\psi\rangle$ of a chosen vector $|\psi\rangle \in \mathcal{H}$ in a given basis $\{|\phi_i\rangle\}_i$ are associated with the numbers α_i defining the vector $\in \ell^2$

Superpositions $a|\psi\rangle + b|\psi'\rangle$ mapped onto: $\begin{pmatrix}a\alpha_1+b\alpha_1'\\ a\alpha_2+b\alpha_2'\\ \vdots\end{pmatrix}$

Scalar product represented by: $\langle\psi|\psi'\rangle \equiv \sum_i \alpha_i^*\alpha_i' = (\,\alpha_1^*,\alpha_2^*,\ldots\,)\begin{pmatrix}\alpha_1'\\ \alpha_2'\\ \vdots\end{pmatrix}$

▶ **Nonseparable Hilbert spaces**

$\mathcal{H}$ is nonseparable if it has no countable basis. This applies in systems with unbounded particle numbers, quantum fields, continuum...

◄ Historical remark
1900-10: David Hilbert (with E. Schmidt) introduces the ∞-dimensional space of square-integrable functions and elaborates the theory of such spaces
1927: John von Neumann (working under Hilbert) introduces abstract Hilbert spaces into QM (1932: book *Mathematische Grundlagen der Quantenmechanik*)

■ Rigged Hilbert space

Although the standard Hilbert space is sufficient for consistent formulation of QM, we will see soon that its suitable extension is very helpful.

► Hierarchy of spaces based on $\mathcal{H} \equiv \ell^2$

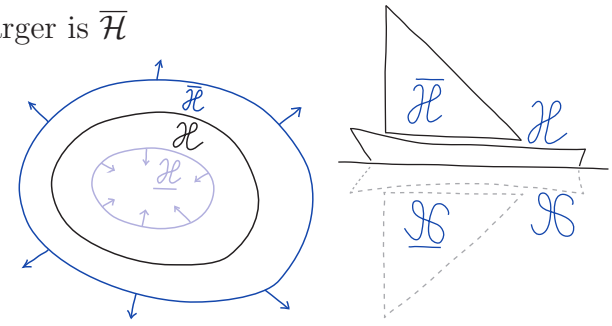
$\underline{\mathcal{H}}$ is a space of sequences $\{\alpha_i\}_{i=1}^{\infty} \equiv |\psi\rangle$ satisfying $\sum_i |\alpha_i|^2 i^m < \infty$ for m=0,1,2....
These form a dense subset of ℓ^2

$\overline{\mathcal{H}}$ (conjugate space to $\underline{\mathcal{H}}$) is a space of sequences $\{\alpha'_i\}_{i=1}^{\infty} \equiv |\psi'\rangle$ satisfying $\langle\psi|\psi'\rangle < \infty$ for any $|\psi\rangle \in \underline{\mathcal{H}}$. This set contains ℓ^2 as a subset.

$\langle\psi|\psi'\rangle \equiv \sum_i \alpha_i^* \alpha'_i < \infty \quad \Rightarrow \sum_i |\alpha'_i|^2 \frac{1}{i^m} < \infty \quad \Rightarrow |\alpha'_i|^2$ may polynomially diverge

In general, the smaller is $\underline{\mathcal{H}}$, the larger is $\overline{\mathcal{H}}$

$\underline{\mathcal{H}}$ and $\overline{\mathcal{H}}$ are linear vector spaces, but not Hilbert spaces:
$\underline{\mathcal{H}}$ is not complete
$\overline{\mathcal{H}}$ does not have scalar product



► Gelfand triple $\boxed{\underline{\mathcal{H}} \subset \mathcal{H} \subset \overline{\mathcal{H}}}$

This "sandwich" of spaces is sometimes called the "rigged Hilbert space", indicating that only such an extended structure allows one to "safely sail the sea" of quantum physics. It turns out that solutions of some basic quantum problems is out of $\mathcal{H}$ but belongs to the larger space $\overline{\mathcal{H}}$, while the definition domain of some quantum operators is not $\mathcal{H}$ but rather its subspace $\underline{\mathcal{H}}$ (see Secs. 2a & 2b).

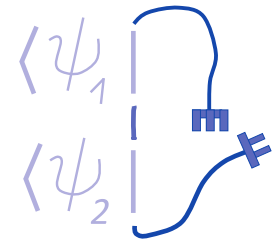
■ Dirac notation

Physicists are proud to master a symbolic technique that makes some involved mathematical reductions much easier to follow. Although the "bra-ket" formalism is not always fully rigorous, it is extremely efficient especially when dealing with the action of linear operators in Hilbert spaces.

► Kets and bras

For any vector $|\psi\rangle \in \mathcal{H}$, called **ket**, there exists a linear functional $F_\psi \equiv \langle\psi|$,

called **bra**, such that the value assigned by F_ψ to $|\phi\rangle \in \mathcal{H}$ is $\boxed{F_\psi(\phi) \equiv \langle\psi|\phi\rangle}$ (the words following from "bra-c-ket")



The bras also satisfy the superposition principle:

$$\alpha\langle\psi_1| + \beta\langle\psi_2| \equiv \langle\alpha^*\psi_1 + \beta^*\psi_2|$$

and the spaces of kets & bras are isomorphic.

Matrix forms: $\langle\psi| \equiv (\,\alpha_1^*, \alpha_2^*, \dots\,)$ $\quad \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix} \equiv |\psi\rangle$

▸ Linear operators

Linear operators play a very important role in QM. They will be subject to systematic study from Sec. 2a. Here we just introduce basic notions.

Linear operator $\boxed{\hat{O}|\psi\rangle = |\psi'\rangle}$ is a mapping $\mathcal{H} \to \mathcal{H}$ of the Hilbert space to itself satisfying the **linearity condition**: $\boxed{\hat{O}(\alpha|\psi_1\rangle + \beta|\psi_2\rangle) = \alpha\hat{O}|\psi_1\rangle + \beta\hat{O}|\psi_2\rangle}$

$\Rightarrow \hat{O}$ is completely defined via its action on any basis: $\{|\phi_i\rangle\}_{i=1}^{d_\mathcal{H}} \xrightarrow{\hat{O}} \{|\phi_i'\rangle\}_{i=1}^{d_\mathcal{H}}$

$$\Rightarrow \hat{O}\underbrace{|\psi\rangle}_{\sum_i \langle\phi_i|\psi\rangle|\phi_i\rangle} = \sum_{i=1}^{d_\mathcal{H}} \langle\phi_i|\psi\rangle \underbrace{\hat{O}|\phi_i\rangle}_{|\phi_i'\rangle} = \sum_{i=1}^{d_\mathcal{H}} |\phi_i'\rangle\langle\phi_i|\psi\rangle \quad \Rightarrow \quad \boxed{\hat{O} \equiv \sum_{i=1}^{d_\mathcal{H}} |\phi_i'\rangle\langle\phi_i|} \quad \begin{matrix} |\phi_i'\rangle\langle\phi_i| \\ \Updownarrow \\ |\phi_i\rangle \xrightarrow{\hat{O}} |\phi_i'\rangle \end{matrix}$$

Any expression of the form $|\phi'\rangle\langle\phi|$ is a linear operator: $|\psi\rangle \xrightarrow{\hat{O}} \langle\phi|\psi\rangle|\phi'\rangle$.

Any linear operator $\hat{O}$ can be expressed as a sum over terms $\propto |\phi_j\rangle\langle\phi_i|$ containing vectors of the *same* basis. This is achieved via the identity (unit) operator:

$\boxed{\sum_{i=1}^{d_\mathcal{H}} |\phi_i\rangle\langle\phi_i| = \hat{I}}$ $\equiv$ **unit operator** $\Rightarrow$ $\quad \{|\phi_i\rangle\} \xrightarrow{\hat{I}} \{|\phi_i\rangle\}$

$$\boxed{\underbrace{\hat{O}}_{\hat{I}\hat{O}\hat{I}} = \sum_{i=1}^{d_\mathcal{H}} \sum_{j=1}^{d_\mathcal{H}} \underbrace{\langle\phi_j|\hat{O}|\phi_i\rangle}_{\langle\phi_j|\hat{O}|\phi_i\rangle \equiv O_{ji}} |\phi_j\rangle\langle\phi_i|}$$

Matrix form general linear operator: $\hat{O} \equiv \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \\ \vdots & & \ddots \end{pmatrix}$

▸ Projectors

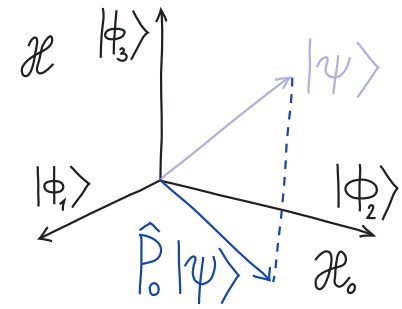
Projection operators (projectors) are linear operators satisfying $\boxed{\hat{P}^2 = \hat{P}}$

(i.e., repeated projection is redundant)

Let $\{|\phi_i\rangle\}_{i=1}^{d_0} \equiv$ orthonormal basis of a subspace $\mathcal{H}_0 \subset \mathcal{H}$. We have $\langle\phi_i|\phi_j\rangle = \delta_{ij}$

$\boxed{\hat{P}_0 = \sum_{i=1}^{d_0} |\phi_i\rangle\langle\phi_i|}$ is a projector to $\mathcal{H}_0$:

$$\hat{P}_0|\psi\rangle \begin{cases} = 0 & \text{for } |\psi\rangle \perp \mathcal{H}_0 \\ \in \mathcal{H}_0 & \text{otherwise} \end{cases}$$



Completeness relation: the projector to the whole $\mathcal{H}$ is the identity operator (see above):

$$\hat{P}_\mathcal{H} = \sum_{i=1}^{d_\mathcal{H}} |\phi_i\rangle\langle\phi_i| = \hat{I}$$

Probability to identify $|\psi\rangle$ with *any* state from the subspace $\mathcal{H}_0$:
In generalization of the above formula $\mathfrak{p}_\psi(\psi_0) = |\langle\psi_0|\psi\rangle|^2 = \langle\psi|\psi_0\rangle\langle\psi_0|\psi\rangle$, the overall probability to (incorrectly) associate a given state $|\psi\rangle \in \mathcal{H}$ with an arbitrary state $|\psi'\rangle \in \mathcal{H}_0$ is given by:

$$\boxed{\mathfrak{p}_\psi(\mathcal{H}_0) \equiv \langle\psi|\hat{P}_0|\psi\rangle = \sum_{i=1}^{d_0} |\langle\phi_i|\psi\rangle|^2}$$

Matrix form of projector operators:
In an orthonormal basis $\{|\phi_i\rangle\}_{i=1}^{d_\mathcal{H}}$ of $\mathcal{H}$ containing as a subset the basis $\{|\phi_{i_j}\rangle\}_{j=1}^{d_0}$ of $\mathcal{H}_0$ (with $i_j \equiv$ indices of the $\mathcal{H}_0$ basis vectors in the $\mathcal{H}$ basis), the projector is expressed as a diagonal matrix with d_0 units and $(d_\mathcal{H}{-}d_0)$ zeros on the diagonal:

$$\hat{P}_0 = \begin{pmatrix} X_1 & 0 & \cdots \\ 0 & X_2 & \\ \vdots & & \ddots \end{pmatrix} \text{ with } X_i = \begin{cases} 1 \text{ for } i \in \{i_1, i_2, \ldots, i_{d_0}\} \\ 0 \text{ for } i \notin \{i_1, i_2, \ldots, i_{d_0}\} \end{cases}$$

◄ Historical remark
1930: Paul Dirac writes the book *The Principles of Quantum Mechanics*, which provides a more intuitive (compared to von Neumann) path to quantum theory, using non-normalizable vectors and δ-function (bra-kets in 3rd edition 1947)
1950-60's: I.M. Gelfand & N.Y. Vilenkin introduce rigged Hilbert spaces, putting Dirac's approach on more rigorous grounds. Systematic use in QM since 1966 (by A. Böhm et al.) but up to now rather scarce

■ Summing Hilbert spaces

One can combine one or more Hilbert spaces in the style of summation. The resulting space then contains the summed spaces as ordinary subspaces.

► Direct sum

Let $\{|\phi_{1i}\rangle\}_{i=1}^{d_1}$ be an orthonormal basis of $\mathcal{H}_1$ and $\{|\phi_{2j}\rangle\}_{j=1}^{d_2}$ one of $\mathcal{H}_2$

Direct sum space $\boxed{\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2}$ has the "summed" basis $\boxed{|\Phi_{ki}\rangle \equiv \begin{cases} |\phi_{1i}\rangle \text{ for } k{=}1 \\ |\phi_{2i}\rangle \text{ for } k{=}2 \end{cases}}$

Hence $\mathcal{H}_1 \oplus \mathcal{H}_2$ consists of all normalizable linear combinations of the basis vectors $|\Phi_{ki}\rangle$ formed by a unification of the basis vectors of $\mathcal{H}_1$ and $\mathcal{H}_2$.

Dimension: $\boxed{d_{\mathcal{H}_1 \oplus \mathcal{H}_2} = d_1 + d_2}$ Orthonormality of basis: $\langle\Phi_{ki}|\Phi_{k'i'}\rangle = \delta_{kk'}\delta_{ii'}$

► State decomposition

Any vector $|\Psi\rangle = \sum_{k,i} \alpha_{ki}|\Phi_{ki}\rangle \in \mathcal{H}$ can be written as $|\Psi\rangle = |\psi_1\rangle + |\psi_2\rangle$ with $|\psi_k\rangle \in \mathcal{H}_k$ $(k = 1, 2)$

$$|\Psi\rangle = \underbrace{\sum_{i=1}^{d_1} \alpha_{1i}|\phi_{1i}\rangle}_{|\psi_1\rangle \equiv \hat{P}_1|\Psi\rangle \in \mathcal{H}_1} + \underbrace{\sum_{j=1}^{d_2} \alpha_{2j}|\phi_{2j}\rangle}_{|\psi_2\rangle \equiv \hat{P}_2|\Psi\rangle \in \mathcal{H}_2}$$

Projectors to the subspaces $\mathcal{H}_k$

$$\hat{P}_k = \sum_{i=1}^{d_k} |\Phi_{ki}\rangle\langle\Phi_{ki}| \;\Rightarrow \begin{cases} \text{orthogonality}: & \hat{P}_1\hat{P}_2 = \hat{P}_2\hat{P}_1 = 0 \\ \text{completeness}: & \hat{P}_1 + \hat{P}_2 = \hat{I}_\mathcal{H} \end{cases}$$

Scalar product: $\boxed{\langle\Psi|\Psi'\rangle_\mathcal{H} = \langle\psi_1|\psi_1'\rangle_{\mathcal{H}_1} + \langle\psi_2|\psi_2'\rangle_{\mathcal{H}_2}}$ where $\begin{cases} |\psi_k\rangle = \hat{P}_k|\Psi\rangle \\ |\psi_k'\rangle = \hat{P}_k|\Psi'\rangle \end{cases}$

▶ Finite-dimensional matrix representation:

$$|\psi_1\rangle = \begin{pmatrix} \alpha_{11} \\ \vdots \\ \alpha_{1d_1} \end{pmatrix},\ |\psi_2\rangle = \begin{pmatrix} \alpha_{21} \\ \vdots \\ \alpha_{2d_2} \end{pmatrix} \quad \Rightarrow \quad |\Psi\rangle = \begin{pmatrix} \alpha_{11} \\ \vdots \\ \alpha_{1d_1} \\ \cdots\cdots \\ \alpha_{21} \\ \vdots \\ \alpha_{2d_2} \end{pmatrix}$$

▶ Multiple sums of Hilbert spaces: $\boxed{\mathcal{H} = \bigoplus_{k=1}^{n} \mathcal{H}_k}$

▶ **The use in QM**: $\mathcal{H}_k \subset \mathcal{H}$ can be associated with subspaces corresponding to various values a_k of an observable A (states $|\psi\rangle \in \mathcal{H}_k$ yield output a_k with certainty; see Sec. 2a). Subspaces in the direct sum can also collect vectors with different symmetry properties (e.g., subspaces of even and odd wavefunctions).

■ Multiplying Hilbert spaces

Hilbert spaces can also be combined in the style of multiplication. This commonly happens in **composite quantum systems** that consist of two or more subsystems (several particles or distinct subsets of degrees of freedom). The multiplication is a rather interesting operation since it allows one to create so called *entangled quantum states* which have no analogue in the classical world.

▶ Direct (tensor) product

Let $\{|\phi_{1i}\rangle\}_{i=1}^{d_1}$ be an orthonormal basis of $\mathcal{H}_1$ and $\{|\phi_{2j}\rangle\}_{j=1}^{d_2}$ one of $\mathcal{H}_2$

Tensor product space $\boxed{\boxed{\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2}}$ has the product basis $\boxed{|\Phi_{ij}\rangle \equiv |\phi_{1i}\rangle|\phi_{2j}\rangle}$

This means that $\mathcal{H}_1 \otimes \mathcal{H}_2$ consists of all normalizable linear combinations of the basis vectors $|\Phi_{ij}\rangle$ formed by direct products of $\mathcal{H}_1$ and $\mathcal{H}_2$ basis vectors. Note that non-product bases of $\mathcal{H}_1 \otimes \mathcal{H}_2$ can also be constructed.

Dimension: $\boxed{\boxed{d_{\mathcal{H}_1 \otimes \mathcal{H}_2} = d_1 \cdot d_2}}$ Orthonormality of basis: $\langle \Phi_{ij}|\Phi_{i'j'}\rangle = \delta_{ii'}\delta_{jj'}$

▶ Factorized states

For any pair of states $\left\{ \begin{array}{l} |\psi_1\rangle = \sum_i \alpha_i |\phi_{1i}\rangle \in \mathcal{H}_1 \\ |\psi_2\rangle = \sum_j \beta_j |\phi_{2j}\rangle \in \mathcal{H}_2 \end{array} \right\}$ there exists the product state

$$\boxed{|\Psi_\otimes\rangle \equiv \underbrace{|\psi_1\rangle \otimes |\psi_2\rangle}_{\equiv |\psi_1\rangle_1 |\psi_2\rangle_2} = \sum_{i=1}^{d_1}\sum_{j=1}^{d_2} \underbrace{\alpha_i\beta_j}_{\gamma_{ij}} |\Phi_{ij}\rangle}$$

A factorized state allows one to uniquely identify the associated state vectors of individual subsystems

Scalar product for factorized states: $\langle \Psi_\otimes | \Psi'_\otimes \rangle_{\mathcal{H}} = \langle \psi_1 | \psi'_1 \rangle_{\mathcal{H}_1} \cdot \langle \psi_2 | \psi'_2 \rangle_{\mathcal{H}_2}$

▶ Entangled states

The possibility to express coefficients γ_{ij} of a general superposition $\sum_{ij} \gamma_{ij} |\Phi_{ij}\rangle$ in the above factorized form ($\gamma_{ij} = \alpha_i\beta_j$) is rather scarce. Almost all states in $\mathcal{H}_1 \otimes \mathcal{H}_2$ are unfactorizable, so called entangled states:

$$\boxed{\boxed{|\Psi\rangle = \sum_{i=1}^{d_1}\sum_{j=1}^{d_2} \underbrace{\gamma_{ij}}_{\neq \alpha_i\beta_j} |\Phi_{ij}\rangle \neq |\psi_1\rangle_1 |\psi_2\rangle_2}}$$

An entangled state does *not* have any associated state vectors of individual subsystems

► Multiple products of Hilbert spaces: $\boxed{\mathcal{H} = \bigotimes_{k=1}^{n} \mathcal{H}_k}$

More and less precise notations:

$\boxed{\mathcal{H}_k \ni |\psi\rangle \equiv |\psi\rangle_k}$ and $\bigotimes_{k=1}^{n} \mathcal{H}_k \ni |\psi_1\rangle_1 \otimes |\psi_2\rangle_2 ... \otimes |\psi_n\rangle_n \equiv |\psi_1\rangle_1 |\psi_2\rangle_2 ... |\psi_n\rangle_n$

► **The use in QM**

Hilbert space $\mathcal{H}$ of a composite system is the $\otimes$ product of partial spaces $\mathcal{H}_k$

The multiplied spaces $\mathcal{H}_k$ can be associated with the spaces corresponding to different parts of the system (e.g. different particles) or to different dynamical variables (e.g., spatial and spin degrees of freedom). Entangled state vectors correspond to *non-classical* situations in which only the whole system and not its individual parts are attributed by a pure quantum-mechanical state (the subsystems are in so called mixed states, see Sec. 6a). Entanglement represents a genuinely **quantum correlation** of the system's parts.

◄ **Historical remark**

1935: A. Einstein, B. Podolsky & N. Rosen use an entangled state to claim that QM is incomplete. E. Schrödinger analyzes such states and coins the term "entanglement"

1b. EXAMPLES OF QUANTUM HILBERT SPACES

In the following, we describe specific state spaces for particles with spin 0 and $\frac{1}{2}$, and the spaces assigned to collections of such particles. We meet another essentially quantum phenomenon: indistinguishability of particles. And we introduce the space of qubits — the playground of quantum information technologies.

■ Single structureless and spinless particle

Particles with no internal degrees of freedom are described by ordinary scalar wavefunctions (cf. Intro.).

► **Wavefunction** $\psi(\vec{x}) \equiv |\psi\rangle \in \boxed{\mathcal{H} \equiv \mathcal{L}^2(\mathbb{R}^3)}$ Hilbert space of **square-integrable functions**

$\boxed{\langle\psi_1|\psi_2\rangle \equiv \int \psi_1^*(\vec{x})\psi_2(\vec{x})\, d\vec{x}} \equiv \int \psi_1^*(\vec{y})\psi_2(\vec{y}) \left|\mathrm{Det}\frac{\partial(x_1...x_3)}{\partial(y_1...y_3)}\right| d\vec{y}$ scalar product

Cartesian & curvilinear coordinates

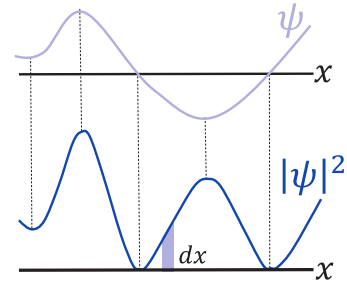
Expansion of $\psi(\vec{x})$ in a discrete **basis of orthonormal functions** $\{\phi_i(\vec{x})\}_{i=1}^{\infty}$

$\Rightarrow$ isomorphism of $\mathcal{L}^2(\mathbb{R}^3)$ with ℓ^2

Normalization: $\langle\psi|\psi\rangle = \int |\psi(\vec{x})|^2 d\vec{x} = 1$

Probabilistic interpretation:

$|\psi(\vec{x})|^2 \equiv \rho(\vec{x})$ is the probability density for finding the particle at position $\vec{x}$. This follows from the association of the state $|\vec{x}\,'\rangle$ of the particle at a single sharp position $\vec{x}\,'$ with the



Dirac δ-function $\delta(\vec{x}-\vec{x}\,')$ (see Sec. 0). Hence the amplitude & probability densities read:

$$\boxed{\begin{array}{l}\mathfrak{a}_\psi(\vec{x}\,')=\langle\vec{x}\,'|\psi\rangle=\int\delta(\vec{x}-\vec{x}\,')\psi(\vec{x})d\vec{x}=\psi(\vec{x}\,')\\ \mathfrak{p}_\psi(\vec{x}\,')=|\mathfrak{a}_\psi(\vec{x}\,')|^2=|\psi(\vec{x}\,')|^2\equiv\rho(\vec{x}\,')\end{array}}$$

Probability expressions for other observables will be treated in Secs. 2a & 2b.

► Rigged Hilbert space of wavefunctions

There is a problem that localized states $|\vec{x}\,'\rangle\equiv\delta(\vec{x}-\vec{x}\,')$ as well as other important states (like plane waves $e^{i\vec{k}\cdot\vec{x}}$, see Sec. 2b) are not in $\mathcal{L}^2(\mathbb{R}^3)$ (they are not quadratically integrable). The rescue comes with the introduction of a convenient Gelfand triple $\underline{\mathcal{H}}\subset\mathcal{H}\subset\overline{\mathcal{H}}$ of spaces. In the 1D case, we define:

$\underline{\mathcal{H}}\equiv$ dense subset of functions: $\int_{-\infty}^{+\infty}|\psi(x)|^2(1+|x|)^m dx<\infty$ for $m=0,1,2,\ldots$

$\overline{\mathcal{H}}\equiv$ functions satisfying $\int_{-\infty}^{+\infty}\psi'^*\psi\,dx<\infty\ \forall\psi'\in\underline{\mathcal{H}}$

Then $\overline{\mathcal{H}}$ includes also polynomially diverging functions, plane waves, δ-functions

An alternative mathematically consistent approach (see Sec. 2a) is to consider only imperfectly localized states, like those within interval $x_i\in[x_i'-\frac{\epsilon_i}{2},x_i'+\frac{\epsilon_i}{2}]$ around $\vec{x}\,'$ represented by wavefucntions $\delta_{\vec{\epsilon}}(\vec{x}-\vec{x}\,')\in\mathcal{L}^2(\mathbb{R}^3)$.

◄ Historical remark

1926: Erwin Schrödiger formulates QM in terms of wavefunction and Max Born develops its probabilistic interpretation

■ Single structureless particle with spin $\frac{1}{2}$

Electrons have spin $\frac{1}{2}$. The spin is a genuinely quantum feature of a particle, which (even for point-like elementary particles) is understood as an intrinsic unstoppable rotation. The general theory of angular momentum in QM will be developed in Secs. 3b & 4b, here we just introduce spinor wavefunctions as the simplest two-component generalization of scalar wavefunctions.

► Spin = intrinsic angular momentum of a particle

The lowest nonzero spin is $s=\frac{1}{2}$, having only 2 possible projections (spin states) $s_\bullet=\pm s\hbar$ in an arbitrarily chosen spatial direction $\bullet$ (conventionally $\bullet=z$):

$$\left.\begin{array}{lll}\textbf{spin up} & s_z=+\frac{\hbar}{2} & \Rightarrow\ |\uparrow\rangle\equiv\binom{1}{0}\equiv|\chi_1\rangle\\ \textbf{spin down} & s_z=-\frac{\hbar}{2} & \Rightarrow\ |\downarrow\rangle\equiv\binom{0}{1}\equiv|\chi_2\rangle\end{array}\right\}\Rightarrow$$

general state

$$\boxed{|\psi\rangle=\alpha_1|\uparrow\rangle+\alpha_2|\downarrow\rangle\equiv\binom{\alpha_1}{\alpha_2}}$$

► Spin Hilbert space: $\boxed{\mathcal{H}\equiv\mathbb{C}^2}$ with $\langle\psi|\psi'\rangle\equiv\binom{\alpha_1^*,\alpha_2^*}{}\binom{\alpha_1'}{\alpha_2'}=\alpha_1^*\alpha_1'+\alpha_2^*\alpha_2'$

Normalization: $|\alpha_1|^2+|\alpha_2|^2=1$

Probability to find the spin up/down:

$$\boxed{\begin{array}{l}\mathfrak{p}_\psi(\uparrow)=|\mathfrak{a}_\psi(\uparrow)|^2=|\langle\uparrow|\psi\rangle|^2=|\alpha_1|^2\\ \mathfrak{p}_\psi(\downarrow)=|\mathfrak{a}_\psi(\downarrow)|^2=|\langle\downarrow|\psi\rangle|^2=|\alpha_2|^2\end{array}}$$

For probabilities of spin projections in an arbitrary direction see Sec. 2b.

Note: General spin $s=0,\frac{1}{2},1,\frac{3}{2},2,\ldots$ has $(2s+1)$ spin projections $s_\bullet=-s\hbar$, $(-s+1)\hbar,\ldots,(+s-1)\hbar,+s\hbar$ to any direction, so $\mathcal{H}\equiv\mathbb{C}^{2s+1}$ (see Sec. 3b).

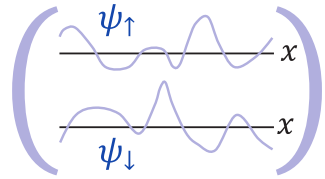
► **Both spatial and spin degrees of freedom**
⇒ direct product of spatial and spin Hilbert spaces: $\boxed{\mathcal{H} \equiv \mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^2}$

Basis vectors: $|\Phi_{ij}\rangle = |\phi_i\rangle|\chi_j\rangle$, where $\{|\phi_i\rangle\}_{i=1}^{\infty}$ is an arbitrary basis in $\mathcal{L}^2(\mathbb{R}^3)$

General state expansion: $|\psi\rangle = \sum_{i=1}^{\infty}\sum_{j=1}^{2}\alpha_{ij}|\phi_i\rangle|\chi_j\rangle = \sum_{i=1}^{\infty}\big[\alpha_{i1}\phi_i(\vec{x})|\uparrow\rangle + \alpha_{i2}\phi_i(\vec{x})|\downarrow\rangle\big]$

$$= \sum_{i=1}^{\infty}\begin{pmatrix}\alpha_{i1}\\ \alpha_{i2}\end{pmatrix}\phi_i(\vec{x}) = \begin{pmatrix}\sum_i \alpha_{i1}\phi_i(\vec{x})\\ \sum_i \alpha_{i2}\phi_i(\vec{x})\end{pmatrix} = \boxed{\begin{pmatrix}\psi_\uparrow(\vec{x})\\ \psi_\downarrow(\vec{x})\end{pmatrix} \equiv \boldsymbol{\psi}(\vec{x}) \equiv \psi(\vec{x}, \underbrace{m_s}_{\pm\frac{1}{2}})} \quad \textbf{spinor}$$

Spinor is a two-component wavefunction equivalent to a wavefunction with a continuous variable $\vec{x}$ and a discrete two-valued variable m_s (the spin projection to z-direction). Note that transformation properties of spinors under spatial rotations are different from ordinary vectors (they will be derived in Sec. 4b).



Simplified notation: $\boxed{(\vec{x}, m_s) \equiv \boldsymbol{\xi}}$ with $\boxed{\int d\boldsymbol{\xi} \equiv \Sigma_{m_s}\int d\vec{x}}$

► **Scalar product** $\langle\psi|\psi'\rangle = \sum_{ij}\sum_{i'j'}\alpha^*_{ij}\alpha'_{i'j'}\underbrace{\langle\phi_i|\phi_{i'}\rangle}_{\delta_{ii'}}\underbrace{\langle\chi_j|\chi_{j'}\rangle}_{\delta_{jj'}} = \sum_{ij}\alpha^*_{ij}\alpha'_{ij}$
can be expressed as:

$$\langle\psi|\psi'\rangle \equiv \int \begin{pmatrix}\psi^*_\uparrow(\vec{x}), \psi^*_\downarrow(\vec{x})\end{pmatrix}\begin{pmatrix}\psi'_\uparrow(\vec{x})\\ \psi'_\downarrow(\vec{x})\end{pmatrix}d\vec{x} = \sum_{m_s}\int \psi^*(\vec{x}, m_s)\psi'(\vec{x}, m_s)d\vec{x} = \int \psi^*(\boldsymbol{\xi})\psi'(\boldsymbol{\xi})d\boldsymbol{\xi}$$

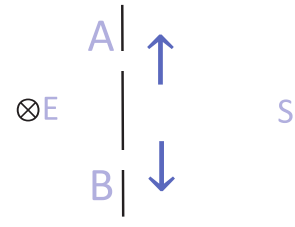
Normalization: $\int |\psi_\uparrow(\vec{x})|^2 d\vec{x} + \int |\psi_\downarrow(\vec{x})|^2 d\vec{x} = 1$

Probability density for particle at given position and spin:

$$\mathfrak{p}_\psi(\vec{x}\uparrow) = \big|\mathfrak{a}_\psi(\vec{x}\uparrow)\big|^2 = \big|\langle\vec{x}\uparrow|\psi\rangle\big|^2 = \left|\int \begin{pmatrix}\delta(\vec{x}'-\vec{x}), 0\end{pmatrix}\begin{pmatrix}\psi_\uparrow(\vec{x}')\\ \psi_\downarrow(\vec{x}')\end{pmatrix}d\vec{x}'\right|^2 = \big|\psi_\uparrow(\vec{x})\big|^2 = \big|\psi(\vec{x}, +\tfrac{1}{2})\big|^2$$
$$\mathfrak{p}_\psi(\vec{x}\downarrow) = \big|\mathfrak{a}_\psi(\vec{x}\downarrow)\big|^2 = \big|\langle\vec{x}\uparrow|\psi\rangle\big|^2 = \left|\int \begin{pmatrix}0, \delta(\vec{x}'-\vec{x})\end{pmatrix}\begin{pmatrix}\psi_\uparrow(\vec{x}')\\ \psi_\downarrow(\vec{x}')\end{pmatrix}d\vec{x}'\right|^2 = \big|\psi_\downarrow(\vec{x})\big|^2 = \big|\psi(\vec{x}, -\tfrac{1}{2})\big|^2$$

► **Coordinate-spin entanglement**: Almost all spinor states are entangled. A factorized state has a special structure $\boldsymbol{\psi}(\vec{x}) = \psi(\vec{x})(\alpha_1|\uparrow\rangle + \alpha_2|\downarrow\rangle) = \psi(\vec{x})\begin{pmatrix}\alpha_1\\ \alpha_2\end{pmatrix}$

► **Application in a which-path version of the double-slit experiment**
Consider a modification of the double-slit experiment (see Intro.) such that **both slits are equipped with spin polarizers**: $\begin{cases}\text{A polarizes electron in direction } \uparrow\\ \text{B polarizes electron in direction } \downarrow\end{cases}$
⇒ paths through slits A & B are distinguishable
The electron's state inside the interferometer is $\boldsymbol{\psi}(\vec{x}) = \alpha\psi_{\rm A}(\vec{x})|\uparrow\rangle + \beta\psi_{\rm B}(\vec{x})|\downarrow\rangle$, where $\psi_{\rm A}, \psi_{\rm B}$ are spatial wavefunctions for particles propagating from the respective slit and α, β some coefficients.



Probability density to detect the electron at place $\vec{x}$ reads $\mathfrak{p}_\psi(\vec{x}) = \langle\psi|\hat{P}_{\vec{x}}|\psi\rangle$, where $\hat{P}_{\vec{x}} = |\vec{x}\uparrow\rangle\langle\vec{x}\uparrow| + |\vec{x}\downarrow\rangle\langle\vec{x}\downarrow|$ is the projector to the subspace of $\mathcal{H}$ (more precisely $\overline{\mathcal{H}}$) spanned by vectors $|\vec{x}\rangle|\uparrow\rangle$ and $|\vec{x}\rangle|\downarrow\rangle$:

$$\mathfrak{p}_\psi(\vec{x}) = \big(\alpha^* \overbrace{\langle\psi_{\rm A}|\vec{x}\rangle}^{\psi_{\rm A}^*(\vec{x})} \overbrace{\langle\uparrow|\uparrow\rangle}^{1} + \beta^* \overbrace{\langle\psi_{\rm B}|\vec{x}\rangle}^{\psi_{\rm B}^*(\vec{x})} \overbrace{\langle\downarrow|\uparrow\rangle}^{0}\big)\big(\alpha \overbrace{\langle\vec{x}|\psi_{\rm A}\rangle}^{\psi_{\rm A}(\vec{x})} \overbrace{\langle\uparrow|\uparrow\rangle}^{1} + \beta \overbrace{\langle\vec{x}|\psi_{\rm B}\rangle}^{\psi_{\rm B}(\vec{x})} \overbrace{\langle\uparrow|\downarrow\rangle}^{0}\big) +$$
$$\big(\alpha^* \underbrace{\langle\psi_{\rm A}|\vec{x}\rangle}_{\psi_{\rm A}^*(\vec{x})} \underbrace{\langle\uparrow|\downarrow\rangle}_{0} + \beta^* \underbrace{\langle\psi_{\rm B}|\vec{x}\rangle}_{\psi_{\rm B}^*(\vec{x})} \underbrace{\langle\downarrow|\downarrow\rangle}_{1}\big)\big(\alpha \underbrace{\langle\vec{x}|\psi_{\rm A}\rangle}_{\psi_{\rm A}(\vec{x})} \underbrace{\langle\downarrow|\uparrow\rangle}_{0} + \beta \underbrace{\langle\vec{x}|\psi_{\rm B}\rangle}_{\psi_{\rm B}(\vec{x})} \underbrace{\langle\downarrow|\downarrow\rangle}_{1}\big)$$

$= |\alpha\psi_{\rm A}(\vec{x})|^2 + |\beta\psi_{\rm B}(\vec{x})|^2 \;\Rightarrow$ **no interference appears** (the same holds if paths A & B are recorded by two *perpendicular* states of *any* spectator system)

◂ Historical remark

1922: O. Stern & W. Gerlach observe the first indication of spin

1924: Wolfgang Pauli introduces "two-valued quantum degree of freedom" and formulates the exclusion principle (see below), in 1927 he introduces spinors

1925: R. Kronig and G. Uhlenbeck & S. Goudsmit provide an interpretation of spin in terms of intrinsic rotation (refused at that time)

■ Two or more distinguishable structureless particles with spin $\frac{1}{2}$

We are ready to construct state spaces for collections of particles. At first we assume that the particles are of different types—*distinguishable*. We assume N particles with spin $\frac{1}{2}$, but the same procedure can be applied regardless of spin.

► $\mathcal{H}_1$, $\mathcal{H}_2$, ... $\mathcal{H}_N$= Hilbert spaces of individual particles: $\mathcal{H}_i = \mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^2$

$$\boxed{\mathcal{H}^{(N)} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N}$$

Wavefunction of a general state $|\Psi\rangle \in \mathcal{H}^{(N)}$

$$\Psi(\underbrace{\vec{x}_1, m_1}_{\boldsymbol{\xi}_1}, \underbrace{\vec{x}_2, m_2}_{\boldsymbol{\xi}_2}, \ldots \underbrace{\vec{x}_N, m_N}_{\boldsymbol{\xi}_N}) = \underbrace{\langle \boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N | \Psi \rangle}_{\mathfrak{a}_\Psi(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N)}$$

N-particle amplitude

Scalar product: $\langle\Psi|\Psi'\rangle \equiv$

$$\sum_{m_1} ... \sum_{m_N} \int ... \int \Psi^*(\vec{x}_1, m_1 ... \vec{x}_N, m_N) \Psi'(\vec{x}_1, m_1 ... \vec{x}_N, m_N) d\vec{x}_1 ... d\vec{x}_N$$
$$= \int ... \int \Psi^*(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N) \Psi'(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N) d\boldsymbol{\xi}_1 ... d\boldsymbol{\xi}_N$$

► **Multidimensional entanglement**: Almost all states exhibit all kinds of entanglement (coordinate-coordinate, spin-spin, and coordinate-spin) of different particles and coordinate-spin entanglement of identical particles

► **Probability expressions**

Wavefunction $\Psi(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N)$ lives in the multidimensional configuration space containing generalized coordinates $\boldsymbol{\xi}_i \equiv (\vec{x}_i, m_i)$ of all particles. It contains complete information on mutual correlations between particles and allows one to extract any kind of probability distribution in the generalized coordinate space:

(a) Joint probability density to find particles # $(1, 2 ... N)$ at $(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 ... \boldsymbol{\xi}_N)$

$$\boxed{\mathfrak{p}_\Psi(\boldsymbol{\xi}_1 \ldots \boldsymbol{\xi}_N) = \big|\mathfrak{a}_\Psi(\boldsymbol{\xi}_1 \ldots \boldsymbol{\xi}_N)\big|^2 = \langle\Psi|\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N\rangle\langle\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N|\Psi\rangle = |\Psi(\boldsymbol{\xi}_1 \ldots \boldsymbol{\xi}_N)|^2}$$

Normalization: $\int ... \int \mathfrak{p}_\Psi(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N)\, d\boldsymbol{\xi}_1 ... d\boldsymbol{\xi}_N = 1$

(b) Integrated probability $\mathfrak{p}_\Psi(X)$ of a property defined by $(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N) \in X$, where X is a certain domain in the multidimensional configuration space:

$$\mathfrak{p}_\Psi(X) = \int ... \int \chi_X(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N) \mathfrak{p}_\Psi(\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N)\, d\boldsymbol{\xi}_1 ... d\boldsymbol{\xi}_N \qquad \text{where } \chi_X = \begin{cases} 1 \text{ for } (\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N) \in X \\ 0 \text{ for } (\boldsymbol{\xi}_1 ... \boldsymbol{\xi}_N) \notin X \end{cases}$$

Example: property X identified with the subset of the config. space in which particle #1 is localized in a state between $|\boldsymbol{\xi}\rangle$ and $|\boldsymbol{\xi}+d\boldsymbol{\xi}\rangle$. Probability $\mathfrak{p}_\Psi(X)=\mathfrak{p}_\Psi(\boldsymbol{\xi}_1=\boldsymbol{\xi})d\boldsymbol{\xi}$, where the density: $\mathfrak{p}_\Psi(\boldsymbol{\xi}_1=\boldsymbol{\xi})=\underbrace{\int\!...\!\int}_{N-1}\mathfrak{p}_\Psi(\boldsymbol{\xi},\boldsymbol{\xi}_2,...\boldsymbol{\xi}_N)d\boldsymbol{\xi}_2...d\boldsymbol{\xi}_N$

(c) Single-particle probability density to find *any* of the N particles at $\boldsymbol{\xi}$

$$\boxed{\mathfrak{p}_\Psi(\boldsymbol{\xi})=\frac{1}{N}\sum_{i=1}^{N}\underbrace{\int\!...\!\int}_{N-1}\mathfrak{p}_\Psi(\boldsymbol{\xi}_1...\boldsymbol{\xi}_{i-1}\underbrace{\boldsymbol{\xi}}_{i}\boldsymbol{\xi}_{i+1}...\boldsymbol{\xi}_N)\,d\boldsymbol{\xi}_1...d\boldsymbol{\xi}_{i-1}d\boldsymbol{\xi}_{i+1}...d\boldsymbol{\xi}_N}$$

Normalization $\int\mathfrak{p}_\Psi(\boldsymbol{\xi})\,d\boldsymbol{\xi}=1$. This density is determined from the expression $N\mathfrak{p}_\Psi(\boldsymbol{\xi})d\boldsymbol{\xi}=\sum_{n=0}^{N}n\mathfrak{p}_\Psi(n,\boldsymbol{\xi},d\boldsymbol{\xi})\equiv\varrho_\Psi(\boldsymbol{\xi})d\boldsymbol{\xi}$, where $\mathfrak{p}_\Psi(n,\boldsymbol{\xi},d\boldsymbol{\xi})$ is the integrated probability for finding any $n\leq N$ particles in states between $|\boldsymbol{\xi}\rangle$ and $|\boldsymbol{\xi}+d\boldsymbol{\xi}\rangle$. So $\varrho_\Psi(\boldsymbol{\xi})=N\mathfrak{p}_\Psi(\boldsymbol{\xi})$ normalized as $\int\varrho_\Psi(\boldsymbol{\xi})\,d\boldsymbol{\xi}=N$ is an **average particle concentration** (not accounting for particle identity) at generalized coordinate $\boldsymbol{\xi}$.

■ Two indistinguishable particles

In quantum physics, if some particles are really the same, we cannot define any kind of their individuality. In particular, we cannot assign to these particles any intrinsic names/numbers as there exists no property that would enable us to recognize whether a given particle is "Fred" or "Bruno". Consider two electrons localized at distinct places A and B. We can name them "the electron at place A" and "the electron at place B"; these are two distinguished single-particle states. However, it is impossible to say whether the present electron at place A is the same electron as the one observed at place A some time ago.

► The Hilbert space of two indistinguishable particles is constructed from the Hilbert space $\mathcal{H}^{(2)}\equiv\mathcal{H}_1\otimes\mathcal{H}_2\ni|\Psi\rangle\equiv\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)$ of two formally distinguishable (though physically identical) particles #1 & #2. We introduce in this space the **particle exchange operator**: $\boxed{\hat{E}_{1\rightleftharpoons2}\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)=\Psi(\boldsymbol{\xi}_2,\boldsymbol{\xi}_1)}$ $\quad\hat{E}^2_{1\rightleftharpoons2}=\hat{I}$

$\hat{E}_{1\rightleftharpoons2}$ exchanges states of particles #1 & #2 in the expansion of $|\Psi\rangle$ in any factorized basis: $|\Psi\rangle=\sum_{ij}\alpha_{ij}|\phi_i\rangle_1|\phi_j\rangle_2\quad\Rightarrow\quad\hat{E}_{1\rightleftharpoons2}|\Psi\rangle=\sum_{ij}\alpha_{ij}|\phi_j\rangle_1|\phi_i\rangle_2$

► For indistinguishable particles we require that the exchange affects only the overall phase of the state since it is physically irrelevant, so $\hat{E}_{1\rightleftharpoons2}|\Psi\rangle=e^{i\varphi}|\Psi\rangle$ with $\varphi\in\mathbb{R}$, and that two subsequent exchanges yield the original state: $e^{2i\varphi}=1$

$$\Rightarrow\quad\begin{cases}\varphi=0\\ \varphi=\pi\end{cases}\qquad\boxed{\begin{array}{rcl}\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)&=&+\Psi(\boldsymbol{\xi}_2,\boldsymbol{\xi}_1)\\ \Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)&=&-\Psi(\boldsymbol{\xi}_2,\boldsymbol{\xi}_1)\end{array}}\qquad\begin{array}{ll}\textbf{symmetric}&\text{for }\textbf{bosons}\\ \textbf{antisymmetric}&\text{for }\textbf{fermions}\end{array}$$

The two possibilities of phase φ define two fundamental types of elementary particles in nature: bosons (with exchange-symmetric wave functions) and fermions (with exchange-antisymmetric wave functions). It turns out (proof given only

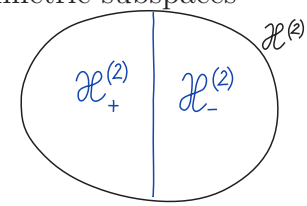
in the relativistic QM) that particles with spin $\frac{1}{2}$ (or spins $\frac{3}{2}, \frac{5}{2}$...) are fermions, while those with no spin (spin 0 or spins 1,2...) are bosons.

► Any two-body wavefunction can be uniquely decomposed into the symmetric & antisymmetric parts that belong to distinct subspaces of $\mathcal{H}^{(2)}$:

$$\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2) = \underbrace{\tfrac{1}{2}\big[\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)+\Psi(\boldsymbol{\xi}_2,\boldsymbol{\xi}_1)\big]}_{\hat{P}_+\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)} + \underbrace{\tfrac{1}{2}\big[\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)-\Psi(\boldsymbol{\xi}_2,\boldsymbol{\xi}_1)\big]}_{\hat{P}_-\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)} \qquad \hat{P}_\pm = \tfrac{1}{2}[\hat{I}\pm\hat{E}_{1\rightleftharpoons 2}]$$

$\hat{P}_+$ and $\hat{P}_-$ are projectors to the symmetric and antisymmetric subspaces

$$\hat{P}_+ + \hat{P}_- = \hat{I} \quad \Rightarrow \quad \boxed{\mathcal{H}^{(2)} = \mathcal{H}^{(2)}_+ \oplus \mathcal{H}^{(2)}_-}$$



General form of decomposition for $|\Psi\rangle = \sum_{ij} \alpha_{ij}|\phi_i\rangle_1|\phi_j\rangle_2$:

$$\hat{P}_\pm|\Psi\rangle = \sum_{ij} \alpha_{ij}\tfrac{1}{2}\big[|\phi_i\rangle_1|\phi_j\rangle_2 \pm |\phi_j\rangle_1|\phi_i\rangle_2\big]$$

► **Pauli principle**: $\boxed{\hat{P}_-|\psi\rangle_1|\psi\rangle_2 = 0}$ (states $|\psi\rangle_1|\psi\rangle_2$ are $\perp$ to subspace $\mathcal{H}^{(2)}_-$)

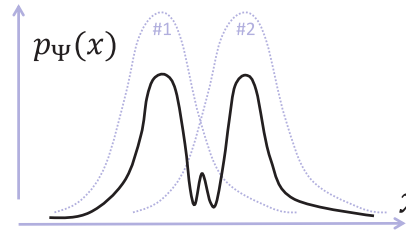
⇒ Two (or more) fermions cannot occur in the same single-particle state. Each single-particle state can be occupied at most by one fermion. This has tremendous consequences for the structure of matter! Without Pauli principle, the world would be a boring place (probably with no bored creature present).

► **Interference effects caused by indistinguishability**

Two **distinguishable** particles in a factorized state: $\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2) = \psi_1(\boldsymbol{\xi}_1)\psi_2(\boldsymbol{\xi}_2)$
Joint probability density: $\mathfrak{p}_\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2) = \mathfrak{p}_1(\boldsymbol{\xi}_1)\mathfrak{p}_2(\boldsymbol{\xi}_2)$
Single-particle prob.density: $\mathfrak{p}_\Psi(\boldsymbol{\xi}) = \frac{1}{2}\,[\mathfrak{p}_1(\boldsymbol{\xi}) + \mathfrak{p}_2(\boldsymbol{\xi})]$ ⇒ no interference
Here $\mathfrak{p}_i(\boldsymbol{\xi}_i) \equiv \mathfrak{p}_{\psi_i}(\boldsymbol{\xi}_i) = |\psi_i(\boldsymbol{\xi}_i)|^2$ is prob.density associated with particle $\#i = 1,2$

Two **indistinguishable** particles: $\hat{P}_\pm\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2) \propto [\psi_1(\boldsymbol{\xi}_1)\psi_2(\boldsymbol{\xi}_2) \pm \psi_1(\boldsymbol{\xi}_2)\psi_2(\boldsymbol{\xi}_1)]$
Joint: $\mathfrak{p}_\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2) \propto \mathfrak{p}_1(\boldsymbol{\xi}_1)\mathfrak{p}_2(\boldsymbol{\xi}_2) + \mathfrak{p}_1(\boldsymbol{\xi}_2)\mathfrak{p}_2(\boldsymbol{\xi}_1) \pm 2\mathrm{Re}[\psi_1(\boldsymbol{\xi}_1)\psi_2^*(\boldsymbol{\xi}_1)\psi_1^*(\boldsymbol{\xi}_2)\psi_2(\boldsymbol{\xi}_2)]$
Single-particle: $\mathfrak{p}_\Psi(\boldsymbol{\xi}) \propto \mathfrak{p}_1(\boldsymbol{\xi}) + \mathfrak{p}_2(\boldsymbol{\xi}) \pm 2\mathrm{Re}\,[\langle\psi_1|\psi_2\rangle\psi_1^*(\boldsymbol{\xi})\psi_2(\boldsymbol{\xi})]$

The state $\hat{P}_\pm\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)$ is entangled and this immediate consequence of particle indistinguishability creates interference effects in both probability densities $\mathfrak{p}_\Psi(\boldsymbol{\xi}_1,\boldsymbol{\xi}_2)$ & $\mathfrak{p}_\Psi(\boldsymbol{\xi})$. However, the interference is significant only if the states $\psi_1(\boldsymbol{\xi})$ & $\psi_2(\boldsymbol{\xi})$ have a sufficient overlap. No interference effects are observed e.g. for very distant particles or for particles with opposite spins (⇒ entanglement of electrons in different galaxies, for instance, is practically unmeasurable).



■ Many indistinguishable particles

It is straightforward (but more laborious) to generalize the above results to $N>2$ indistinguishable particles. In short, particle permutations are decomposed into

pairwise exchanges and the states of identical bosons (fermions) are identified with symmetric (antisymmetric) subspaces with respect to these exchanges. A general theory of bosonic & fermionic systems will be elaborated in Sec. 14.

▶ N distinguishable particles: $\Psi(\boldsymbol{\xi}_1,\dots\boldsymbol{\xi}_N)\equiv|\Psi\rangle\in\mathcal{H}^{(N)}\equiv\otimes_{k=1}^{N}\mathcal{H}_k$

Factorized basis: $|\phi_{i_1}\rangle_1|\phi_{i_2}\rangle_2\dots|\phi_{i_N}\rangle_N\equiv|\Phi_{i_1i_2\dots i_N}\rangle$ with $i_k=1,2,3,\dots$

▶ **Particle exchanges and permutations**

Exchange operators

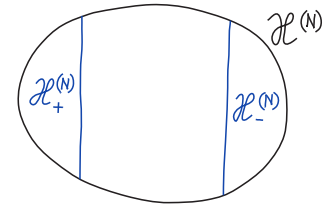
$$\boxed{\hat{E}_{k\rightleftharpoons l}|\Phi_{i_1\dots i_k\dots i_l\dots i_N}\rangle=|\Phi_{i_1\dots i_l\dots i_k\dots i_N}\rangle}$$

Permutation operators

$$\boxed{\hat{\mathcal{E}}_\pi|\Phi_{i_1i_2\dots i_N}\rangle=|\Phi_{i_{k_1^\pi}i_{k_2^\pi}\dots i_{k_N^\pi}}\rangle}$$

Permutation $(k_1^\pi,k_2^\pi,\dots k_N^\pi)$ is an arbitrary reordering of the original sequence $(1,2,\dots N)$. Index $\pi=1,\dots N!$ is the permutation identifier and number $k_i^\pi\in\{1,2,\dots,N\}$ stands for the ith term of the πth reordered sequence. For example $(1,2,3)\to(1,2,3),(3,1,2),(2,3,1),(1,3,2),(3,2,1),(2,1,3)$ for $N=3$. Any permutation $\hat{\mathcal{E}}_\pi$ can be written as a product of exchanges $\hat{E}_{k\rightleftharpoons l}$. The factorization of a given $\hat{\mathcal{E}}_\pi$ is not unique, but all factorizations have either even or odd number of exchanges. This defines even & odd permutations.

Permutation sign $\sigma_\pi=\begin{cases}+ & \text{for even permutation}\\ - & \text{for odd permutation}\end{cases}$



▶ **Hilbert space decomposition**

$$\boxed{\mathcal{H}^{(N)}=\mathcal{H}_+^{(N)}\oplus\cdots\oplus\mathcal{H}_-^{(N)}}$$

The dots represent subspaces with mixed symmetries, while $\mathcal{H}_+^{(N)}$ and $\mathcal{H}_-^{(N)}$ are fully symmetric and antisymmetric subspaces satisfying:

$$\boxed{\hat{\mathcal{E}}_\pi|\Psi\rangle=+|\Psi\rangle}\ \forall|\Psi\rangle\in\mathcal{H}_+^{(N)},\qquad \boxed{\hat{\mathcal{E}}_\pi|\Psi\rangle=\sigma_\pi|\Psi\rangle}\ \forall|\Psi\rangle\in\mathcal{H}_-^{(N)}$$

$$\boxed{\hat{P}_+^{(N)}=\frac{1}{N!}\sum_{\pi=1}^{N!}\hat{\mathcal{E}}_\pi}\qquad\boxed{\hat{P}_-^{(N)}=\frac{1}{N!}\sum_{\pi=1}^{N!}\sigma_\pi\hat{\mathcal{E}}_\pi}\qquad\text{projectors to }\mathcal{H}_+^{(N)}\ \&\ \mathcal{H}_-^{(N)}$$

A sketch of proof: The fact that $\hat{P}_\pm|\Psi\rangle\in\mathcal{H}_\pm^{(N)}$ follows from the closure relations of permutations: (i) for any two permutations π,π' we have $\hat{\mathcal{E}}_\pi\hat{\mathcal{E}}_{\pi'}=\hat{\mathcal{E}}_{\pi''}$, where π'' denotes another permutation satisfying $\sigma_{\pi''}=\sigma_\pi\sigma_{\pi'}$, (ii) if $\{\hat{\mathcal{E}}_{\pi'}\}_{\pi'=1}^{N!}$ represents a complete set of permutations, so does $\{\hat{\mathcal{E}}_\pi\hat{\mathcal{E}}_{\pi'}\}_{\pi'=1}^{N!}$ for any fixed $\hat{\mathcal{E}}_\pi$. In this way we can show that $\hat{\mathcal{E}}_\pi\hat{P}_+^{(N)}|\Psi\rangle=\hat{P}_+^{(N)}|\Psi\rangle$ and $\hat{\mathcal{E}}_\pi\hat{P}_-^{(N)}|\Psi\rangle=\sigma_\pi\hat{P}_-^{(N)}|\Psi\rangle$. Relations (i) and (ii) also imply that $\sum_\pi\sum_{\pi'}\hat{\mathcal{E}}_\pi\hat{\mathcal{E}}_{\pi'}=N!\sum_{\pi''}\hat{\mathcal{E}}_{\pi''}$ and $\sum_\pi\sum_{\pi'}\sigma_\pi\hat{\mathcal{E}}_\pi\sigma_{\pi'}\hat{\mathcal{E}}_{\pi'}=N!\sum_{\pi''}\sigma_{\pi''}\hat{\mathcal{E}}_{\pi''}$, which prove that $(\hat{P}_\pm^{(N)})^2=\hat{P}_\pm^{(N)}$.

Hilbert space for N identical particles is $\begin{cases}\mathcal{H}_+^{(N)} & \text{for } \textbf{bosons}\\ \mathcal{H}_-^{(N)} & \text{for } \textbf{fermions}\end{cases}$

$\hat{P}_+^{(N)} + \hat{P}_-^{(N)} \neq \hat{I}$ for $N > 2$: the rest of the space contains mixed symmetry subspaces (corresponding e.g. to mixtures of several types of identical particles)

► Expression of a **basis in the fermionic space**:

$$\hat{P}_-^{(N)} \underbrace{\Big[|\phi_1\rangle_1 |\phi_2\rangle_2 \ldots |\phi_N\rangle_N \Big]}_{|\Phi_{12\ldots N}\rangle} = \frac{1}{N!} \mathrm{Det} \begin{pmatrix} |\phi_1\rangle_1 & |\phi_1\rangle_2 & \ldots & |\phi_1\rangle_N \\ |\phi_2\rangle_1 & |\phi_2\rangle_2 & \ldots & |\phi_2\rangle_N \\ \vdots & & \ldots & \vdots \\ |\phi_N\rangle_1 & |\phi_N\rangle_2 & \ldots & |\phi_N\rangle_N \end{pmatrix}$$

Slater determinant

Normalization: The above projected state is not normalized. For the normalization coefficient we calculate $\langle \hat{P}_-^{(N)} \Phi_{12\ldots N} | \hat{P}_-^{(N)} \Phi_{12\ldots N} \rangle = \langle \Phi_{12\ldots N} | (\hat{P}_-^{(N)})^2 \Phi_{12\ldots N} \rangle = \langle \Phi_{12\ldots N} | \hat{P}_-^{(N)} \Phi_{12\ldots N} \rangle = 1/N!$ (the 2nd eq. follows from the hermiticity of projectors, see Sec. 2a, the last from the fact that any nontrivial permutation of $|\phi_1\rangle_1 \ldots |\phi_N\rangle_N$, where all $|\phi_1\rangle$s are mutually different, yields zero overlap with the original state) $\Rightarrow$ the normalized state reads $\sqrt{N!}\, \hat{P}_-^{(N)} |\Phi_{12\ldots N}\rangle = \frac{1}{\sqrt{N!}} \mathrm{Det}\,(\ldots)$

Notes: (a) Analogous expression for bosons can be formally written with "Det" replaced by a symbol denoting the exchange-symmetric sum of permutations. (b) Slater-determinant or analogous symmetrized states originate from *factorized* states in the space of distinguishable particles. They carry just a minimal unavoidable entanglement caused by indistinguishability of particles. These states form a basis in $\mathcal{H}_-^{(N)}$ or $\mathcal{H}_+^{(N)}$, so a general N-body fermionic or bosonic state can be expressed as a *superposition* of these basis states.

◄ Historical remark

1924: S.N. Bose derives Planck blackbody law from indistinguishability of photons
1924: Wolfgang Pauli formulates the exclusion principle to explain periodic table
1926: Werner Heisenberg and Paul Dirac relate Pauli principle to antisymmetric wavefunctions and Bose-Einstein statistics to symmetric wavefunctions. Dirac and Enrico Fermi derive statistical law for "fermions"
1927: D. Hartree & V. Fock derive approximation for atomic N-electron wavefunctions, in 1929 J. Slater facilitates the description by using the determinant
1939-50: M. Fierz, W. Pauli, J. Schwinger provide proofs (within the relativistic quantum theory) of the general theorem relating the "type of statistics" to spin

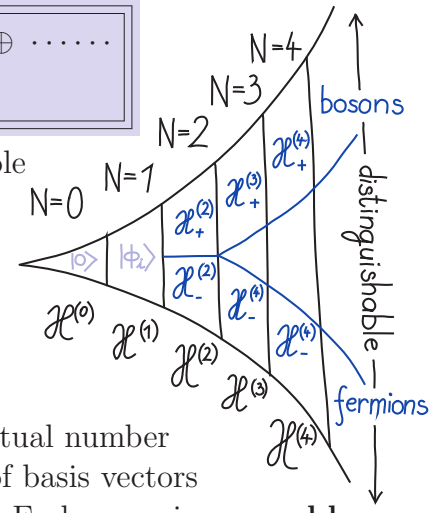
■ Systems with unbounded number of particles

We come to many-particle systems in which the particle number is not fixed. One can think of an exchange of particles with a bath. More fundamentally, if the special relativity is applied to processes involving elementary particles, the number of particles (the sum of their rest masses) is not conserved. Particles can be repeatedly created and annihilated, conserving only the total energy $\Leftrightarrow$ mass of the system. It turns out that considering no upper bound on the

particle number we leave the safe harbor of separable Hilbert spaces and face the limitless ocean of continuum. This is a transition to the field theory. Work with the Fock space within the nonrelativistic QM will be practiced in Secs. 14 & 15.

► **Fock space**
Sum of spaces for all particle numbers $N = 0, 1, 2, 3, \ldots$

$$\mathcal{H} \equiv \underbrace{\mathcal{H}^{(0)}}_{\substack{\text{vacuum} \\ \text{state } |0\rangle}} \oplus \underbrace{\mathcal{H}^{(1)}}_{1 \text{ particle}} \oplus \underbrace{\mathcal{H}^{(2)}_{\bullet}}_{2 \text{ particles}} \cdots \oplus \underbrace{\mathcal{H}^{(N)}_{\bullet}}_{N \text{ particles}} \oplus \cdots\cdots$$



This applies for distinguishable/indistinguishable particles of the same type:

$$\mathcal{H}^{(N)}_{\bullet} \equiv \begin{cases} \mathcal{H}^{(N)}_{+} & \text{indistinguishable bosons} \\ \mathcal{H}^{(N)}_{-} & \text{indistinguishable fermions} \\ \mathcal{H}^{(N)} & \text{distinguishable particles} \end{cases}$$

► **Separability versus non-separability**
In nonrelativistic QM it is assumed that the actual number of particles N is *unlimited* but *finite*. The set of basis vectors subject to this constraint is countable and such Fock space is **separable**. However, the *closure* of the Fock space including $\mathcal{H}^{(\infty)}_{\bullet}$ is **non-separable**. Reasoning: basis states $|\Phi_{i_1 i_2 \ldots}\rangle \equiv |\phi_{i_1}\rangle_1 |\phi_{i_2}\rangle_2 \ldots$. for $N{=}\infty$ are specified by an infinite number of integer indices $i_1, i_2, \ldots$. identifying basis states of individual particles. This set is uncountable in analogy to real numbers (infinite sequences of digits; see Cantor's "diagonal slash" argument).

◄ **Historical remark**
1932: Vladimir Fock introduced the space for indefinite particle number
1958: Paul Dirac relates the Fock space to field quantization & continuum problems

■ Artificial systems (qubits...)

Since recently, various artificial quantum systems are assembled in the laboratory to be harnessed in potential applications of quantum information technologies (Sec. 9). Such systems (formed by ensembles of trapped atoms, nuclear spins, superconducting circuits etc.) are designed so that they allow for controlled manipulations and show minimal sensitivity to external perturbations. The specific physical content of individual states is not essential (this being just an "engineering" issue) and the only focus is set to the mathematical properties of complex superpositions of arbitrary basis states in the finite Hilbert space.

► **Qubit**: any system with the 2-dimensional Hilbert space $\boxed{\mathcal{H} = \mathbb{C}^2}$ can be considered as a quantum analog of classical bit. The basis of $\mathcal{H}$ (formed by two selected states of the underlying system) is denoted as $\{|0\rangle, |1\rangle\}$.

General normalized states of the qubit are mapped to the unit sphere (points with spherical angles ϑ, φ), where classical logical states correspond to the north ($|0\rangle$) and south ($|1\rangle$) poles.

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle = \overbrace{e^{i\varphi_0}}^{\text{irrel. global phase}}\Big(\cos\tfrac{\vartheta}{2}|0\rangle + e^{i\overbrace{(\varphi_1-\varphi_0)}^{\varphi}}\sin\tfrac{\vartheta}{2}|1\rangle\Big)$$

► **Qudit**: a generalization to any higher dimension d (e.g., qutrit for $d=3$ etc.). Hilbert space $\mathcal{H} = \mathbb{C}^d \equiv \mathrm{Span}\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$. A general normalized state $|\psi\rangle = \sum_{k=0}^{d-1}\alpha_k|k\rangle$ is determined (up to the global phase) by $2(d-1)$ real parameters (e.g., by $d-1$ hyperspherical angles and $d-1$ relative phase angles).

► **System of N qubits** (Hilbert space of a quantum computer)

$$\mathcal{H} = \bigotimes_{i=1}^{N}\mathcal{H}_i \equiv \mathrm{Span}\Big\{\underbrace{|l_1\rangle_1|l_2\rangle_2\ldots|l_N\rangle_N}_{|x\rangle}\Big\}_{(l_1,l_2,\ldots,l_N)=(0,0,\ldots,0)}^{(1,1,\ldots,1)} \equiv \mathrm{Span}\big\{|x\rangle\big\}_{x=0}^{2^N-1}, \quad d=2^N$$

Factorized basis vectors built from states $|l_i\rangle_i \equiv |0\rangle_i$ or $|1\rangle_i$ can be enumerated by $x = 0, ..., 2^N-1$ so that $l_1 l_2 ... l_N$ is the binary representation of x.

$$|\Psi\rangle = \sum_{x=0}^{2^N-1}\alpha_x|x\rangle$$

General state of the system describes a **quantum register** that can carry integers $x \in \{0, 1, ..., 2^N-1\}$ as well as all their superpositions with any coefficients $\alpha_x \in \mathbb{C}$.

Although the initial state $|\Psi_0\rangle$ of various computational procedures is factorized, $|\Psi_0\rangle = \frac{1}{\sqrt{2^N}}\sum_{x=0}^{2^N-1}|x\rangle = \prod_{i=1}^{N}\frac{1}{\sqrt{2}}(|0\rangle_i+|1\rangle_i)$ the space $\mathcal{H}$ supports all kinds of *bi-* & *multi-partite entanglement*. Splitting the whole register to 2 subregisters A and B with n and $N-n$ qubits, respectively, $\mathcal{H}_\mathrm{A} = \bigotimes_{i=1}^{n}\mathcal{H}_i = \mathrm{Span}\{|x\rangle_\mathrm{A}\}_{x=0}^{2^n-1}$, $\mathcal{H}_\mathrm{B} = \bigotimes_{i=n+1}^{N}\mathcal{H}_i = \mathrm{Span}\{|x'\rangle_\mathrm{B}\}_{x'=0}^{2^{N-n}-1}$, so $\mathcal{H} = \mathcal{H}_\mathrm{A}\otimes\mathcal{H}_\mathrm{B}$, we can express a general state $\in \mathcal{H}$ in the form

$$|\Psi\rangle = \sum_{x=0}^{2^n-1}\sum_{x'=0}^{2^{N-n}-1}\alpha_{xx'}|x\rangle_\mathrm{A}|x'\rangle_\mathrm{B} \quad \alpha_{xx'}\in\mathbb{C},$$

It is **almost always entangled!**

The space $\mathcal{H}$ can be decomposed to subspaces with various **exchange symmetries** of individual qubit states. Consider concrete splitting s to 2 subregisters with n and $N-n$ qubits (e.g., $s = \{1,3,4\}\{2,5\}$ for $N=5$) and define the subspace $\mathcal{H}_s^{(N,n)}$ such that $\hat{E}_{i\rightleftharpoons j}|\Psi\rangle = \pm|\Psi\rangle$ for any $|\Psi\rangle \in \mathcal{H}_s^{(N,n)}$, with $\begin{cases} + & \text{for } i,j \text{ in the same subregister,} \\ - & \text{for } i,j \text{ in different subregisters.} \end{cases}$ Let $r(N,n)$ is the number such (nonequivalent) subspaces. It can be shown that $\mathcal{H} = \bigoplus_{n=\lceil N/2\rceil}^{N}\bigoplus_{s=1}^{r(N,n)}\mathcal{H}_s^{(N,n)}$

◄ Historical remark

1980's: P. Benioff, R. Feynman, D. Deutsch and others pioneer the idea of using controllable quantum systems for simulation and computation purposses

1995-present: construction of increasingly complex controllable quantum devices

2a. REPRESENTATION OF QUANTUM OBSERVABLES

The Hilbert space and its scalar product allowed us to calculate probabilities for mistaking a given state vector $|\psi\rangle$ with another state vector $|\psi'\rangle$. However, we do not know how to assign the vectors $|\psi\rangle$, $|\psi'\rangle$... to actual states of the system. This unavoidably requires definition of real observable quantities (shortly observables) that determine the system's actual properties. Hence our next task is to introduce observables into the Hilbert space structure.

In classical mechanics, observables were just ordinary functions in the phase space. In quantum mechanics, the thing is more complicated since many observables yield *discrete values* and results of measurements are generally *indeterministic*. We seek for an elegant mathematical tool capable to cope with these properties.

■ Operators associated with observables

Consider an arbitrary observable denoted as A. Associated with each state $|\psi\rangle \in \mathcal{H}$ there must be a probability distribution $\mathfrak{p}_\psi(a)$ characterizing all possible measurement outputs $\{a\}$ of A on this state. A suitable path to obtain such a distribution proceeds via the association of each quantity A with an operator $\hat{A}$, which represents a specific mapping $\mathcal{H} \to \mathcal{H}$ (see Sec. 1a). We first present a plausible (but not unique) motivation for launching out in this direction and then briefly outline some rudiments of the operator theory.

► Moments of statistical distribution

The **probability distribution** $\mathfrak{p}_\psi(a)$ of all possible measurement outcomes a of observable A in state $|\psi\rangle$ can be characterized by **statistical moments**:

$$\boxed{\langle A^n\rangle_\psi \equiv \int a^n\, \mathfrak{p}_\psi(a)\, da}$$

$n{=}1$: $\langle A\rangle_\psi$ **average (expectation) value**
$n{=}2$: $\langle (A-\langle A\rangle_\psi)^2\rangle_\psi = \langle A^2\rangle_\psi - \langle A\rangle_\psi^2$ **variance (dispersion)**
.....
.....

The knowledge of all moments $\langle A^1\rangle_\psi, \langle A^2\rangle_\psi, \langle A^3\rangle_\psi, \langle A^4\rangle_\psi, \ldots\ldots$ under some conditions uniquely determines the whole distribution $\mathfrak{p}_\psi(a)$.

► Calculation of moments via operators

Consider an operator $\hat{A}|\psi\rangle \equiv |\hat{A}\psi\rangle \equiv |\psi'\rangle \in \mathcal{H}$. Integer powers of this operator can be calculated in a straightforward way: $\hat{A}^n|\psi\rangle \equiv \underbrace{\hat{A}\hat{A}\ldots\hat{A}}_{n\,\text{times}}|\psi\rangle \equiv |\hat{A}^n\psi\rangle \in \mathcal{H}$. This motivates us to set the following postulate:

Any physical observable A is associated with a **linear Hermitian operator** $\hat{A}$ acting on the Hilbert space $\mathcal{H}$ of states. Statistical moments of the distribution $\mathfrak{p}_\psi(a)$ are calculated as:

$$\boxed{\langle A^n\rangle_\psi = \langle\psi|\hat{A}^n\psi\rangle}$$

Requirement 1: linearity
Because all QM is linear!

$$\boxed{\hat{A}\big(\alpha|\psi_1\rangle + \beta|\psi_2\rangle\big) = \alpha\hat{A}|\psi_1\rangle + \beta\hat{A}|\psi_2\rangle}$$

$$\boxed{\hat{A} \equiv \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \\ \vdots & & \ddots \end{pmatrix}}$$

matrix representation of lin. operators with arbitrary basis $\{|\phi_i\rangle\} \Rightarrow$ matr. elements $A_{ij} = \langle\phi_i|\hat{A}\phi_j\rangle$ (see Sec. 1a)

Requirement 2: Hermiticity $\boxed{\langle\psi_1|\hat{A}\psi_2\rangle = \langle\hat{A}\psi_1|\psi_2\rangle} = \langle\psi_2|\hat{A}\psi_1\rangle^*$

$\boxed{\langle\psi|\hat{A}^n\psi\rangle \in \mathbb{R}}$ Hermiticity is sufficient (though not necessary) condition for the statistical moments being **real numbers** (as needed)

$\Rightarrow$ the matrices associated with $\hat{A}$ satisfy: $\boxed{A_{ij} = A^*_{ji} \text{ for } i{\neq}j \text{ and } A_{ii} \in \mathbb{R}}$

▶ Some mathematical definitions

Definition domain: Operator $\hat{A}$ is defined for $|\psi\rangle \in \mathrm{Def}(\hat{A}) \subseteq \mathcal{H}$

For physics purposes it often suffices if $\boxed{\mathrm{Def}(\hat{A}) \equiv \text{a } \textbf{dense subset } \underline{\mathcal{H}} \subset \mathcal{H}}$

Operator norm: $||\hat{A}||^2 \equiv \mathrm{Sup}\left\{\frac{\langle\hat{A}\psi|\hat{A}\psi\rangle}{\langle\psi|\psi\rangle}\right\}_{|\psi\rangle\in\mathrm{Def}(\hat{A})}$ (cf. rigged Hilbert space, Sec. 1a)

$||\hat{A}|| < \infty$ for **bounded** operators, $||\hat{A}|| = \infty$ for **unbounded** operators

Hermitian adjoint operator $\hat{A}^\dagger$ is an operator satisfying the condition:

$\boxed{\langle\psi_1|\hat{A}\psi_2\rangle = \langle\hat{A}^\dagger\psi_1|\psi_2\rangle} = \langle\psi_2|\hat{A}^\dagger\psi_1\rangle^* \quad \begin{cases}\forall|\psi_2\rangle{\in}\mathrm{Def}(\hat{A})\\ \forall|\psi_1\rangle{\in}\mathrm{Def}(\hat{A}^\dagger){\supseteq}\mathrm{Def}(\hat{A})\end{cases}$

$\boxed{\hat{A}^\dagger = \begin{pmatrix} A^*_{11} & A^*_{21} & \cdots \\ A^*_{12} & A^*_{22} & \\ \vdots & & \ddots \end{pmatrix} \equiv \hat{A}^{\mathrm{T}*}}$ matrix representation of Hermitian adjoint operator (= transpose & complex conjugate matrix)

Adjoint of a product: $\boxed{(\hat{A}_1\hat{A}_2)^\dagger = \hat{A}^\dagger_2\hat{A}^\dagger_1}$ and similarly for multiple products

$\langle\psi_1|\hat{A}_1\hat{A}_2\psi_2\rangle = \langle\hat{A}^\dagger_1\psi_1|\hat{A}_2\psi_2\rangle = \langle\hat{A}^\dagger_2\hat{A}^\dagger_1\psi_1|\psi_2\rangle$

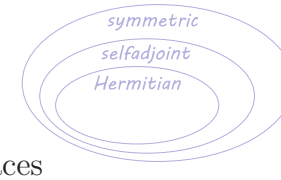
Symmetric, selfadjoint vs. Hermitian operators

All these operators satisfy the following condition: but for different domains of vectors $|\psi\rangle$ $\boxed{\hat{A}|\psi\rangle = \hat{A}^\dagger|\psi\rangle}$

Symmetric operator: $|\psi\rangle \in \mathrm{Def}(\hat{A}) \subseteq \mathrm{Def}(\hat{A}^\dagger) \subseteq \mathcal{H}$

Selfadjoint operator: $|\psi\rangle \in \mathrm{Def}(\hat{A}) = \mathrm{Def}(\hat{A}^\dagger) \subseteq \mathcal{H}$

Hermitian operator: $|\psi\rangle \in \mathrm{Def}(\hat{A}) = \mathrm{Def}(\hat{A}^\dagger) = \mathcal{H}$



These definitions are equivalent in finite-dimensional spaces but not in ∞-dim. spaces. Nevertheless, most textbooks including this one make use of the term "Hermitian operator" regardless of the definition domain.

▶ Function of operator

Physical observables are often defined as functions of other observables.

We first define a function of operator for functions of the form $f(x) = \sum_k f_k\, x^k$, i.e. expressible as Taylor series: $\boxed{f(\hat{A}) \equiv \sum_k f_k\, \hat{A}^k}$

A more general definition will be given below $f_k \in \mathbb{R} \Rightarrow f(\hat{A})$ Hermitian

▶ Tensor products of operators

We will need to use operators in product spaces. Here are some constructions:

Let $\begin{Bmatrix}\hat{A}_1 \text{ on } \mathcal{H}_1\\ \hat{A}_2 \text{ on } \mathcal{H}_2\end{Bmatrix}$ be operators defined by basis actions $\begin{Bmatrix}\hat{A}_1|\phi_{1i}\rangle \equiv |\phi'_{1i}\rangle\\ \hat{A}_2|\phi_{2j}\rangle \equiv |\phi'_{2j}\rangle\end{Bmatrix}$. Then:

(a) Operator $\boxed{\hat{A}=\hat{A}_1\otimes\hat{A}_2}$ on $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$ is defined by: $\hat{A}|\psi\rangle=\hat{A}\big[\sum_{i,j}\gamma_{ij}\overbrace{|\phi_{1i}\rangle|\phi_{2j}\rangle}^{|\Phi_{ij}\rangle}\big]=\sum_{i,j}\gamma_{ij}\overbrace{|\phi'_{1i}\rangle|\phi'_{2j}\rangle}^{|\Phi'_{ij}\rangle}$

(b) Possible extension of $\hat{A}_1$, $\hat{A}_2$ to $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$ is obtained from:

$$\boxed{\begin{array}{l}\hat{A}_1^{(\mathrm{ext})}=\hat{A}_1\otimes\hat{I}_2\equiv\hat{A}_1\\ \hat{A}_2^{(\mathrm{ext})}=\hat{I}_1\otimes\hat{A}_2\equiv\hat{A}_2\end{array}}\quad\begin{array}{l}\hat{I}_1\equiv\text{unit op. in }\mathcal{H}_1\\ \hat{I}_2\equiv\text{unit op. in }\mathcal{H}_2\end{array}$$

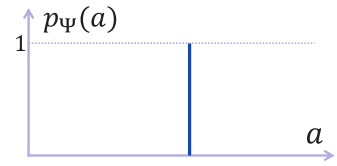
Similarly for multiple products $\bigotimes_i\mathcal{H}_i$

■ Eigenvalues and eigenvectors of Hermitian operators

The key characteristic of any operator in the Hilbert space is its spectrum of eigenvalues and the set of the corresponding eigenvectors. Not only these eigensolutions constitute a subject of an involved mathematical theory, they also play the most essential role in the formulation of quantum mechanics.

▶ "Dispersion-free" states and possible measurement outcomes

Consider state $|\psi_a\rangle$ in which observable A yields a "sharp" value, i.e. a single possible output a with probability $\mathfrak{p}_\psi(a)=1$. Hence the average $\langle A\rangle_{\psi_a}=a$ and variance $\boxed{\langle\!\langle A^2\rangle\!\rangle_{\psi_a}\equiv\langle A^2\rangle_{\psi_a}-\langle A\rangle^2_{\psi_a}}=0$



$$\underbrace{\langle\psi_a|\hat{A}^2\psi_a\rangle}_{\langle A^2\rangle_{\psi a}}-\underbrace{\langle\psi_a|\hat{A}\psi_a\rangle^2}_{\langle A\rangle^2_{\psi_a}=a^2}=\langle\psi_a|\underbrace{\hat{A}^2-2a\hat{A}+a^2\hat{I}}_{(\hat{A}-a\hat{I})^2}|\psi_a\rangle=\langle(\hat{A}-a\hat{I})\psi_a|(\hat{A}-a\hat{I})\psi_a\rangle=0$$

$$\Rightarrow(\hat{A}-a\hat{I})|\psi_a\rangle=0\Rightarrow\boxed{\hat{A}|\psi_a\rangle=a|\psi_a\rangle}\Rightarrow\left\{\begin{array}{ll}|\psi_a\rangle&\equiv\textbf{eigenvector}\\ a&\equiv\textbf{eigenvalue}\end{array}\right\}\text{ of operator }\hat{A}$$

For $\hat{A}=\hat{A}^\dagger$ the eigenvalues $a=\langle a|\hat{A}|a\rangle\in\mathbb{R}$

These considerations lead to a plausible determination of the set $\mathcal{S}(\hat{A})$ of possible measurement outcomes of observable $A\leftrightarrow\hat{A}$. We assume that *each possible outcome is associated with a state in which it is measured with certainty*, hence $\forall\ a\in\mathcal{S}(\hat{A})$ there $\exists$ dispersion-free state $|\psi_a\rangle$. This leads to the postulate:

$$\mathcal{S}(\hat{A})\equiv\{\,\text{possible measurement outcomes of A}\,\}\equiv\{\,\text{eigenvalues of }\hat{A}\,\}$$

Below we will use a "stammering" notation with $|\psi_a\rangle\equiv|a\rangle$, so: $\boxed{\hat{A}|a\rangle=a|a\rangle}$

▶ **Orthogonality** of eigenvectors with different eigenvalues (valid for Hermitian operators)

$$\left.\begin{array}{ll}\hat{A}|a\rangle=a|a\rangle & \Rightarrow\langle a'|\hat{A}|a\rangle=a\langle a'|a\rangle\\ \hat{A}|a'\rangle=a'|a'\rangle & \Rightarrow\underbrace{\langle a|\hat{A}|a'\rangle}_{\langle a'|\hat{A}|a\rangle^*}=\underbrace{a'}_{a'^*}\underbrace{\langle a|a'\rangle}_{\langle a'|a\rangle^*}\end{array}\right\}\Rightarrow0=\underbrace{(a-a')}_{\neq0}\langle a'|a\rangle\Rightarrow\boxed{\langle a'|a\rangle=0}$$

⇒ Different dispersion-free states (i.e., eigenstates with different eigenvalues) are *perfectly distinguishable*

▶ Degeneracy

A single eigenvalue a of $\hat{A}$ may have *more than one linearly independent eigenvectors* $\{|a;k\rangle\}_{k=1}^n$. Due to linearity of $\hat{A}$, any superposition of $\{|a;k\rangle\}_{k=1}^n$ is also

an eigenvector with the same eigenvalue: $\hat{A}\left(\sum_{k=1}^{n}\alpha_k|a;k\rangle\right)=a\sum_{k=1}^{n}\alpha_k|a;k\rangle$. Hence all eigenvectors with the same eigenvalue a form a **degeneracy subspace** $\mathcal{H}_a$ whose dimension $\boxed{d_{\mathcal{H}_a}\equiv d_a\leq d_{\mathcal{H}}}$ is the maximal number of linearly independent eigenvectors, i.e. the maximal size $n_{\max}$ of the set $\{|a;k\rangle\}_{k=1}^{n}$. One can choose in $\mathcal{H}_a$ an **orthonormal basis** $\{|a^{(k)}\rangle\}_{k=1}^{d_a}$ satisfying $\boxed{\langle a^{(k')}|a^{(k)}\rangle=\delta_{k'k}}$

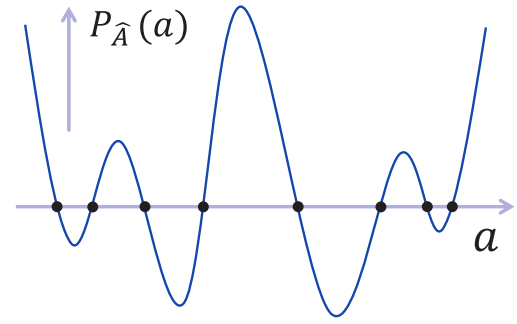
▶ Eigensolutions for finite dimension

$$\hat{A}|a\rangle=a|a\rangle \qquad \Leftrightarrow \qquad (\hat{A}-a\hat{I})|a\rangle=0 \qquad \Rightarrow \qquad \boxed{\underbrace{\mathrm{Det}(\hat{A}-a\hat{I})}_{\mathcal{P}_{\hat{A}}(a)}=0}$$

For $d_{\mathcal{H}}<\infty$ the middle relation represents a finite set of linear equations with r.h.s.=0. Its solution exists *iff* a is a root of the **characteristic polynomial**

$$\boxed{\mathcal{P}_{\hat{A}}(a)=\mathrm{Det}\begin{pmatrix} A_{11}-a & A_{12} & \dots \\ A_{21} & A_{22}-a & \\ \vdots & & \ddots \end{pmatrix}}$$

of order $d_{\mathcal{H}}$. The eq. $\mathcal{P}_{\hat{A}}(a)=0$ has $n\in\{1,2,...,d_{\mathcal{H}}\}$ solutions $\{a_i\}_{i=1}^{n}$, all $a_i\in\mathbb{R}$ (from Hermiticity of $\hat{A}$).



The corresponding eigenvectors $|a_i\rangle$ satisfy $(\hat{A}-a_i\hat{I})|a_i\rangle=0$, which for an expansion $|a_i\rangle=\sum_m\alpha_{mi}|\phi_m\rangle$ in arbitrary basis $\{|\phi_m\rangle\}_{m=1}^{d_{\mathcal{H}}}$ yields a linear set of equations for coefficients $\{\alpha_{mi}\}$. It can be solved due to the the nullity of its determinant.

$$\boxed{\begin{pmatrix} A_{11}-a_i & A_{12} & \dots \\ A_{21} & A_{22}-a_i & \\ \vdots & & \ddots \end{pmatrix}\begin{pmatrix} \alpha_{1i} \\ \alpha_{2i} \\ \vdots \end{pmatrix}=0}$$

Theorem: For any Hermitian operator $\hat{A}$ in $\mathcal{H}$, there exists $d_{\mathcal{H}}$ orthonormal eigenvectors (irrespectively of the number $1\leq n\leq d_{\mathcal{H}}$ of eigenvalues).
Sketch of proof: For any matrix $\hat{A}$ of dim. $d_{\mathcal{H}}$, the fundamental theorem of algebra guarantees the existence of at least one eigenvalue a and the corresponding eigenvector $|a\rangle$. The eigenvector can be normalized to $\langle a|a\rangle=1$ since $\hat{A}|a\rangle=a|a\rangle$ $\Rightarrow$ $\hat{A}(\alpha|a\rangle)=a(\alpha|a\rangle)$ $\forall\alpha\in\mathbb{C}$. Consider the orthogonal complement $\mathcal{H}^{\perp}$ of $|a\rangle$, which is a $(d_{\mathcal{H}}-1)$ dimensional subspace of $\mathcal{H}$ such that $\langle a|\psi\rangle=0$ $\forall$ $|\psi\rangle\in\mathcal{H}^{\perp}$. From Hermiticity of $\hat{A}$ we get: $\langle a|\hat{A}\psi\rangle=a\langle a|\psi\rangle$, so $\mathcal{H}^{\perp}$ is invariant under the action of $\hat{A}$. Hence the same procedure can be repeated for $\mathcal{H}^{\perp}$, finding a new normalized eigenvector $|a'\rangle\in\mathcal{H}^{\perp}$. The theorem is then proven by induction.

$\Rightarrow$ If the number of eigenvalues $n<d_{\mathcal{H}}$, some of them must be degenerate. Dimensions of the degeneracy subspaces satisfy: $\boxed{\sum_{i=1}^{n}d_{a_i}=d_{\mathcal{H}}}$

▶ Completeness for finite dimension

Given any Hermitian operator $\hat{A}$ in $\mathcal{H}$ of dimension $d_{\mathcal{H}}<\infty$, one can introduce an **orthonormal basis** of $\mathcal{H}$ **formed by eigenvectors** of $\hat{A}$:

Detailed notation (i runs over different eigenvalues, k over different eigenvectors in a single deg. subspace):
$$\left\{ \begin{array}{ll} |a_i\rangle \equiv |a_i^{(1)}\rangle & \text{eigenvector for nondeg. eigenvalue } a_i \\ \left\{|a_i^{(k)}\rangle\right\}_{k=1}^{d_{a_i}} & \text{eigenvectors for degenerate eigenvalue } a_i \\ & \text{(selected orthonormal basis of } \mathcal{H}_{a_i}) \end{array} \right\}_{i=1}^{n}$$

Simplified notation: $\{a_j\}_{j=1}^{d_\mathcal{H}} \longleftrightarrow \{|a_j\rangle\}_{j=1}^{d_\mathcal{H}} \equiv$ { eigenvalues, some of them maybe equal } $\longleftrightarrow$ { the corresponding eigenvectors, all orthonormal }

Orthonormality condition:
$$\boxed{\langle a_{i'}^{(k')}|a_i^{(k)}\rangle = \delta_{i'i}\delta_{k'k} \qquad \langle a_{j'}|a_j\rangle = \delta_{j'j}}$$

The completeness relation reads:
$$\boxed{\sum_{i=1}^{n} \overbrace{\sum_{k=1}^{d_{a_i}} |a_i^{(k)}\rangle\langle a_i^{(k)}|}^{\text{projector } \hat{P}_{a_i}} = \hat{I}_\mathcal{H} = \sum_{j=1}^{d_\mathrm{H}} |a_j\rangle\langle a_j|}$$

► **Diagonal representation (diagonalization)**

Similarity transformation of any Hermitian matrix $\hat{A}$ with matrix $\hat{U}$ build from eigenvector components: $|a_j\rangle = \sum_{m=1}^{d_\mathrm{H}} \alpha_{mj}|\phi_m\rangle \equiv \begin{pmatrix} \alpha_{1j} \\ \alpha_{2j} \\ \vdots \end{pmatrix}$

$$\overbrace{\begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{12}^* & A_{22} & \\ \vdots & & \ddots \end{pmatrix}}^{\hat{A}} = \overbrace{\underbrace{\begin{pmatrix} \boxed{\alpha_{11}} & \boxed{\alpha_{12}} & \dots \\ \boxed{\alpha_{21}} & \boxed{\alpha_{22}} & \\ \vdots & \vdots & \ddots \end{pmatrix}}_{|a_1\rangle \quad |a_2\rangle \quad \dots}}^{\hat{U}} \overbrace{\begin{pmatrix} \boxed{a_1} & 0 & \dots \\ 0 & \boxed{a_2} & \\ \vdots & & \ddots \end{pmatrix}}^{\hat{A}_\mathrm{diag}} \overbrace{\begin{pmatrix} \boxed{\alpha_{11}^* \ \alpha_{21}^* \ \dots} \\ \boxed{\alpha_{12}^* \quad \alpha_{22}^*} \\ \vdots \ \ddots \end{pmatrix}}^{\hat{U}^\dagger} \begin{array}{|l} \langle a_1| \\ \langle a_2| \\ \vdots \end{array}$$

► **Example**: general 2×2 Hermitian matrix $\boxed{\hat{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{pmatrix}}$ has 1 or 2 eigenvalues, but always 2 orthonorm. eigenvectors:

Characteristic polynomial: $\mathcal{P}_{\hat{A}}(a) = (A_{11}-a)(A_{22}-a) - |A_{12}|^2$
$$= a^2 - (A_{11}+A_{22})a + (A_{11}A_{22} - |A_{12}|^2)$$

Roots = eigenvalues: $a_\pm = \frac{A_{11}+A_{22}}{2} \pm \sqrt{\left(\frac{A_{11}-A_{22}}{2}\right)^2 + |A_{12}|^2}$
$\Rightarrow$ degeneracy $a_+ = a_-$ *iff* $A_{11} = A_{22}$ and $A_{12} = 0$

Eigenvector eq.: $\begin{pmatrix} \frac{A_{11}-A_{22}}{2} \mp \sqrt{\left(\frac{A_{11}-A_{22}}{2}\right)^2 + |A_{12}|^2} & A_{12} \\ A_{12}^* & \frac{A_{22}-A_{11}}{2} \mp \sqrt{\left(\frac{A_{11}-A_{22}}{2}\right)^2 + |A_{12}|^2} \end{pmatrix} \begin{pmatrix} \alpha_{1\pm} \\ \alpha_{2\pm} \end{pmatrix} = 0$

Rows of this matrix are dependent, so the solution is determined by any of the two eqs., e.g. the first one: $\left[\frac{A_{11}-A_{22}}{2} \mp \sqrt{\left(\frac{A_{11}-A_{22}}{2}\right)^2 + |A_{12}|^2}\right] \alpha_{1\pm} + A_{12}\alpha_{2\pm} = 0$

It can be checked that $\langle a_-|a_+\rangle = (\alpha_{1-}^*, \alpha_{2-}^*) \begin{pmatrix} \alpha_{1+} \\ \alpha_{2+} \end{pmatrix} = 0$

Counterexample: *non-Hermitian* matrix $\hat{A} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ has *only 1 eigenvector:*
Characteristic polynomial: $\mathcal{P}_{\hat{A}}(a) = (1-a)^2 \quad \Rightarrow$ root: $a = 1$
Eigenvector eq.: $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = 0 \quad \Rightarrow$ single normalized eigenvector $\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

► **Quantization**: Already at this stage we can conclude that discrete character of the observable values of some quantities A is a consequence of the assumption that the observable values coincide with the eigenvalues $a_1, a_2, \dots$ of the corresponding operator $\hat{A}$. However, the full picture cannot be drawn without considering operators in infinite-dimensional spaces.

▶ Eigensolutions for infinite dimension

For $d_{\mathcal{H}} = \infty$, the expression $\mathrm{Det}(\hat{A} - a\hat{I})$ has no sense. To find solutions of the eigenvector equation $(\hat{A} - a\hat{I})|a\rangle = 0$ is much more difficult in this case. In general, an ∞-dimensional operator $\hat{A}$ may have both **discrete & continuous spectrum** of eigenvalues. Moreover, eigenvalues from the continuous spectrum have no eigenvectors $\in \mathcal{H}$. Note that a rigorous analysis of these issues goes beyond our present level of advancement. We will just indicate two alternative mathematical treatments: one by von Neumann, who stays within the standard Hilbert space as he allows only finite intervals of continuous eigenvalues, and one initiated by Dirac, who steps out towards the rigged Hilbert space by taking into account single eigenvalues of continuous quantities.

Example of ∞-dim. operator with **discrete spectrum**:

$$\hat{A} = \begin{pmatrix} \boxed{0} & 0\ 0 & 0\ 0 & \cdots \\ 0 & \boxed{\begin{matrix}0&1\\1&0\end{matrix}} & \begin{matrix}0&0\\0&0\end{matrix} & \\ 0 & \begin{matrix}0&0\\0&0\end{matrix} & \boxed{\begin{matrix}0&2\\2&0\end{matrix}} & \\ \vdots & & & \ddots \end{pmatrix} \Rightarrow \left(\begin{matrix} \boxed{1} \\ \boxed{0} \\ \boxed{0} \\ \vdots \end{matrix} \right), \left(\begin{matrix} \boxed{0} \\ \boxed{\frac{1}{\sqrt{2}}} \\ \boxed{\pm\frac{1}{\sqrt{2}}} \\ \boxed{0} \\ \vdots \end{matrix} \right), \left(\begin{matrix} \boxed{0} \\ \boxed{0} \\ \boxed{0} \\ \boxed{\frac{1}{\sqrt{2}}} \\ \boxed{\pm\frac{1}{\sqrt{2}}} \\ \vdots \end{matrix} \right), ... \equiv \begin{cases} \text{orthonormal} \\ \text{eigenvectors} \\ \text{corresponding} \\ \text{to eigenvalues} \\ 0, \pm 1, \pm 2, ... \end{cases}$$

The spectrum $\mathcal{S}(\hat{A}) \equiv \mathbb{Z} \equiv \{..., -2, -1, 0, +1, +2, ...\}$
The corresponding eigenvectors $|a_i\rangle \in \mathcal{H} \equiv \ell^2$

Example of ∞-dim. operator with **continuous spectrum**:

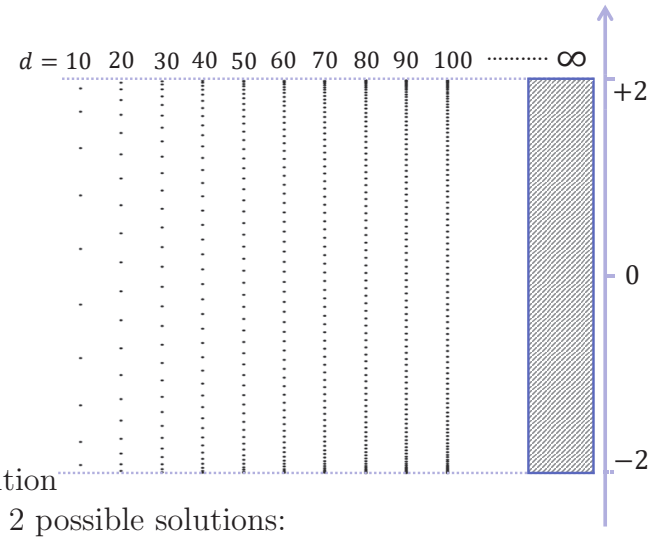
$$\hat{A} = \begin{pmatrix} 0 & \boxed{1} & 0 & 0 & 0 & \cdots \\ \boxed{1} & 0 & \boxed{1} & 0 & 0 & \\ 0 & \boxed{1} & 0 & \boxed{1} & 0 & \\ 0 & 0 & \boxed{1} & 0 & \boxed{1} & \\ \vdots & & \ddots & & \ddots & \end{pmatrix} \quad \Rightarrow \quad \text{eigenvector equation:} \quad \underbrace{\begin{pmatrix} -a & 1 & 0 & 0 & 0 & \cdots \\ 1 & -a & 1 & 0 & 0 & \\ 0 & 1 & -a & 1 & 0 & \\ 0 & 0 & 1 & -a & 1 & \\ \vdots & & \ddots & \ddots & \ddots & \end{pmatrix}}_{\hat{A} - a\hat{I}} \underbrace{\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \vdots \end{pmatrix}}_{|a\rangle} = 0$$

For a finite dimension $d_{\mathrm{H}} \equiv d$ the above eigenvector equation leads to the following set of equations:

$$\left\{ \begin{matrix} \alpha_2 = a\alpha_1 \\ \alpha_1 + \alpha_3 = a\alpha_2 \\ \alpha_2 + \alpha_4 = a\alpha_3 \\ \alpha_3 + \alpha_5 = a\alpha_4 \\ \vdots \\ \alpha_{d-2} + \alpha_d = a\alpha_{d-1} \\ \alpha_{d-1} = a\alpha_d \end{matrix} \right\} \Rightarrow \begin{cases} \text{single recursive eq.} \\ \boxed{\alpha_{l-1} + \alpha_{l+1} = a\alpha_l} \\ \text{valid for } l = 1, 2, ..., d \\ \text{with boundary} \\ \text{conditions: } \alpha_0 = \alpha_{d+1} = 0 \end{cases}$$

Solution for $d < \infty$: Starting from $\alpha_1 = 1$, the above set of equations yields: $\alpha_2 = a$, $\alpha_3 = (a^2 - 1)$, $\alpha_4 = (a^3 - 2a)$, ... However, the last pair of equations will not be satisfied for all values of a. It can be shown that $|\langle\alpha|\hat{A}|\alpha\rangle| \leq 2\langle\alpha|\alpha\rangle\ \forall|\alpha\rangle \in \ell^2$. Hence the solution exists only for some discrete values $a_i \in [-2, +2]$ (see the figure) and the corresponding eigenvectors $|a_i\rangle$ are trivially normalizable.

Solution for $d = \infty$: In this case, the problem with the last pair of equations does not take place, so the solution exists for all $a \in (-\infty, +\infty)$. However, the



eigenvectors obtained in this way are not normalizable, i.e., $|a\rangle \notin \mathcal{H} \equiv \ell^2$. It can be shown that $|a\rangle \notin \overline{\mathcal{H}} \equiv \overline{\ell^2}$ for $|a|>2$, so $|a\rangle$ is out of even the upper space in the Gelfand triple. On the other hand, for $|a|\leq 2$ we find $|a\rangle \in \overline{\ell^2}$.

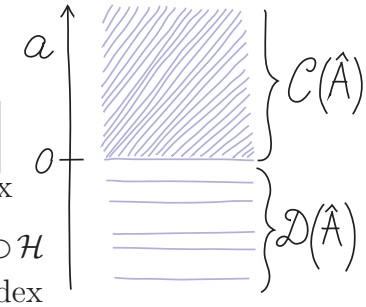
Sketch of proof: We can solve the above recursive equation $\alpha_{l-1}+\alpha_{l+1}=a\alpha_l$ by the ansatz $\alpha_l=r^l$, which leads to the condition $r^{l-1}(1-ar+r^2)=0$. This yields 2 possible solutions: $r=\frac{a}{2}\pm\sqrt{(\frac{a}{2})^2-1}\equiv r_\pm$. The boundary condition $\alpha_0=0$ implies $\alpha_l=(r_+^l-r_-^l)$. For $|a|\leq 2$ we have $r_\pm\in\mathbb{C}$. One can find $\vartheta\in[0,2\pi)$ such that $\frac{a}{2}=\cos\vartheta$ and $r_\pm=\cos\vartheta\pm i\sin\vartheta=e^{\pm i\vartheta}$. Hence $\alpha_l=\sin(l\vartheta)$, which means that the components are bounded and oscillate with l and the resulting vector $|a\rangle\in\overline{\ell^2}$. In contrast, for $|a|>0$ we have $r_\pm\in\mathbb{R}$ with $r_+>1$ and $r_-<1$, so $|\alpha_l|$ diverges exponentially with l, which means that $|a\rangle\notin\overline{\ell^2}$.

Conclusion: Eigensolutions $\in\overline{\mathcal{H}}$ are declared to be generalized eigenvectors of an ∞-dimensional operator $\hat{A}$, while those $\notin\overline{\mathcal{H}}$ are not considered as eigenvectors in any sense. Therefore, the above operator $\hat{A}$ for $d=\infty$ has a continuous spectrum $\mathcal{S}(\hat{A})\equiv[-2,+2]$.

▶ Spectrum of a general operator in infinite dimension

A general Hermitian operator $\hat{A}$ can combine both discrete and continuous spectra:

$$\underbrace{\mathcal{S}(\hat{A})}_{\text{spectrum}} = \underbrace{\mathcal{D}(\hat{A})}_{\text{discrete part}} \cup \underbrace{\mathcal{C}(\hat{A})}_{\text{continuous part}}$$



Eigenvalues $a_i\in\mathcal{D}(\hat{A})$ have eigenvectors $|a_i^{(k)}\rangle\in\mathcal{H}$ where $k\in\{1,2,\ldots d_{a_i}\}$ is a discrete degeneracy index

Eigenvalues $a\in\mathcal{C}(\hat{A})$ have eigenvectors $|a^{(k)}\rangle\in\overline{\mathcal{H}}\supset\mathcal{H}$ where $k\in\mathcal{D}_a$ is a $\left\{\begin{smallmatrix}\text{discrete } (k=1,\ldots d_a)\\ \text{continuous}\end{smallmatrix}\right\}$ degeneracy index

The discrete part of the spectrum fulfills the standard eigenvector relations:

Orthonormality: $\langle a_{i'}^{(k')}|a_i^{(k)}\rangle=\delta_{i'i}\delta_{k'k}$ Projectors: $\hat{P}_{a_i}=\sum_{k=1}^{d_{a_i}}|a_i^{(k)}\rangle\langle a_i^{(k)}|$

The continuous part of spectrum needs special treatment of eigenvector issues. This requires rather involved mathematics, of which we present only a rough outline.

▶ Dirac's approach to the continuous spectrum

An explicit use is made of the **extended space** $\overline{\mathcal{H}}$ in the Gelfand triple $\overline{\mathcal{H}} \supset \mathcal{H} \supset \underline{\mathcal{H}}$ which contains all discrete & continuous eigenvectors. The formal spectral decomposition of $\hat{A}$ in $\overline{\mathcal{H}}$ is analogous to that for a discrete spectrum, which alows us to hide (ignore) most of the mathematical subtleties.

The scalar product is not defined in $\overline{\mathcal{H}}$, nevertheless we introduce the following **"orthonormality" conditions** valid in the sense of distribution theory:

$$\begin{array}{c} \langle a'^{(k')}|a^{(k)}\rangle = \delta(a'-a)\delta_{k'k} \quad (k',k \text{ discrete}) \\ \langle a'^{(k')}|a^{(k)}\rangle = \delta(a'-a)\delta(k'-k) \quad (k',k \text{ continuous}) \end{array} \qquad \langle a^{(k')}|a_i^{(k)}\rangle = 0$$

normalization to δ-function

These relations guarantee consistency of the expansion of a general $|\psi\rangle \in \overline{\mathcal{H}}$ in the "eigenbasis" of $\hat{A}$. We have: $|\psi\rangle = \sum\limits_{i,k} \langle a_i^{(k)} \underbrace{|\psi\rangle}_{*} |a_i^{(k)}\rangle + \int \sum\limits_{l} \langle a^{(l)} \underbrace{|\psi\rangle}_{*} |a^{(l)}\rangle \, da$

(discrete k, l considered) and substitution of the same expression for $*$ yields:

$$|\psi\rangle = \sum_{i,k,i',k'} \underbrace{\langle a_i^{(k)}|a_{i'}^{(k')}\rangle}_{\delta_{ii'}\delta_{kk'}} \langle a_{i'}^{(k')}|\psi\rangle |a_i^{(k)}\rangle + \sum_{i,k,l} \int \underbrace{\langle a^{(l)}|a_i^{(k)}\rangle}_{0} da \langle a_i^{(k)}|\psi\rangle |a_i^{(k)}\rangle +$$

$$+ \int \sum_{i,k} \underbrace{\langle a_i^{(k)}|a^{(l)}\rangle}_{0} \langle a^{(l)}|\psi\rangle |a^{(l)}\rangle \, da + \iint \sum_{ll'} \underbrace{\langle a^{(l)}|a'^{(l')}\rangle}_{\delta(a-a')\delta_{ll'}} \langle a'^{(l')}|\psi\rangle |a^{(l)}\rangle \, da \, da' = \left\{ \begin{array}{l} \text{previous} \\ \text{expression} \end{array} \right.$$

Projectors to eigenspaces of continuous eigenvalues:

$\hat{\Pi}_a \equiv \sum\limits_{k \in \mathcal{D}_a} |a^{(k)}\rangle\langle a^{(k)}| \equiv$ projector to the degeneracy subspace of eigenvalue a, where $\sum\limits_{k \in \mathcal{D}_a} \equiv \left\{ \begin{array}{l} \sum\limits_{k=1}^{d_a} \quad \text{(discrete deg.index)} \\ \int\limits_{\mathcal{D}_a} dk \quad \text{(continuous deg.index)} \end{array} \right.$

Completeness & orthogonality relations are jointly expressed as follows:

$$\sum_{\substack{i \\ a_i \in \mathcal{D}(\hat{A})}} \underbrace{\sum_{k=1}^{d_{a_i}} |a_i^{(k)}\rangle\langle a_i^{(k)}|}_{\hat{P}_{a_i}} + \int_{\mathcal{C}(\hat{A})} \underbrace{\sum_{k \in \mathcal{D}_a} |a^{(k)}\rangle\langle a^{(k)}|}_{\hat{\Pi}_a} \, da = \hat{I}_{\overline{\mathcal{H}}}$$

$$\begin{aligned} \hat{P}_{a_i}\hat{P}_{a_j} &= \delta_{ij}\hat{P}_{a_i} \\ \hat{\Pi}_a\hat{\Pi}_{a'} &= \delta(a-a')\hat{\Pi}_a \\ \hat{P}_{a_i}\hat{\Pi}_a &= 0 \end{aligned}$$

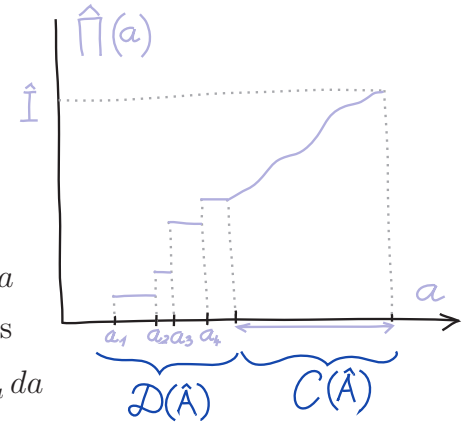
▶ Von Neumann's approach to the continuous spectrum

It works in the **standard Hilbert space** $\mathcal{H}$ which excludes eigenvectors for individual eigenvalues $a \in \mathcal{C}(\hat{A})$, but includes subspaces $\mathcal{H}_{(a',a'')} \subset \mathcal{H}$ corresponding to any interval (a', a'') of eigenvalues $a \in \mathcal{S}(\hat{A})$ in the sense that probability distributions $\mathfrak{p}_\psi(a)$ vanish outside (a', a'') for any state $|\psi\rangle \in \mathcal{H}_{(a',a'')}$

Let $\hat{\mathbf{\Pi}}_{(a',a'')}$ be projector to $\mathcal{H}_{(a',a'')}$, where the interval (a', a'') may generally overlap with both $\mathcal{D}(\hat{A})$ and $\mathcal{C}(\hat{A})$. This projector must naturally satisfy the interval splitting condition: $\hat{\mathbf{\Pi}}_{(a',a''')} = \hat{\mathbf{\Pi}}_{(a',a'')} + \hat{\mathbf{\Pi}}_{(a'',a''')}$ for any $a' \le a'' \le a'''$

Define a "cummulative" projector to a subspace with $a \le a'$: $\boxed{\hat{\mathbf{\Pi}}_{(-\infty,a')} \equiv \hat{\mathbf{\Pi}}(a')}$

Schematic illustration:



Due to the splitting condition, a projector to an infinitesimal eigenvalue interval reads:

$\hat{\mathbf{\Pi}}_{(a',a'+da)} = \hat{\mathbf{\Pi}}(a'+da) - \hat{\mathbf{\Pi}}(a') \equiv \frac{d}{da}\hat{\mathbf{\Pi}}(a)|_{a=a'} da$

Note: in the Dirac language these expressions would read $\frac{d}{da}\hat{\mathbf{\Pi}}(a)|_{a=a'} \sim \hat{\Pi}_{a'}$ $\quad \hat{\mathbf{\Pi}}_{(a',a'')} \sim \int_{a'}^{a''} \hat{\Pi}_a \, da$

Completeness relation in Von Neumann's language is expressed as:

$$\boxed{\int_{\mathcal{S}(\hat{A})} d\hat{\mathbf{\Pi}}(a) = \hat{I}_{\mathcal{H}}}$$

where use is made of Stieltjes method of integration:

$$\int f(x) \underbrace{d\hat{\sigma}(x)}_{\substack{\text{operator} \\ \text{measure}}} \equiv \lim_{n\to\infty} \sum_{k=1}^{n} f(x_k)[\hat{\sigma}(x_{k+1}) - \hat{\sigma}(x_k)]$$

▶ Spectral decomposition of operator

The above completeness relations lead to the expression of any Hermitian operator $\hat{A}$ and its Taylor-expanded functions $f(\hat{A}) \equiv \sum_n f_n \hat{A}^n$ in terms of the eigenvalues and projectors to the corresponding eigenspaces:

For **discrete spectrum**: $\boxed{\hat{A} = \sum_i a_i \hat{P}_{a_i} \quad f(\hat{A}) = \sum_i f(a_i)\hat{P}_{a_i}}$

Proof:

$$|\psi\rangle = \sum_i \sum_{k=1}^{d_i} \langle a_i^{(k)}|\psi\rangle |a_i^{(k)}\rangle \;\Rightarrow\; \hat{A}^n|\psi\rangle = \sum_i a_i^n \underbrace{\sum_{k=1}^{d_i} |a_i^{(k)}\rangle\langle a_i^{(k)}|}_{\hat{P}_{a_i}} \psi\rangle \;\Rightarrow\; \hat{A}^n = \sum_i a_i^n \hat{P}_{a_i}$$

$$\Downarrow$$

$$\Sigma_n f_n \hat{A}^n = \sum_i \underbrace{\Sigma_n f_n a_i^n}_{f(a_i)} \hat{P}_{a_i}$$

For **general (combined) spectrum**:

$$\boxed{\begin{array}{lll} \hat{A} & = \sum\limits_{\mathcal{D}(\hat{A})} a_i \hat{P}_{a_i} + \int\limits_{\mathcal{C}(\hat{A})} a\, \hat{\Pi}_a \, da & \equiv \int\limits_{\mathcal{S}(\hat{A})} a \; d\hat{\mathbf{\Pi}}(a) \\ f(\hat{A}) & = \sum\limits_{\mathcal{D}(\hat{A})} f(a_i)\hat{P}_{a_i} + \int\limits_{\mathcal{C}(\hat{A})} f(a)\, \hat{\Pi}_a \, da & \equiv \int\limits_{\mathcal{S}(\hat{A})} f(a)\, d\hat{\mathbf{\Pi}}(a) \end{array}}$$

▶ This allows us to redefine the **operator function** $f(\hat{A})$ even for functions which are not determined by the Taylor series, i.e. for $f(\hat{A}) \neq \sum_n f_n \hat{A}^n$. Let $\mathrm{Def}[f(a)]$ be the definition domain of function $f(a)$. Then:

$$\boxed{f(\hat{A}) = \sum_{\mathcal{D}(\hat{A})\cap \mathrm{Def}[f(a)]} f(a_i)\hat{P}_{a_i} + \int_{\mathcal{C}(\hat{A})\cap \mathrm{Def}[f(a)]} f(a)\, \hat{\Pi}_a \, da \quad \equiv \int_{\mathcal{S}(\hat{A})\cap \mathrm{Def}[f(a)]} f(a)\, d\hat{\mathbf{\Pi}}(a)}$$

The definition domain $\mathrm{Def}[f(\hat{A})]$ of the operator function defined in this way is the subspace of $\mathcal{H}$ spanned by all eigenvectors whose eigenvalues $a \in \mathrm{Def}[f(a)]$

► Eigenvalue expression of **operator norm**: $||\hat{A}||^2 = \text{Sup}\left\{|a|^2\right\}_{a\in\mathcal{S}(\hat{A})}$
Bounded (unbounded) operator $\hat{A} \Leftrightarrow$ bounded (unbounded) spectrum $\mathcal{S}(\hat{A})$

■ Probability distribution for measurement outcomes

The spectral decomposition of operator $\hat{A}$ associated with observable A and the initial postulate on the statistical moments $\langle A^n\rangle_\psi = \langle\psi|\hat{A}^n\psi\rangle$ (for normalized states) enables us to finally deduce the desired probability distribution $\mathfrak{p}_\psi(a)$ for possible outcomes a of measurement A on state $|\psi\rangle$.

► **Moments** of the probability distribution for observable A in state $|\psi\rangle$:

$$\langle A^n\rangle_\psi \equiv \begin{cases} \displaystyle\sum_{\mathcal{D}(\hat{A})} a_i^n\ \mathfrak{p}_\psi(a_i) \quad + \int_{\mathcal{C}(\hat{A})} a^n\ \mathfrak{p}_\psi(a)\,da & \text{defining formula of the } n\text{th moment} \\ \displaystyle\sum_{\mathcal{D}(\hat{A})} a_i^n\ \langle\psi|\hat{P}_{a_i}\psi\rangle + \int_{\mathcal{C}(\hat{A})} a^n\ \langle\psi|\hat{\Pi}_a\psi\rangle\,da \equiv \langle\psi|\hat{A}^n\psi\rangle & \text{expression from the spectral decomposition} \end{cases}$$

By comparing both lines in this formula we see that the corresponding expressions $\mathfrak{p}_\psi(a_i) \leftrightarrow \langle\psi|\hat{P}_{a_i}\psi\rangle$ and $\mathfrak{p}_\psi(a) \leftrightarrow \langle\psi|\hat{\Pi}_a\psi\rangle$ must be equal. Therefore we arrive at the following crucial conclusion:

► **Probabilities of measurement outcomes as vector overlaps**

Given a state $|\psi\rangle$ satisfying $\langle\psi|\psi\rangle = 1$ and an observable expressed by operator $\hat{A} = \sum_{\mathcal{D}(\hat{A})} a_i\hat{P}_{a_i} + \int_{\mathcal{C}(\hat{A})} a\,\hat{\Pi}_a\,da$, the probabilities of measurement outcomes are:

$$\begin{array}{ll} \text{Discrete case:} & \mathfrak{p}_\psi(a_i) = \langle\psi|\hat{P}_{a_i}\psi\rangle = \displaystyle\sum_{k=1}^{d_{a_i}} |\langle a_i^{(k)}|\psi\rangle|^2 \\ \text{Continuous case:} & \mathfrak{p}_\psi(a)\,da = \langle\psi|\hat{\Pi}_a\psi\rangle\,da = \displaystyle\sum_{k\in\mathcal{D}_a} |\langle a^{(k)}|\psi\rangle|^2\,da \end{array} = \langle\psi|d\hat{\mathbf{\Pi}}(a)\psi\rangle$$

Note that the resulting formula for the probability $\mathfrak{p}_\psi(a_i)$ or probability density $\mathfrak{p}_\psi(a)$ can be used as an alternative (equivalent) postulate of QM instead of that for $\langle A^n\rangle_\psi$ (see above).

For a nondegenerate eigenvalue a with eigenvector $|a\rangle$ we can say that:

$$\left.\begin{array}{ll} \langle a|\psi\rangle & \equiv \text{amplitude} \\ |\langle a|\psi\rangle|^2 & \equiv \text{probability} \end{array}\right\} \text{to measure } a \text{ on } |\psi\rangle \Leftrightarrow \text{to associate } |\psi\rangle \text{ with } |a\rangle$$

◄ Historical remark

1900-10: David Hilbert studies spectral properties of integral operators
1924: D. Hilbert and R. Courant publish the book *Methoden der mathematischen Physik* containing methods that later became relevant in QM
1925: Werner Heisenberg (and M. Born & P. Jordan) formulate "matrix mechanics", introducing the concept of matrix operators to QM (although in a different sense)
1926: Erwin Schrödinger in his wave mechanics makes use of operators associated with observables, he shows the equivalence with matrix mechanics

1926-32: John von Neumann unifies Schrödinger's and Heisenberg's approaches using self-adjoint operators acting on a general Hilbert space, with M. Stone they work out the theory of such operators
1927-30: Paul Dirac develops "symbolic" formalism transcending ordinary Hilbert space, this is formalized in the 1950's in terms of rigged Hilbert spaces

2b. EXAMPLES OF QUANTUM OBSERVABLES

The formalism developed in the previous section is now ready to bear fruit. We will introduce the operators mostly associated with observables characterizing a single particle. At the end we also mention some simple many-body systems.

■ Spin-$\frac{1}{2}$ operators

Spin operators are the clearest examples of quantum observables since they work in the best of all possible Hilbert spaces—that with dimension 2. The same operators (but no more with the physical meaning of spin) can be used in the Hilbert space of a qubit (Sec. 1b).

► **Operators of spin components** along x, y, z axes in $\mathcal{H} \equiv \mathbb{C}^2$

$$\hat{S}_x = \tfrac{\hbar}{2}\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\hat{\sigma}_x} \qquad \hat{S}_y = \tfrac{\hbar}{2}\underbrace{\begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}}_{\hat{\sigma}_y} \qquad \hat{S}_z = \tfrac{\hbar}{2}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\hat{\sigma}_z}$$

Pauli matrices

Together with the unit matrix $\hat{I} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ the Pauli matrices $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ form a complete set of Hermitian operators in $\mathcal{H} \equiv \mathbb{C}^2$ (any $\hat{A}$ is their lin. combination).

► **Projection to general direction** $\vec{n} = (\underbrace{\sin\vartheta\cos\varphi}_{n_x}, \underbrace{\sin\vartheta\sin\varphi}_{n_y}, \underbrace{\cos\vartheta}_{n_z})$
Observable with operator: $|\vec{n}|^2{=}1$

$$\hat{S}_{\vec{n}} = \vec{n}\cdot\hat{\vec{S}} = \tfrac{\hbar}{2}(\vec{n}\cdot\hat{\vec{\sigma}}) = \tfrac{\hbar}{2}\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} = \tfrac{\hbar}{2}\begin{pmatrix} \cos\vartheta & e^{-i\varphi}\sin\vartheta \\ e^{+i\varphi}\sin\vartheta & -\cos\vartheta \end{pmatrix}$$

► **Eigenvalues of spin projection** $\hat{S}_{\vec{n}}$

$$\text{Det}\left[\tfrac{\hbar}{2}\begin{pmatrix} n_z-\lambda & n_x-in_y \\ n_x+in_y & -(n_z+\lambda) \end{pmatrix}\right] = 0 \quad \Rightarrow \quad \lambda^2 = 1 \quad \Rightarrow \quad s_{\vec{n}} = \begin{cases} +\frac{\hbar}{2} \\ -\frac{\hbar}{2} \end{cases}$$

► **Eigenvectors of spin projection** $\hat{S}_{\vec{n}}$

Eigenequation $\begin{pmatrix} n_z & n_x-in_y \\ n_x+in_y & -n_z \end{pmatrix}\begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix} = \pm\begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix}$ has ∞ solutions.

For $n_z \neq \pm 1$ (otherwise solutions known) we get $\alpha_\pm = -\frac{n_x - in_y}{n_z \mp 1}\beta_\pm$,
which yields normalized eigenvectors

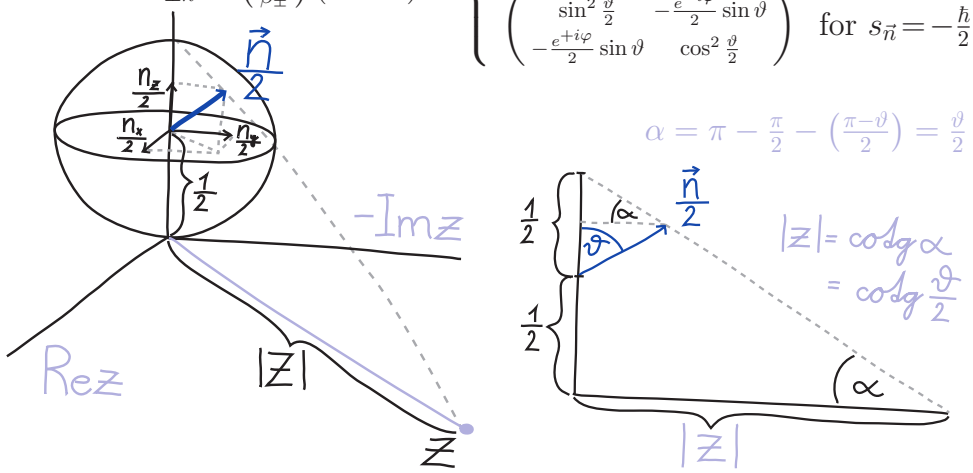
$$|{\uparrow_{\vec{n}}}\rangle = \begin{pmatrix} e^{-i\varphi}\cos\frac{\vartheta}{2} \\ \sin\frac{\vartheta}{2} \end{pmatrix} \quad \text{for } s_{\vec{n}} = +\tfrac{\hbar}{2}$$

$$|{\downarrow_{\vec{n}}}\rangle = \begin{pmatrix} -e^{-i\varphi}\sin\frac{\vartheta}{2} \\ \cos\frac{\vartheta}{2} \end{pmatrix} \quad \text{for } s_{\vec{n}} = -\tfrac{\hbar}{2}$$

satisfying the orthogonality relation $\langle{\downarrow_{\vec{n}}}|{\uparrow_{\vec{n}}}\rangle = \begin{pmatrix} \alpha_-^* & \beta_-^* \end{pmatrix}\begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = 0$

Projectors to eigenspaces:

$$\hat{P}_{\pm\vec{n}} = \begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix} \begin{pmatrix} \alpha_\pm^* & \beta_\pm^* \end{pmatrix} = \begin{cases} \begin{pmatrix} \cos^2\frac{\vartheta}{2} & \frac{e^{-i\varphi}}{2}\sin\vartheta \\ \frac{e^{+i\varphi}}{2}\sin\vartheta & \sin^2\frac{\vartheta}{2} \end{pmatrix} & \text{for } s_{\vec{n}} = +\frac{\hbar}{2} \\ \begin{pmatrix} \sin^2\frac{\vartheta}{2} & -\frac{e^{-i\varphi}}{2}\sin\vartheta \\ -\frac{e^{+i\varphi}}{2}\sin\vartheta & \cos^2\frac{\vartheta}{2} \end{pmatrix} & \text{for } s_{\vec{n}} = -\frac{\hbar}{2} \end{cases}$$



For an unnormalized eigenvector $\boxed{|\uparrow_{\vec{n}}\rangle = z|\uparrow\rangle + |\downarrow\rangle, \quad z = -\frac{n_x - i n_y}{n_z - 1} = e^{-i\varphi}\cot\frac{\vartheta}{2}}$ the point $z \in \mathbb{C}$ represents the stereographic projection of vector $\frac{\vec{n}}{2}$, hence any general superposition $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$ corresponds to a state $|\uparrow_{\vec{n}}\rangle$ of spin pointing in the direction $\vec{n}$ obtained from $z = \alpha/\beta$ by the inverse projection.

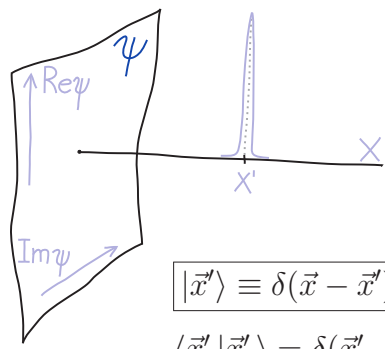
■ Coordinate & momentum

The most important observables in classical mechanics (such that all the other observables are made of them) are the coordinates and momenta. Unfortunately, these are precisely the observables whose QM operators make troubles.

▶ Coordinate & momentum eigenfunctions

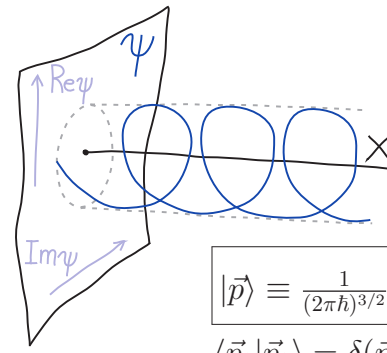
We use the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3)$ and the rigged Hilbert space $\underline{\mathcal{H}} \subset \mathcal{H} \subset \overline{\mathcal{H}}$ with $\underline{\mathcal{H}} \equiv$ differentiable functions (C^∞) satisfying $|\frac{d^n}{dx^n}\psi(\vec{x})|_{|\vec{x}|\to\infty} \lesssim |\vec{x}|^{-m}$ for any $n, m \geq 0$ (Schwartz space of "test functions" for tempered distributions).

Postulate: Eigenstates of position & momentum $\equiv$ δ-function & plane wave



$$\boxed{|\vec{x}'\rangle \equiv \delta(\vec{x} - \vec{x}')}$$

$$\langle \vec{x}_1' | \vec{x}_2' \rangle = \delta(\vec{x}_1' - \vec{x}_2')$$



$$\boxed{|\vec{p}\rangle \equiv \frac{1}{(2\pi\hbar)^{3/2}}\, e^{i\frac{\vec{p}\cdot\vec{x}}{\hbar}}}$$

$$\langle \vec{p}_1 | \vec{p}_2 \rangle = \delta(\vec{p}_1 - \vec{p}_2)$$

These functions $\in \overline{\mathcal{H}}$ are not normalizable (so $\notin \mathcal{L}^2(\mathbb{R}^3)$), but we require at least the above "normalization" to the δ-function.

► Operators of coordinate components

Notation: $\vec{x} = (x, y, z) \equiv (x_1, x_2, x_3)$
Action of operator $\hat{x}_i \equiv$ multiplication by variable x_i:

$$\boxed{\underbrace{\hat{x}_i\psi(\vec{x})}_{[\hat{x}_i\psi](\vec{x})} \equiv \underbrace{x_i\psi(\vec{x})}_{\psi'(\vec{x})}}$$

$$\mathrm{Def}(\hat{x}_i) := \underline{\mathcal{H}}$$

Hermiticity: $\int \psi_1(\vec{x})^*[x_i\psi_2(\vec{x})]d\vec{x} = \int [x_i\psi_1(\vec{x})]^*\psi_2(\vec{x})d\vec{x}$

Eigenstates $\delta(\vec{x}-\vec{x}') \in \overline{\mathcal{H}}$ satisfy $x_i\delta(\vec{x}-\vec{x}') = x_i'\delta(\vec{x}-\vec{x}') \Rightarrow$ continuous spectrum $x_i' \in (-\infty, +\infty)$

► Operators of momentum components

Notation: $\vec{p} = (p_x, p_y, p_z) \equiv (p_1, p_2, p_3)$
Action of operator $\hat{p}_i$ prop. to the derivative in x_i:

$$\boxed{\underbrace{\hat{p}_i\psi(\vec{x})}_{[\hat{p}_i\psi](\vec{x})} \equiv \underbrace{-i\hbar\frac{\partial}{\partial x_i}\psi(\vec{x})}_{\psi'(\vec{x})}}$$

This means $\boxed{\hat{\vec{p}} = -i\hbar\vec{\nabla}}$ $\qquad$ $\mathrm{Def}(\hat{p}_i) := \underline{\mathcal{H}}$

Hermiticity: $\int \psi_1(\vec{x})^*[-i\hbar\frac{\partial\psi_2}{\partial x_i}(\vec{x})]d\vec{x} = \int [-i\hbar\frac{\partial\psi_1}{\partial x_i}(\vec{x})]^*\psi_2(\vec{x})d\vec{x} + \underbrace{[\psi_1(\vec{x})^*\psi_2(\vec{x})]_{-\infty}^{+\infty}}_{0}$

Eigenstates $e^{i\vec{p}\cdot\vec{x}/\hbar} \in \overline{\mathcal{H}}$ satisfy $-i\hbar\frac{\partial}{\partial x_i}e^{i\vec{p}\cdot\vec{x}/\hbar} = p_i e^{i\vec{p}\cdot\vec{x}/\hbar} \Rightarrow$ continuous spectrum $p_i \in (-\infty, +\infty)$

Since $\boxed{\vec{p} = \hbar\vec{k} = \frac{2\pi\hbar}{\lambda}\vec{n}}$ with $\vec{k} \equiv$ **wavevector**, $\vec{n} \equiv$ unit vector (flight direction), we reproduce the old **de Broglie relation** for the wavelength: $\boxed{\lambda_{\mathrm{B}} = \frac{2\pi\hbar}{p} \equiv \frac{h}{p}}$

◄ Historical remark

1924: Louis de Broglie associates plane waves with moving particles
1926: Erwin Schrödinger applies operators within the wave mechanics
1927: Wolfgang Pauli introduces spin matrices
1930: Paul Dirac introduces explicit momentum and position operators
1940's-60's: Rigorous mathematical treatment in terms of the distribution theory (L. Schwartz *et al.*) and rigged Hilbert spaces (I. Gelfand *et al.*)

■ Hamiltonian of a structureless particle

The incorrigible *enfants terribles*—the coordinate and momentum operators—give birth to a respected (although not always well-behaved) operator named Hamiltonian. This is a crucial operator in quantum theory as it represents the total energy of the system (here mostly a single nonrelativistic particle with no internal structure) and generates its quantum evolution (see Sec. 5a).

► Operator of total energy $\hat{H} \equiv$ Hamiltonian of the system

Eigenequation $\boxed{\hat{H}|E\rangle = E|E\rangle}$ **stationary Schrödinger equation**

Solutions of this equation yield measurable energies of the system.

▶ Hamiltonian of free particle (no external field) with mass M

$$\hat{H} = \frac{1}{2M}(\hat{\vec{p}}\cdot\hat{\vec{p}}) = -\frac{\hbar^2}{2M}\underbrace{\left(\vec{\nabla}\cdot\vec{\nabla}\right)}_{\Delta}$$

operator of **kinetic energy**

$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ Laplace operator

Eigenequation $\left(\Delta + \underbrace{\frac{2ME}{\hbar^2}}_{\pm k^2 = \pm(k_1^2+k_2^2+k_3^2)}\right)\psi(\vec{x}) = 0$

Solutions
for $E \geq 0$ physical: $\psi \propto e^{\pm i\vec{k}\cdot\vec{x}} \in \overline{\mathcal{H}}$
for $E < 0$ nonphysical: $\psi \propto e^{\pm\vec{k}\cdot\vec{x}} \notin \overline{\mathcal{H}}$

Continuous spectrum $E \in [0, +\infty)$ infinitely degenerate (except $E=0$)

Eigenstates: $|E_{\vec{k}}\rangle = e^{i\vec{k}\cdot\vec{x}} \equiv |\vec{p} = \hbar\vec{k}\rangle$ with eigenvalues $E \equiv E_{\vec{k}} = \frac{(\hbar k)^2}{2M}$

▶ Hamiltonian of massive particle in scalar potential field

Potential energy of the particle in an external field $\equiv V(\vec{x})$

$$\hat{H} = \underbrace{\frac{1}{2M}(\hat{\vec{p}}\cdot\hat{\vec{p}})}_{\substack{\hat{T}\\ \text{kinetic}}} + \underbrace{V(\hat{\vec{x}})}_{\substack{\hat{V}\\ \text{potential energy}}} \equiv -\frac{\hbar^2}{2M}\Delta + V(\vec{x})$$

Stationary Schrödinger eq.
$\left[-\frac{\hbar^2}{2M}\Delta + V(\vec{x}) - E\right]\psi(\vec{x}) = 0$

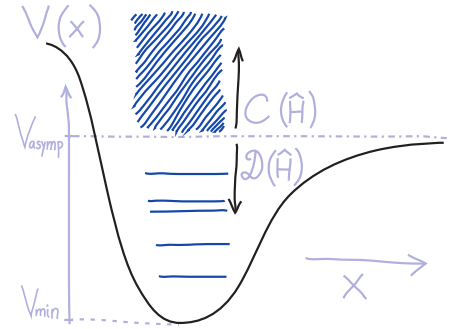
▶ Bound and unbound states of particle in potential

Eigensolutions of the Schrödinger equation with potential may be of two types:
Bound states (correspond to motions of the particle in a bounded spatial domain with lower potential energy) ⇒ discrete spectrum, normalizable wavefunction $\psi(\vec{x}) \in \mathcal{H} = \mathcal{L}^2(\mathbb{R}^3)$
Unbound states (correspond to unbounded particle motions across the whole space) ⇒ continuous spectrum, non-normalizable wavefunction $\psi(\vec{x}) \in \overline{\mathcal{H}}$

Consider potentials $V(\vec{x})$ of two types:

(a) Potential wells of a general shape
Such potentials support the existence of bound states of the particle inside the well
Define values:

$$V_{\text{asymp}} = \lim_{r\to\infty} \text{Min}\{V(\overbrace{r,\vartheta,\varphi}^{\text{sph.coord.}})\}_{\vartheta,\varphi}$$
$$V_{\text{min}} \equiv \text{Min}\{V(\vec{x})\}_{\vec{x}}$$



The spectrum of such $\hat{H}$ consists of two parts:

discrete part	$\mathcal{D}(\hat{H})$	(bound states):	$E_i \in (V_{\text{min}}, V_{\text{asymp}})$
continuous part	$\mathcal{C}(\hat{H})$	(unbound states):	$E \in (V_{\text{asymp}}, +\infty)$

Reasoning: In the asymptotic domain $r \to \infty$ for $(\vartheta, \varphi) = (\vartheta_0, \varphi_0)$ corresponding to the minimal $V(\vec{x})$ the Schrödinger equation $\left[-\frac{\hbar^2}{2M}\Delta + (V_{\text{asymp}} - E)\right]\psi \approx 0$ yields asymptotic solutions $\psi(r, \vartheta_0, \varphi_0) \sim e^{-\frac{1}{\hbar}\sqrt{2M(V_{\text{asymp}}-E)}r}$, which are normalizable for $E < V_{\text{asymp}}$ and unnormalizable for $E > V_{\text{asymp}}$.

(b) Periodic potentials of a general shape (solids, crystals):
The limit V_{asymp} does not exist. The whole spectrum is continuous and has a **band structure** (alternating zones of allowed and forbidden values of E). The eigenfunctions are not normalizable and all correspond to unbound states. Note that proofs of these statements are not presented here (but see Sec. 4b).

▶ **Nonanalytic potentials: conditions upon eigenfunctions**

From the stationary Schrödinger equation it follows that:

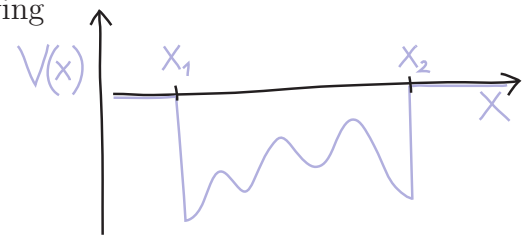
$\left(V, \frac{\partial V}{\partial x_i}, \dots \frac{\partial^n V}{\partial x_i^n}\right)\Big|_{\vec{x}=\vec{a}}$ continuous $\Leftrightarrow$ $\left(\psi, \frac{\partial \psi}{\partial x_i}, \dots \frac{\partial^n \psi}{\partial x_i^n}, \frac{\partial^{n+1} \psi}{\partial x_i^{n+1}}, \frac{\partial^{n+2} \psi}{\partial x_i^{n+2}}\right)\Big|_{\vec{x}=\vec{a}}$ continuous

If $V(\vec{x})|_{\vec{x}=\vec{a}}$ is discontinuous (the potential has a **finite jump** at $\vec{x}=\vec{a}$), then both $\psi, \frac{\partial \psi}{\partial x_i}\Big|_{\vec{x}=\vec{a}}$ must be continuous as well as the **logarithmic derivative**:

$$\boxed{\beta_i(\vec{x})|_{\vec{x}=\vec{a}} \equiv \frac{\frac{\partial \psi}{\partial x_i}(\vec{x})}{\psi(\vec{x})}\Big|_{\vec{x}=\vec{a}} = \frac{\partial}{\partial x_i} \ln \psi(\vec{x})\Big|_{\vec{x}=\vec{a}}}$$

Example: 1D potential well of a finite range $x \in [x_1, x_2]$

We assume an arbitrary potential satisfying
$V(x) \begin{cases} = 0 & \text{for } x < x_1 \ \& \ x > x_2, \\ < 0 & \text{for } x_1 \le x \le x_2, \end{cases}$
such that at both edges x_1 and x_2 $V(x)$ has discontinuities (**finite jumps**)



Eigenfunctions for bound ($E<0$) and unbound ($E \ge 0$) states read as

	$x < x_1$	$x_1 \le x \le x_2$	$x_2 < x$
$E<0$	$A_1 e^{+kx} + \cancel{A_2 e^{-kx}}$	$B_1\psi_1(x)_E + B_2\psi_2(x)_E$	$\cancel{C_1 e^{+kx}} + C_2 e^{-kx}$
$E \ge 0$	$A_1 \cos(kx) + A_2 \sin(kx)$	$B_1\psi_1(x)_E + B_2\psi_2(x)_E$	$C_1 \cos(kx) + C_2 \sin(kx)$

where $\{\psi_1(x)_E, \psi_2(x)_E\}$ are 2 independent eigensolutions inside the well,
$k = \frac{\sqrt{2ME}}{\hbar}$, and $\{A_1, A_2, B_1, B_2, C_1, C_2\}$ are coefficients to be determined.

$E<0$: (2 matching conditions at x_1)+(2 match.conds.at x_2)+(1 norm.condition)
$\Rightarrow$ cannot be solved with 4 free parameters $\forall E \Rightarrow$ discrete E spectrum

$E \ge 0$: (2 matching conditions at x_1)+(2 matching conditions at x_2)
$\Rightarrow$ can be solved with 6 free parameters $\forall E \Rightarrow$ continuous E spectrum

For **infinite jump** of $V(\vec{x})|_{\vec{x}=\vec{a}}$ only $\psi(\vec{x})|_{\vec{x}=\vec{a}}$ must be continuous

■ Hamiltonian with a separable potential

We look now at the special case of potential that has a trivial separated form $\boxed{V(\vec{x}) = V_1(x_1) + V_2(x_2) + V_3(x_3)}$ with each $V_k(x_k)$, $k=1,2,3$, being an arbitrary 1D potential in coordinate x_k. There are just a few (two?) practical

examples of such trivially separable potentials, but the analysis will help us to understand a rather important technique: separation of variables in differential equations in more general cases.

► **Form of solution**

Let us solve 3 × 1D equation $\overbrace{\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_k^2}+V_k(x_k)\right]}^{\hat{H}_k}\psi_{i_k}(x_k)=E_{i_k}\psi_{i_k}(x_i)$

The solution of the 3D problem can then be written as:

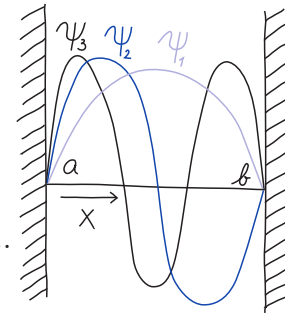
$$\underbrace{[\hat{H}_1+\hat{H}_2+\hat{H}_3]}_{\hat{H}}\underbrace{\psi_{i_1}(x_1)\psi_{i_2}(x_2)\psi_{i_3}(x_3)}_{\psi_{i_1i_2i_3}(\vec{x})}=\underbrace{(E_{i_1}+E_{i_2}+E_{i_3})}_{E_{i_1i_2i_3}}\underbrace{\psi_{i_1}(x_1)\psi_{i_2}(x_2)\psi_{i_3}(x_3)}_{\psi_{i_1i_2i_3}(\vec{x})}$$

1D eigenfunctions $\{\psi_{i_k}(x_k)\equiv|\psi_{i_k}\rangle\}_{i_k=1,2,...}$ ≡ basis in Hilbert space $\mathcal{H}_k$

$\{\psi_{i_1}(x_1)\psi_{i_2}(x_2)\psi_{i_3}(x_3)\equiv|\psi_{i_1}\rangle|\psi_{i_2}\rangle|\psi_{i_3}\rangle\}_{i_k=1,2,...}$ ≡ basis in $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2\otimes\mathcal{H}_3$

► **Examples**

(a) Particle in a box $V(\vec{x})=\left\{\begin{array}{l}0 \text{ for } x_k\in(a_k,b_k),\ k=1,2,3\\ \infty \text{ otherwise}\end{array}\right\}$



So $V(\vec{x})=V_{(a_1,b_1)}(x_1)+V_{(a_2,b_2)}(x_2)+V_{(a_3,b_3)}(x_3)$,
where each $V_{(a_k,b_k)}(x_k)$ is a 1D infinite square well potential, for which the 1D problem has solutions

$$\underbrace{\left(\frac{1}{2M}\hat{p}_k^2+V_{(a_k,b_k)}\right)}_{\hat{H}_k}|\psi_{n_k}\rangle=\underbrace{\left(\frac{\pi\hbar}{\sqrt{2M}L_k}n_k\right)^2}_{E_{n_k}}|\psi_{n_k}\rangle,\quad n_k=1,2,3,...$$

with eigenvectors $|\psi_{n_k}\rangle\equiv\psi_{n_k}(x_k)\propto\sin\left[\frac{n_k\pi}{L_k}(x-a_k)\right]$, where $L_k=b_k-a_k$

The solution of the whole 3D problem reads as:

$$\underbrace{[\hat{H}_1+\hat{H}_2+\hat{H}_3]}_{\hat{H}}\underbrace{|\psi_{n_1}\rangle|\psi_{n_2}\rangle|\psi_{n_3}\rangle}_{|\psi_{n_1n_2n_3}\rangle}=\underbrace{\frac{(\pi\hbar)^2}{2M}\left[\left(\frac{n_1}{L_1}\right)^2+\left(\frac{n_2}{L_2}\right)^2+\left(\frac{n_3}{L_3}\right)^2\right]}_{E_{n_1n_2n_3}}\underbrace{|\psi_{n_1}\rangle|\psi_{n_2}\rangle|\psi_{n_3}\rangle}_{|\psi_{n_1n_2n_3}\rangle}$$

Equilateral case: $L_k=L\quad\Rightarrow E_{n_1n_2n_3}\to\boxed{E_N=\frac{(\pi\hbar)^2}{2ML^2}\underbrace{(n_1^2+n_2^2+n_3^2)}_{N}}$

Various choices of (n_1,n_2,n_3) yield the following values of N and the corresponding degeneracy dimensions d_N:

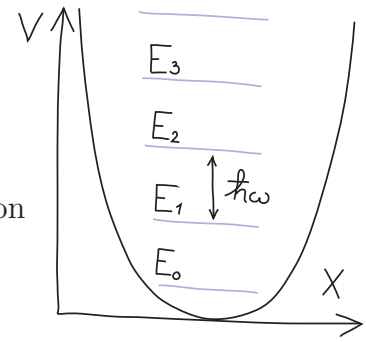
N	d_N
3	1
6	3
9	3
11	3
14	6
⋮	⋮

Consequence: The ground-state energy $E_{\rm gs}\propto\frac{1}{V^{2/3}}$ grows with volume V, which implies **"Schrödinger pressure"** against any decrease of V (increase of particle containment). This is closely related to the uncertainty relations (see Sec. 3a) and has crucial consequences (together with the Pauli principle) for the collapse of dying stars to red giants, neutron stars or black holes (though one would need relativistic equations for a qualitative analysis).

(b) Harmonic oscillator $V(\vec{x})=\frac{M}{2}(\omega_1^2x_1^2+\omega_2^2x_2^2+\omega_3^2x_3^2)$

The 1D problems have solutions

$$\underbrace{\left(\tfrac{1}{2M}\hat{p}_k^2+\tfrac{M\omega_k^2}{2}\hat{x}_k^2\right)}_{\hat{H}_k}|\psi_{n_k}\rangle=\underbrace{\hbar\omega_k\left(n_k+\tfrac{1}{2}\right)}_{E_{n_k}}|\psi_{n_k}\rangle$$



with $n_k=0,1,2,3,\ldots$ The eigenfunctions obtained from the differential form of the Schrödinger equation $\left[\frac{d^2}{d\xi_k^2}+(\lambda-\xi_k^2)\right]\psi(\xi_k)=0$, with $\xi_k=\sqrt{\frac{M\omega_k}{\hbar}}x_k$, $\lambda=\frac{2E}{M\omega}$, are $|\psi_{n_k}\rangle\equiv\psi_{n_k}(x_k)\propto e^{-\xi_k^2/2}H_{n_k}(\xi_k)$, $\overbrace{e^{\xi^2-(\xi-\eta)^2}}^{\text{generating function}}|_{\eta=0}$ where $H_n(\xi)\equiv\frac{d^n}{d\eta^n}$ are **Hermite polynomials**

The 3D case:

$$\underbrace{[\hat{H}_1+\hat{H}_2+\hat{H}_3]}_{\hat{H}}\underbrace{|\psi_{n_1}\rangle|\psi_{n_2}\rangle|\psi_{n_3}\rangle}_{|\psi_{n_1n_2n_3}\rangle}=\underbrace{\hbar\left[\omega_1(n_1+\tfrac{1}{2})+\omega_2(n_2+\tfrac{1}{2})+\omega_3(n_3+\tfrac{1}{2})\right]}_{E_{n_1n_2n_3}}\underbrace{|\psi_{n_1}\rangle|\psi_{n_2}\rangle|\psi_{n_3}\rangle}_{|\psi_{n_1n_2n_3}\rangle}$$

Isotropic case: $\omega_k=\omega \quad\Rightarrow E_{n_1n_2n_3}\to\boxed{E_N=\hbar\omega(\underbrace{n_1+n_2+n_3}_{N}+\tfrac{3}{2})}$

N	d_N
0	1
1	3
2	6
3	10
⋮	⋮

Various choices of (n_1,n_2,n_3) yield $N=0,1,2,3,4,\ldots$ and the corresponding degeneracy dimensions $d_N=\frac{(N+1)(N+2)}{2}$:

Alternative method of solution:

Hamiltonian of each 1D oscillator can be expressed as $\boxed{\hat{H}_k=\hbar\omega_k\left(\underbrace{\hat{b}_k^\dagger\hat{b}_k}_{\hat{n}_k}+\tfrac{1}{2}\right)}$ where $\hat{b}_k^\dagger=\frac{\hat{x}_k}{\sqrt{2\hbar/M\omega_k}}-i\frac{\hat{p}_k}{\sqrt{2\hbar M\omega_k}}$, $\hat{b}_k=\frac{\hat{x}_k}{\sqrt{2\hbar/M\omega_k}}+i\frac{\hat{p}_k}{\sqrt{2\hbar M\omega_k}}$ are **ladder operators**, whose algebraic properties (see Secs. 3b & 14) ensure that the operator $\hat{n}_k$ has eigenvalues $n_k=0,1,2,\ldots$. The operators $\hat{b}_k^\dagger$ and $\hat{b}_k$, respectively, are interpreted as creation and annihilation operators of the (kth) oscillator excitaton quantum (so called **phonon**) and the operator $\hat{n}_k$ has the meaning of the number of these quanta. This procedure has a crucial importance for quantization of physical fields, such as the electromagnetic field, in the relativistic formulation of the quantum theory (Sec. 14).

■ Orbital angular momentum

Before we continue with other Hamiltonians and potentials in the 3D space, it is useful to construct operators of angular momentum associated with the orbital motions of any particle.

► **Operators** of orbital ang. momentum are analogous to classical expressions:

components $\boxed{\hat{L}_i=\varepsilon_{ijk}\hat{x}_j\hat{p}_k}$ $\Leftrightarrow$ **vector** $\boxed{\hat{\vec{L}}=\hat{\vec{x}}\times\hat{\vec{p}}=-i\hbar\left[\vec{x}\times\vec{\nabla}\right]}$

Hermiticity: $\hat{L}_i^\dagger=\varepsilon_{ijk}\hat{p}_k^\dagger\hat{x}_j^\dagger=\varepsilon_{ijk}\hat{p}_k\hat{x}_j=\varepsilon_{ijk}\hat{x}_j\hat{p}_k=\hat{L}_i$ (since $j\neq k$)

▶ Expression in spherical coordinates

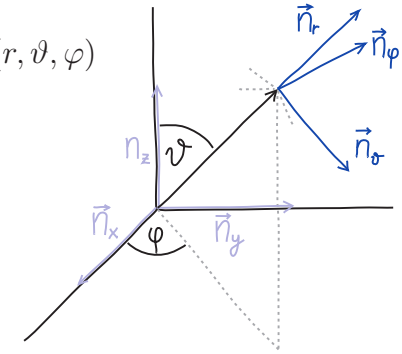
Transformation of wavefunctions: $\psi(x,y,z) \mapsto \psi(r,\vartheta,\varphi)$

Unit vectors in coordinate directions:

$$\begin{pmatrix} \vec{n}_r \\ \vec{n}_\vartheta \\ \vec{n}_\varphi \end{pmatrix} = \begin{pmatrix} \sin\vartheta\cos\varphi & \sin\vartheta\sin\varphi & \cos\vartheta \\ \cos\vartheta\cos\varphi & \cos\vartheta\sin\varphi & -\sin\vartheta \\ -\sin\varphi & \cos\varphi & 0 \end{pmatrix} \begin{pmatrix} \vec{n}_x \\ \vec{n}_y \\ \vec{n}_z \end{pmatrix}$$

$$\begin{pmatrix} \vec{n}_x \\ \vec{n}_y \\ \vec{n}_z \end{pmatrix} = \begin{pmatrix} \sin\vartheta\cos\varphi & \cos\vartheta\cos\varphi & -\sin\varphi \\ \sin\vartheta\sin\varphi & \cos\vartheta\sin\varphi & \cos\varphi \\ \cos\vartheta & -\sin\vartheta & 0 \end{pmatrix} \begin{pmatrix} \vec{n}_r \\ \vec{n}_\vartheta \\ \vec{n}_\varphi \end{pmatrix}$$

Orthogonal matrix $\Rightarrow$ [inverse = transpose]



Vector of orbital angular momentum expressed in spherical coordinates:

$$\hat{\vec{L}} = -i\hbar \Big[\underbrace{r\vec{n}_r}_{\vec{x}} \times \underbrace{\Big(\vec{n}_r \tfrac{\partial}{\partial r} + \vec{n}_\vartheta \tfrac{1}{r}\tfrac{\partial}{\partial\vartheta} + \vec{n}_\varphi \tfrac{1}{r\sin\vartheta}\tfrac{\partial}{\partial\varphi} \Big)}_{\vec{\nabla}} \Big]$$

$\vec{n}_r\times\vec{n}_r=0$
$\vec{n}_r\times\vec{n}_\vartheta=\vec{n}_\varphi$
$\vec{n}_r\times\vec{n}_\varphi=-\vec{n}_\vartheta$

$$\boxed{\hat{\vec{L}} = -i\hbar \Big[\vec{n}_\varphi \tfrac{\partial}{\partial\vartheta} - \vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi} \Big]}$$ acts only on the angular part of $\psi(r,\vartheta,\varphi)$

$\Rightarrow$ we consider factorized wavefunctions $\boxed{\psi(r,\vartheta,\varphi) \equiv R(r)\,\Omega(\vartheta,\varphi)}$

▶ Angular-momentum component along the z-axis

$$\vec{n}_z = \cos\vartheta\,\vec{n}_r - \sin\vartheta\,\vec{n}_\vartheta \qquad \Rightarrow \qquad \vec{n}_z \cdot \hat{\vec{L}} \;\equiv\; \boxed{\hat{L}_z = -i\hbar\tfrac{\partial}{\partial\varphi}}$$

Eigenvalue equation allows for further factorization:

$$\hat{L}_z \underbrace{\Omega(\vartheta,\varphi)}_{f(\vartheta)g(\varphi)} = l_z\Omega(\vartheta,\varphi) \qquad -i\hbar\tfrac{\partial}{\partial\varphi}g(\varphi) = l_z g(\varphi) \text{ with condition } g(\varphi{+}2\pi) = g(\varphi)$$

$$\Rightarrow \qquad \boxed{l_z = m\hbar} \text{ with } m = 0, \pm1, \pm2, \pm3, \ldots \text{ and } \boxed{g_m(\varphi) = e^{im\varphi}}$$

Additional condition $l_z^2 \le L^2 \Rightarrow \boxed{|m| \le m_{\max}}$ (see below and in Sec. 3b)

From the symmetry argument, the same form of eigenvalues must be valid for *any component* of $\hat{\vec{L}}$, but as we will see in Sec. 3b, the system *cannot* be in a simultaneous eigenstate of all angular-momentum components.

▶ Squared orbital angular momentum

The size of the angular-momentum vector is determined by the square:

$$\boxed{\hat{L}^2 = \hat{\vec{L}}\cdot\hat{\vec{L}}} = -\hbar^2 \Big[\vec{n}_\varphi \tfrac{\partial}{\partial\vartheta} - \vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi} \Big] \cdot \Big[\vec{n}_\varphi \tfrac{\partial}{\partial\vartheta} - \vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi} \Big] =$$

$$= -\hbar^2 \Big[\underbrace{\vec{n}_\varphi \tfrac{\partial}{\partial\vartheta} \cdot \vec{n}_\varphi \tfrac{\partial}{\partial\vartheta}}_{\frac{\partial^2}{\partial\vartheta^2}} - \underbrace{\vec{n}_\varphi \tfrac{\partial}{\partial\vartheta} \cdot \vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi}}_{0} - \underbrace{\vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi} \cdot \vec{n}_\varphi \tfrac{\partial}{\partial\vartheta}}_{-\cot\vartheta\frac{\partial}{\partial\vartheta}} + \underbrace{\vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi} \cdot \vec{n}_\vartheta \tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\varphi}}_{\frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}} \Big]$$

$$= -\hbar^2 \Big[\underbrace{\tfrac{\partial^2}{\partial\vartheta^2} + \cot\vartheta\tfrac{\partial}{\partial\vartheta}}_{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial}{\partial\vartheta}} + \tfrac{1}{\sin^2\vartheta}\tfrac{\partial^2}{\partial\varphi^2} \Big] \;\Rightarrow\; \boxed{\hat{L}^2 = -\hbar^2 \Big[\tfrac{1}{\sin\vartheta}\tfrac{\partial}{\partial\vartheta}\sin\vartheta\tfrac{\partial}{\partial\vartheta} + \tfrac{1}{\sin^2\vartheta}\tfrac{\partial^2}{\partial\varphi^2} \Big]}$$

▶ Eigenequation $\hat{L}^2\Omega_{\lambda m}(\vartheta,\varphi) = \lambda^2\Omega_{\lambda m}(\vartheta,\varphi)$

solved with a factorized function $\Omega_{\lambda m}(\vartheta,\varphi) \equiv f_{\lambda m}(\vartheta)\, e^{im\varphi}$

$$\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial}{\partial\vartheta} - \frac{m^2}{\sin^2\vartheta} + \frac{\lambda^2}{\hbar^2}\right] f_{\lambda m}(\vartheta) = 0 \xrightarrow[\xi=\cos\vartheta]{\text{subst.}} \left[\frac{\partial}{\partial\xi}(1-\xi^2)\frac{\partial}{\partial\xi} - \frac{m^2}{1-\xi^2} + \frac{\lambda^2}{\hbar^2}\right] f_{\lambda m}(\xi) = 0$$

The solution known in the form (for derivation see elsewhere):

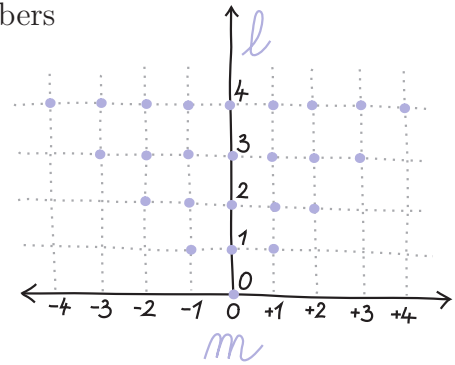
$f_{\lambda m}(\xi) \equiv P_{lm}(\xi) \propto (1-\xi^2)^{\frac{m}{2}} \frac{d^{l+m}}{d\xi^{l+m}}(\xi^2-1)^l$ **associated Legendre polynomial**

Eigenvalues $\boxed{\lambda^2 = l(l+1)\hbar^2 \text{ with } \begin{cases} l = 0, 1, 2 \dots \\ m = -l, (-l{+}1) \dots 0 \dots (+l{-}1), +l \end{cases}}$

Eigenfunctions

$$\Omega_{\lambda m}(\vartheta,\varphi) = \boxed{\underbrace{\mathcal{N}_{lm}}_{\text{normalization}} P_{lm}(\cos\vartheta)\; e^{im\varphi} \equiv Y_{lm}(\vartheta,\varphi)}$$ **spherical harmonics**

Relation between l and m quantum numbers is represented by the following diagram:



Note: The existence of **simultaneous eigenstates** of $\hat{L}^2$ and $\hat{L}_z$ is not accidental. It follows from the fact that both operators commute, see Sec. 3b, where also the selection rules for m and l are derived.

■ Hamiltonian with isotropic (spherically symmetric) potential

Equipped with the angular momentum operators, we can return to the Hamiltonian of a single structureless nonrelativistic particle moving in a spherically symmetric potential field $\boxed{V(\vec{x}) = V(r)}$ This is a rather important situation in general since nature likes rotational invariance. Besides the general discussion we will briefly report three well known examples, including the famous solution of the hydrogen atom, which was at the very beginning of quantum theory.

▶ Hamiltonian in spherical coordinates

$$\boxed{\hat{H} = -\tfrac{\hbar^2}{2M}\Delta + V(r)} = \frac{1}{2M}\Big[\underbrace{\frac{-\hbar^2}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}}_{\hat{p}_r^2} + \underbrace{\frac{-\hbar^2}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial}{\partial\vartheta} + \frac{-\hbar^2}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}}_{r^{-2}\hat{L}^2}\Big] + V(r)$$

This can be decomposed into three parts:

$$\boxed{\hat{H} = \underbrace{\frac{1}{2M}\hat{p}_r^2}_{\substack{\text{radial} \\ \text{kin.energy}}} + \underbrace{\frac{1}{2Mr^2}\hat{L}^2}_{\substack{\text{orbital} \\ \text{kin.energy}}} + \underbrace{V(r)}_{\substack{\text{potential} \\ \text{energy}}}}$$

with $\boxed{\hat{p}_r \equiv -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)}$ **radial momentum**

The radial momentum operator has spherical waves as its eigenfunctions (see below) and in this sense it differs from any Cartesian component of momentum (with planar waves as eigenfunctions). The decomposition of the kitetic energy into the radial and angular (orbital) components has a clear physical meaning.

▶ Separation of variables

The isotropic form of the Hamiltonian enables one to separate radial and angular variables through the wavefunction ansatz:

$$\boxed{\psi_{nlm}(r,\vartheta,\varphi) \equiv \underbrace{R_{nl}(r)}_{\frac{u_{nl}(r)}{r}} Y_{lm}(\vartheta,\varphi)}$$

$\hat{L}^2 Y_{lm}(\vartheta,\varphi) = \hbar^2 l(l+1) Y_{lm}(\vartheta,\varphi)$

The equation for R_{nl} reads: $\left[-\frac{\hbar^2}{2M}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\hbar^2 l(l+1)}{2Mr^2} + V(r)\right] R_{nl}(r) = E_{nl} R_{nl}(r)$

$$\boxed{\left[-\frac{\hbar^2}{2M}\frac{d^2}{dr^2} + \underbrace{\frac{\hbar^2 l(l+1)}{2Mr^2} + V(r)}_{V_{\text{eff}}^{(l)}(r)}\right] u_{nl}(r) = E_{nl} u_{nl}(r)} \quad \textbf{radial Schrödinger eq.}$$

The **centrifugal term** (the first term in the effective potential $V_{\text{eff}}^{(l)}$) describes rotational kinetic energy of the particle with orbital q. number l at distance r.

▶ Unbound-state asymptotics (eigenfunctions of radial momentum)

For $V(r) \xrightarrow{r\to\infty} 0$ we write down an $E > 0$ asymptotic radial solution for $l = 0$:

spherical wave (for $r \gg 0$):

$-i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\frac{e^{ip_r r/\hbar}}{r} = p_r \frac{e^{ip_r r/\hbar}}{r}$

$$\boxed{R_{p_r}(r) \propto \frac{e^{i\frac{p_r r}{\hbar}}}{r}} \quad \equiv \text{plane wave of } u(r)$$

▶ Bound state near the origin

From the normalization we know that $u(r)r^2 \xrightarrow{r\to 0} 0$ and we further assume that $V(r)u(r)r^2 \xrightarrow{r\to 0} 0$ (the potential is not too crazy for $r \to 0$). Then the approximate $r \to 0$ equation $\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u \approx 0$ can be solved with $u(r) \propto r^k$

$$k(k-1) = l(l+1) \quad \Rightarrow \quad k = \begin{cases} l+1 \\ -l \ \text{(nonphysical)} \end{cases} \quad \Rightarrow \quad \boxed{u_{nl}(r)|_{r\sim 0} \approx r^{l+1} \xrightarrow{r\to 0} 0}$$

Why the $k = -l$ solution is nonphysical? Because for $l > 0$ it is not normalizable, while for $l = 0$ the action of Δ on $R(r) \propto r^{-1}$ would yield a singularity $\propto \delta(r)$, which is not supposed to be involved in $V(r)$.

▶ Example: (a) finite spherical square well

$$\boxed{V(r) = \begin{cases} -V_0 < 0 & \text{for } r < R \\ 0 & \text{for } r \geq R \end{cases}}$$

Radial equation: $\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2M(E-V)}{\hbar^2}\right] u_{nl}(r) = 0$ with $V = \begin{cases} -V_0 \\ 0 \end{cases}$

Discrete spectrum $E_n \in (-V_0, 0)$, continuous spectrum $E \in (0, +\infty)$

$$\kappa = \frac{\sqrt{2M(E+V_0)}}{\hbar} \quad k = \frac{\sqrt{2ME}}{\hbar} \begin{cases} > 0 & \text{for } E \geq 0 \\ = i\varkappa & \text{for } E < 0 \end{cases} \quad r \to \rho \equiv \begin{cases} \kappa r & \text{for } r < R \\ kr & \text{for } r \geq R \end{cases}$$

The eigenfunctions in a general case can expressed through **Bessel & Neumann functions**, or alternatively through **Hankel functions**:

$$R_{nl}(\rho)=\frac{u_{nl}(\rho)}{\rho}=\begin{cases}\text{Bessel} & j_l(\rho)\ \propto_{\rho\to 0}\ \rho^l\\ \text{Neumann} & n_l(\rho)\ \propto_{\rho\to 0}\ \rho^{-(l+1)}\\ \text{Hankel} & h_l^+(\rho)=j_l(\rho)+in_l(\rho)\ \propto_{r\to\infty}\ \frac{e^{i(\rho-l\pi/2)}}{i\rho}\\ \text{functions} & h_l^-(\rho)=j_l(\rho)-in_l(\rho)\ \propto_{r\to\infty}\ \frac{e^{-i(\rho-l\pi/2)}}{i\rho}\end{cases}$$

Normalizable bound states ($E<0$): the $r=0$ and $r\to\infty$ conditions restrict the solution to the form

$$\boxed{R_{nl}(r)=\begin{cases}Aj_l(\kappa r) & \text{for } r<R\\ B\,\mathrm{Re}h_l^+(i\varkappa r) & \text{for } r\geq R\end{cases}}$$

Constants A, B and energy levels E_{nl} are obtained from numerical solution of a pair of equations $\left\{\begin{array}{l}\frac{\frac{d}{d\rho}j_l(\kappa R)}{j_l(\kappa R)}=\frac{\frac{d}{d\rho}\mathrm{Re}h_l^{(1)}(i\varkappa R)}{\mathrm{Re}h_l^+(i\varkappa R)}\\ \kappa^2+\varkappa^2=\frac{2MV_0}{\hbar^2}\end{array}\right\}$

► **Example: (b) isotropic harmonic oscillator** (revisited) $\boxed{V(r)=\frac{M\omega^2}{2}r^2}$

From the previous treatment we know: $E_N=\hbar\omega(N+\frac{3}{2})$, where $N=n_1+n_2+n_3$

The solution in spherical coordinates: $\boxed{R_{nl}(\xi)\propto\xi^l L_n^{l+1/2}(\xi^2)}$ with $\xi=\sqrt{\frac{M\omega}{\hbar}}r$

$L_i^a(\rho)\equiv\rho^{-a}e^\rho\frac{d^i}{d\rho^i}(\rho^{i+a}e^{-\rho})$ **generalized Laguerre polynomial**

Relation between quantum numbers from both solutions: $\boxed{\underbrace{N+1}_{1,2,3\ldots}=2n_r+l+1}$

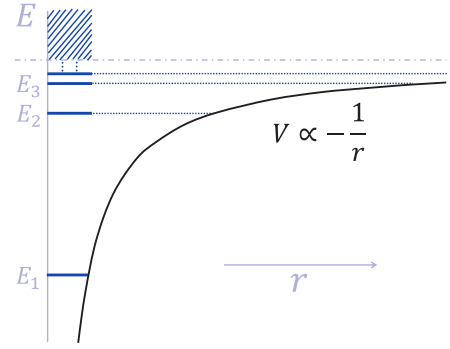
with $n_r=0,1,2,\ldots$ **radial quantum number** = number of nodes of $R_{nl}(r)$

► **Example: (c) attractive Coulomb field** $\boxed{V(r)=-\frac{K}{r}}$

This also describes electron in the hydrogen atom: $K=\frac{e^2}{4\pi\epsilon_0}$

Discrete spectrum $E_n<0$, continuous spectrum $E\geq 0$

Determination of the discrete spectrum: Using $\rho=\sqrt{\frac{8M|E|}{\hbar^2}}r$, $\lambda=\sqrt{\frac{MK^2}{2\hbar^2|E|}}$ we look for solutions of the radial equation $\left[\frac{d^2}{d\rho^2}-\frac{l(l+1)}{\rho^2}+\frac{\lambda}{\rho}\right]u(\rho)=0$ with the required boundary conditions in the form $u(\rho)=\rho^{l+1}e^{-\rho/2}p(\rho)$, where $p(\rho)=\sum_{k=0}^\infty c_k\rho^k$ with some coefficients c_k. The resulting condition $c_{k+1}=\frac{k+l+1-\lambda}{(k+l+2)(k+l+1)-l(l+1)}c_k$ ($\Rightarrow\ c_k\sim\frac{1}{k!}$ for large k $\Rightarrow$ exponential growth of $p(\rho)$ for large ρ) yields a normalizable solution *iff* $c_k=0$ for $k\geq k_{\max}$. The value $k_{\max}\equiv n_r$, which is the degree of the polynomial $p(\rho)$, i.e., the number of nodes of $u(\rho)$, is given by $n_r+l+1-\lambda=0$. So $n_r+l+1=\frac{\alpha}{\hbar}\sqrt{\frac{M}{2|E|}}$



$\Rightarrow\ \boxed{E_n=-\frac{MK^2}{2\hbar^2}\frac{1}{n^2}}$ $\quad\boxed{\begin{array}{ll}n&=n_r+l+1\\&=1,2,3,\ldots\end{array}}$

with the principal quantum number n derived from the radial and orbital quantum numbers $n_r=0,1,2,\ldots$ and $l=0,1,2,\ldots$

Degeneracy dimension of level n is given by $\left\{ \begin{smallmatrix} l=0,1,\dots(n-1) \\ m=-l,\cdots+l \end{smallmatrix} \right\} \Rightarrow d_n = \sum_{l=0}^{n-1}(2l+1) = n^2$

$\boxed{R_{nl}(\rho) \propto \rho^l e^{-\rho/2} L^{2l+1}_{n-l-1}(\rho)}$ with $L^j_i(\rho) \equiv \frac{d^j}{d\rho^j} e^\rho \frac{d^i}{d\rho^i}(\rho^i e^{-\rho})$

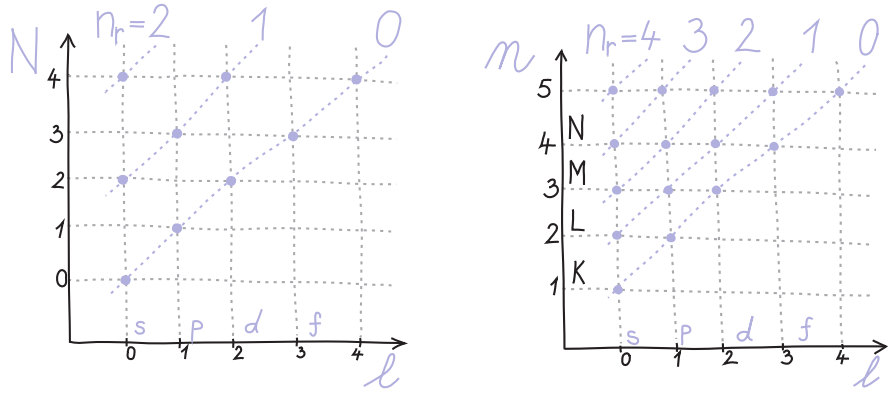
associated Laguerre polynomial

Hydrogen atom:

Defining the **Compton wavelength** $\lambda\!\!\!^{-}_{\rm C}$ for electron and introducing the dimensionless **fine-structure constant** $\alpha = V(\lambda\!\!\!^{-}_{\rm C})/Mc^2$, we express the hydrogen energies as $\boxed{E_n = -\frac{1}{2}Mc^2\alpha^2\frac{1}{n^2}}$ (the ground state has $E_1 \doteq -13.6$ eV). The above dimensionless length reads $\rho = \frac{2}{na_{\rm B}}r$, where $\boxed{a_{\rm B} = \frac{\lambda\!\!\!^{-}_{\rm C}}{\alpha}} \doteq 0.053$ nm is the **Bohr radius**.

$\boxed{\lambda\!\!\!^{-}_{\rm C} = \frac{\hbar}{Mc} \doteq 386\,\text{fm}}$
$\boxed{\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \doteq \frac{1}{137}}$

► Graphical expression of oscillator and hydrogen selection rules for quantum numbers



◄ Historical remark

1913-24: Development of atomic physics in terms of "old quantum mechanics"
1926: Erwin Schrödinger presents 4 papers introducing the wavefunction and explaining the energy quantization in terms of an eigenvalue problem, with solutions for Coulomb and harmonic potentials obtained via the orbital angular momentum
1928-30: Application to molecules and solids; L. Pauling explains chemical bond, P.M. Morse describes vibrations of diatomic molecules (Morse potential), F. Bloch and L. Brillouin analyze eigenstates in periodic potentials
1929: First numerical algorithm for solving the eigenvalue problem
1932-49: Early development of quantum theory of atomic nuclei: two-nucleon potential (H. Yukawa), shell model (D. Ivanenko, M. Goeppert-Mayer, J.H.D. Jensen)

■ Hamiltonian of a spin-$\frac{1}{2}$ particle in static electromagnetic field

We now look at the Hamiltonian of an structureless, electron-like particle moving in general (but static) electric and magnetic fields. The interaction now includes not only the electric charge of the particle, but also its magnetic dipole moment. This is a very important case, in atomic physics and beyond. We will also discuss the invariance of the Schrödinger equation under the gauge

transformation—the concept that in a generalized form plays an essential role in the present theory of all particle interactions.

▶ We assume a charged particle with a nonzero magnetic dipole moment and all other static electromagnetic moments equal zero. In analogy with the classical expression, the quantum Hamiltonian reads as:

$$\boxed{\hat{H} = \tfrac{1}{2M}\left[\hat{\vec{p}} - q\vec{A}(\hat{\vec{x}})\right]^2 + qV(\hat{\vec{x}}) - \hat{\vec{\mu}}\cdot\vec{B}(\hat{\vec{x}})}$$

$q \equiv$ particle charge
$\hat{\vec{\mu}} \equiv$ particle magnetic dipole moment
$V(\vec{x}) \equiv$ **scalar potential**
$\vec{A}(\vec{x}) \equiv$ **vector potential**

$\vec{B}(\vec{x}) = \vec{\nabla}\times\vec{A}(\vec{x}) \equiv$ magnetic induction,
$\vec{E}(\vec{x}) = -\vec{\nabla}V(\vec{x}) - \underbrace{\frac{\partial}{\partial t}\vec{A}(\vec{x})}_{0} \equiv$ electric intensity of a stationary elmg. field

▶ **Magnetic dipole moment operator** $\hat{\vec{\mu}}$ is proportional to the operator of the particle spin. We suppose particles with spin $\frac{1}{2}$, specifically electrons, protons and neutrons:

$$\boxed{\hat{\vec{\mu}} = g\,\mu\,\left(\tfrac{1}{\hbar}\hat{\vec{S}}\right) = g\,\tfrac{q\hbar}{2M}\,\left(\tfrac{1}{2}\hat{\vec{\sigma}}\right)}$$

$g \equiv$ **gyromagnetic ratio** $\left\{\begin{array}{cc} g{=}2 & \text{electron} \\ g{=}5.5856 & \text{proton} \\ g{=}-3.8263 & \text{neutron}\end{array}\right.$

$\boxed{\mu = \frac{e\hbar}{2M}} = \left\{\begin{array}{c}\textbf{Bohr}\\ \textbf{nuclear}\end{array}\right\}$ **magneton** for $M = \left\{\begin{array}{c} M_{\rm e} \\ M_{\rm p}\end{array}\right\}$

The ratio $g = \frac{\vec{\mu}/\mu}{\vec{S}/\hbar}$ is dimensionless, its value for a structureless spin-$\frac{1}{2}$ particle being predicted by the relativistic Dirac theory to $g = 2$. The proton and neutron values of g reflect the internal quark structure. Small quantum-field corrections exist also for structureless particles like electrons or muons.

▶ Evaluation of the **kinetic term** (mind that $\hat{\vec{p}}$ and $\vec{A}(\hat{\vec{x}}) \equiv \hat{\vec{A}}$ do *not* commute):

$$\left[\hat{\vec{p}} - q\hat{\vec{A}}\right]^2 = \underbrace{\hat{\vec{p}}^2}_{-\hbar^2\Delta} \underbrace{-q\left[\hat{\vec{p}}\cdot\hat{\vec{A}} + \hat{\vec{A}}\cdot\hat{\vec{p}}\right]}_{+i\hbar q[\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}]} + q^2\hat{\vec{A}}^2 = -\hbar^2\Delta + i\hbar q\left[(\vec{\nabla}\cdot\vec{A}) + 2\vec{A}\cdot\vec{\nabla}\right] + q^2\vec{A}^2$$

▶ **Pauli equation** (the stationary version)

Eigenequation $\hat{H}\boldsymbol{\psi} = E\boldsymbol{\psi}$ with spinor $\boldsymbol{\psi}(\vec{x}) = \begin{pmatrix}\psi_\uparrow(\vec{x}) \\ \psi_\downarrow(\vec{x})\end{pmatrix}$ yields

$$\boxed{-\tfrac{\hbar^2}{2M}\Delta\boldsymbol{\psi} + \tfrac{i\hbar q}{2M}\underbrace{(\vec{\nabla}\cdot\vec{A})}_{=0\text{ in Lorentz calibration}}\boldsymbol{\psi} + \tfrac{i\hbar q}{M}(\vec{A}\cdot\vec{\nabla}\boldsymbol{\psi}) + qV\boldsymbol{\psi} + \tfrac{q^2}{2M}\vec{A}^2\boldsymbol{\psi} - g\tfrac{q\hbar}{2M}\tfrac{1}{2}\underbrace{(\hat{\vec{\sigma}}\cdot\vec{B})}_{\begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z\end{pmatrix}}\boldsymbol{\psi} = E\boldsymbol{\psi}}$$

▶ Special case: **homogeneous magnetic field**

$\vec{B}(\vec{x}) \equiv (0,0,B)$ can be obtained from $\vec{A}(\vec{x}) = \frac{B}{2}(-y,+x,0)$ satisfying $\vec{\nabla}\cdot\vec{A} = 0$.
The second term of the above equation, $\frac{i\hbar q}{M}(\vec{A}\cdot\vec{\nabla}\boldsymbol{\psi}) = \frac{qB}{2M}\underbrace{i\hbar\left[-y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}\right]}_{-\hat{L}_z}\boldsymbol{\psi}$,
corresponds to the energy $E = -\vec{B}\cdot\vec{\mu}_{\rm orb}$ of the orbital magnetic dipole with moment $\hat{\vec{\mu}}_{\rm orb} = \frac{q\hbar}{2M}\frac{1}{\hbar}\hat{\vec{L}}$ in mag. field $\vec{B}$.

The Pauli equation reads as:

$$\Big[\underbrace{-\tfrac{\hbar^2}{2M}\Delta}_{\substack{\text{translational}\\ \text{kinitic}\\ \text{energy}}} \underbrace{+qV}_{\substack{\text{electrostat.}\\ \text{energy}}} \underbrace{-\tfrac{qB}{2M}\left(\hat{L}_z+g\hat{S}_z\right)}_{\substack{\text{mag. moment interaction}\\ \Rightarrow\textbf{Zeeman splitting}}} + \underbrace{\tfrac{q^2B^2}{8M}(x^2+y^2)}_{\substack{\frac{1}{2}M\omega_{\mathrm{L}}^2\\ \text{kinetic energy of }\textbf{precession}\ \approx\ 0}}\Big]\boldsymbol{\psi} = E\boldsymbol{\psi}$$

The last expression (arising from the $\propto \vec{A}^2$ term) represents the kinetic energy of the precesional motion of the magnetic dipole in the field $\vec{B}$ with the **Larmor frequency** $\omega_{\mathrm{L}} \equiv \frac{qB}{2M}$. For electron in hydrogen $\omega_{\mathrm{L}} \lesssim \omega_{\mathrm{orbital}}$ for $B \lesssim 10^5\,\mathrm{T}$. So this term can be neglected unless the field is extremely large.

▶ Invariance under gauge transformations

The effect of classical electromagnetic field is invariant under the gauge transformations generated by $f(\vec{x},t)$:

$$\boxed{\vec{A} \mapsto \vec{A}' = \vec{A} - \vec{\nabla} f} \qquad \boxed{V \mapsto V' = V + \underbrace{\frac{\partial}{\partial t} f}_{=0 \text{ in stac. case}}}$$

These transformations do not change $\vec{E}$ and $\vec{B}$, but they *do* change the Pauli equation! Does quantum physics depend on $\vec{A}$ instead of the "physical fields" $\vec{E}$ and $\vec{B}$? The complete answer is not quite straightforward, but for the time being it is enough to show that the gauge transformation of $\vec{A}$ in the Pauli equation is always compensated by a local phase transformation of the wavefunction. This means that the gauge transformation does not alter energies and spatial probability densities corresponding to individual eigenstates of the Hamiltonian.

$$\boxed{\boldsymbol{\psi}(\vec{x}) \mapsto \boldsymbol{\psi}'(\vec{x}) \equiv \boldsymbol{\psi}(\vec{x}) e^{-i\frac{q}{\hbar}f(\vec{x})}}$$

Direct verification: $(-i\hbar\vec{\nabla} - q\vec{A}')^2\boldsymbol{\psi}' = (-i\hbar\vec{\nabla} - q\vec{A}')\cdot(-i\hbar\vec{\nabla} - q\vec{A}')e^{-i\frac{q}{\hbar}f}\boldsymbol{\psi} = (-i\hbar\vec{\nabla} - q\vec{A}')\cdot e^{-i\frac{q}{\hbar}f}(-i\hbar\vec{\nabla} - q\vec{A})\boldsymbol{\psi} = e^{-i\frac{q}{\hbar}f}(-i\hbar\vec{\nabla} - q\vec{A})^2\boldsymbol{\psi}$

Therefore: $\hat{H}\boldsymbol{\psi} = E\boldsymbol{\psi} \quad\Rightarrow\quad \hat{H}'\boldsymbol{\psi}' = E\boldsymbol{\psi}' \quad\Rightarrow\quad |\psi(\vec{x},m_s)|^2 = |\psi'(\vec{x},m_s)|^2$

However, as discussed in Sec. 8, not all mystery is gone.

◀ Historical remark

1927: Wolfgang Pauli writes down the spinor equation for particle in mag.field
1928: Hermann Weyl shows that gauge transformations in QM are related to local phase changes of the wavefunction

■ Hamiltonians of simple coupled systems

At last, we give a few elementary examples of many-body Hamiltonians. Please note that the list of diverse important Hamiltonians is practically endless.

▶ Many-electron atom

Atom with Z electrons (coordinates $\vec{x}^{(i)}$ and Laplacians $\Delta^{(i)}$, $i = 1, ..., Z$) and a point-like nucleus with charge Ze. Nonrelativistic Hamiltonian describing only electric effects (neglecting effects of the magnetic moments):

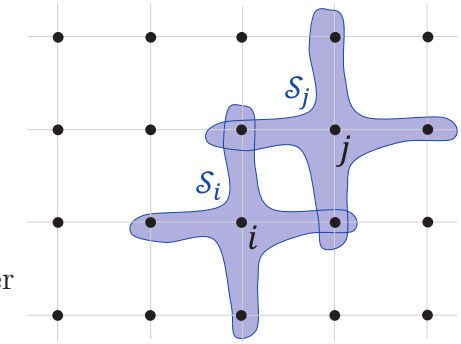
$$\hat{H} = -\frac{\hbar^2}{2M}\sum_{i=1}^{Z}\Delta^{(i)} - \frac{Ze^2}{4\pi\epsilon_0}\sum_{i=1}^{Z}\frac{1}{|\vec{x}^{(i)}|} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{Z}\frac{1}{|\vec{x}^{(i)}-\vec{x}^{(j)}|}$$

The solution of $\hat{H}|\Psi\rangle = E|\Psi\rangle$ is an atisymmetrized many-body wavefunction $\propto \hat{P}_-^{(Z)}\Psi(\vec{x}^{(1)}, m^{(1)}, \ldots, \vec{x}^{(Z)}, m^{(Z)}) \in \mathcal{H}_-^{(Z)}$, with $m^{(i)}$ denoting electron spin projections (arbitrary for the present spin-independent $\hat{H}$). However, because of an exponential increase of the dimension of a suitably truncated Hilbert space, the numerical solution is practically impossible even for medium Z and efficient approximation methods are needed.

▶ Interacting spin (qubit) systems: Ising model

Consider a system composed of N qubits (spin-$\frac{1}{2}$ particles with frozen spatial degrees of freedom, $i = 1, ..., N$). The Hamiltonian can read as:

$$\hat{H} = \frac{\varepsilon}{2}\sum_{i=1}^{N}\hat{\sigma}_z^{(i)} - \frac{\kappa}{2n}\sum_{i=1}^{N}\sum_{j\in\mathcal{S}_i}\hat{\sigma}_x^{(i)}\hat{\sigma}_x^{(j)} = \begin{cases} \varepsilon\sum\limits_i \hat{I}\otimes\cdots\otimes\hat{I}\otimes\hat{\sigma}_z^{(i)}\otimes\hat{I}\otimes\cdots\otimes\hat{I} \\ -\frac{\kappa}{2n}\sum\limits_{\langle i,j\rangle}\hat{I}\otimes\cdots\otimes\hat{I}\otimes\hat{\sigma}_x^{(i)}\otimes\hat{I}\otimes\cdots\otimes\hat{I}\otimes\hat{\sigma}_x^{(j)}\otimes\hat{I}\otimes\cdots\otimes\hat{I} \end{cases}$$



where ε sets the single-qubit energies ($=\pm\frac{\varepsilon}{2}$) and κ quantifies two-qubit interactions. It is assumed that the ith qubit interacts with n qubits contained in a set $\mathcal{S}_i$. We can think of the qubits as arranged to a lattice with $\mathcal{S}_i$ coinciding with a certain neighborhood of qubit i (for a finite lattice we may consider periodic boundary conditions). This Hamiltonian may describe a lattice of interacting magnetic dipoles in an external magnetic field or a system of interacting qubits. For some particular arrangements, an analytic solution is known, but in majority of cases a numerical diagonalization of $\hat{H}$ in the $d = 2^N$ Hilbert space is necessary. The model is known for its phase transitions.

▶ Qubits interacting with an oscillator: Rabi and Dicke models

Consider a system composed of (1) 1D harmonic oscillator with the single-quantum energy $\hbar\omega \equiv \varepsilon_1$, described by dimensionless coordinate & momentum operators $\hat{\mathrm{x}} = \frac{\hat{x}}{\sqrt{2\hbar/M\omega}}$ & $\hat{\mathrm{p}} = \frac{\hat{p}}{\sqrt{2\hbar M\omega}}$ (it can be a quantized one-mode field), and (2) set of N qubits (two-level atoms, $\frac{1}{2}$-spins etc.). A possible Hamiltonian is:

$$\hat{H} = \varepsilon_1\left(\hat{\mathrm{p}}^2 + \hat{\mathrm{x}}^2\right) + \frac{\varepsilon_2}{2}\sum_{i=1}^{N}\hat{\sigma}_z^{(i)} - \frac{\kappa}{\sqrt{N}}\,\hat{\mathrm{x}}\sum_{i=1}^{N}\hat{\sigma}_x^{(i)} = \begin{cases} \varepsilon_1\frac{\hat{\mathrm{p}}^2+\hat{\mathrm{x}}^2}{2}\otimes\hat{I} + \varepsilon_2\,\hat{I}\otimes\hat{\mathrm{S}}_z \\ -\frac{\kappa}{\sqrt{N-1}}\,\hat{\mathrm{x}}\otimes\hat{\mathrm{S}}_x \end{cases}$$

The model is solved numerically in a truncated $d = \infty$ Hilbert space. For $N \to \infty$ (this requires the $\frac{1}{\sqrt{N}}$ scaling of the interaction term) the ground state

shows a nonanalytic change from "normal" to "superradiant" phase at some critical coupling κ. The $N = 1$ case is sometimes called the Rabi model.

◂ Historical remark
1925: E. Ising solves the 1D spin model with nearest-neighbor interactions
1944: L. Onsager solves of the 2D square-lattice spin model with $\varepsilon = 0$
1954: R. Dicke presents his schematic model of coherent atom-field interaction
since 2010: experimental realizations of the Dicke model and its quantum effects

3a. COMPATIBLE AND INCOMPATIBLE OBSERVABLES

Operators, in contrast to ordinary numbers and functions used in classical physics, have one revolutionary property: they *may not* be commuting. The product $\hat{A}\hat{B}$ does not have to be the same operator as $\hat{B}\hat{A}$. This property turns out to be of essential importance for physics. For instance, we will see that it is responsible for the key feature of the quantum world: uncertainty.

We introduce the **commutator** of operators,

$$\boxed{[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}} = \begin{cases} 0 & \text{if } \hat{A}\hat{B}=\hat{B}\hat{A} \\ i\hat{C}\neq 0 & \text{if } \hat{A}\hat{B}\neq\hat{B}\hat{A} \end{cases}$$

and rise the relative classification of observables:
(1) compatible observables A, B with $[\hat{A},\hat{B}] = 0$,
(2) incompatible observables A, B with $[\hat{A},\hat{B}] \neq 0$.

■ Compatible observables

We first explore the case when $\hat{A}\hat{B} = \hat{B}\hat{A}$. We show that such commuting operators $\hat{A}$ and $\hat{B}$ can be diagonalized simultaneously, i.e., can be associated with a common set of eigenvectors. A maximal set of commuting operators selects a unique basis in the Hilbert space and in this way creates a particular representation of all physical state vectors and observables–operators.

► $[\hat{A},\hat{B}] = 0 \;\Rightarrow$ eigenspaces of $\hat{B}$ are invariant under the action of $\hat{A}$ and vice versa: $\hat{B}|\psi\rangle = b|\psi\rangle \;\Rightarrow\; \hat{B}\underbrace{(\hat{A}|\psi\rangle)}_{|\psi'\rangle} = \hat{A}\hat{B}|\psi\rangle = b\underbrace{(\hat{A}|\psi\rangle)}_{|\psi'\rangle} \;\Rightarrow\; \hat{A}|\psi\rangle$ is eigenvector of $\hat{B}$ with eigenvalue b

► Commuting operators have a **complete set of common eigenvectors**
Intuitively, this is obvious from the invariance of the eigenspaces $\mathcal{H}_a$ of $\hat{A}$ under the action of $\hat{B}$. The subspace $\mathcal{H}_a$ can therefore be considered as the Hilbert space where operator $\hat{B}$ finds eigenvectors $|b\rangle$.
A more rigorous proof: Let $\{|a_i^{(k)}\rangle\}_{i,k}$ and $\{|b_j^{(l)}\rangle\}_{j,l}$ be orthonormal eigenbases of $\hat{A}$ and $\hat{B}$, respectively (with i, j enumerating the respective eigenvalues a_i and b_j, and k, j the basis vectors in degeneracy subspaces)

Unique expansion: $|a_i^{(k)}\rangle = \sum_j \underbrace{\sum_l \alpha_{ij}^{(kl)} |b_j^{(l)}\rangle}_{|\psi_{ij}^{(k)}\rangle} = \sum_j |\psi_{ij}^{(k)}\rangle$, where: $\hat{B}|\psi_{ij}^{(k)}\rangle = b_j |\psi_{ij}^{(k)}\rangle$

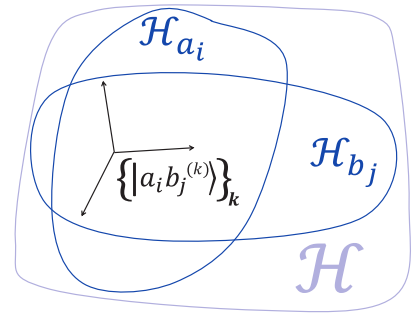
Eigenstate condition reads as: $(\hat{A}-a_i\hat{I})|a_i^{(k)}\rangle = 0 = \sum_j \overbrace{(\hat{A}-a_i\hat{I})|\psi_{ij}^{(k)}\rangle}^{|\tilde{\psi}_{ij}^{(k)}\rangle}$ $\left\{\begin{array}{l}\text{where: } \hat{B}|\tilde{\psi}_{ij}^{(k)}\rangle = b_j|\tilde{\psi}_{ij}^{(k)}\rangle \\ \text{(from invariance of } \mathcal{H}_{b_j} \text{ under } \hat{A})\end{array}\right.$

$|\tilde{\psi}_{ij}^{(k)}\rangle$ with different j orthogonal $\Rightarrow$ the condition satisfied *iff* $|\tilde{\psi}_{ij}^{(k)}\rangle = 0\ \forall j$

$\Rightarrow |\psi_{ij}^{(k)}\rangle$ is a simultaneous eigenvector of $\hat{A}$ and $\hat{B}$ (eigenvalues a_i and b_j)

The same procedure repeated $\forall\ |a_i^{(k)}\rangle \Rightarrow$ the resulting set $\{|\psi_{ij}^{(k)}\rangle\}_{i,j,k}$ of simultaneous eigenvectors is complete since it allows one to expand the basis $\{|a_i^{(k)}\rangle\}_{i,k}$

$\Rightarrow$ There exists a simultaneous orthonormal eigenbasis $\{|a_i b_j{}^{(k)}\rangle\}_{i,j,k}$ of both $\hat{A}$ and $\hat{B}$, where $^{(k)}$ enumerates the states with the same combination of eigenvalues a_i and b_j. In this sense, the observables A and B are *compatible*.



► $\boxed{[\hat{A},\hat{B}]=0 \quad \Leftrightarrow \quad [\hat{P}_{a_i},\hat{P}_{b_j}]=0 \quad \forall\ i,j}$

That means: Operators commute *iff* all their eigenspace projectors commute.

$\Leftarrow$ follows from spectral decompositions: $\hat{A} = \sum_i a_i \hat{P}_{a_i}$ and $\hat{B} = \sum_j b_j \hat{P}_{b_j}$

$\Rightarrow$ follows from $\hat{P}_{a_i} = \sum_{j' \in \mathcal{S}_B^{a_i}} \sum_k |a_i b_{j'}{}^{(k)}\rangle\langle a_i b_{j'}{}^{(k)}|$, $\hat{P}_{b_j} = \sum_{i' \in \mathcal{S}_A^{b_j}} \sum_l |a_{i'} b_j{}^{(l)}\rangle\langle a_{i'} b_j{}^{(l)}|$

$\{\begin{smallmatrix}\mathcal{S}_B^{a_i}\\ \mathcal{S}_A^{b_j}\end{smallmatrix}\} \equiv$ the set of eigenvalues $\{\begin{smallmatrix}b_{j'}\\ a_{i'}\end{smallmatrix}\}$ contained in the eigenspace of $\{\begin{smallmatrix}a_i\\ b_j\end{smallmatrix}\}$

$\hat{P}_{a_i}\hat{P}_{b_j} = \sum_{i',j'}\sum_{k,l} |a_i b_{j'}{}^{(k)}\rangle \underbrace{\langle a_i b_{j'}{}^{(k)}|a_{i'} b_j{}^{(l)}\rangle}_{\delta_{ii'}\delta_{jj'}\delta_{kl}} \langle a_{i'} b_j{}^{(l)}| = \sum_k |a_i b_j{}^{(k)}\rangle\langle a_i b_j{}^{(k)}| = \hat{P}_{b_j}\hat{P}_{a_i}$

► **Complete set of commuting operators (of compatible observables)**

The above conclusions concerning 2 commuting operators can be generalized to an arbitrary number n of mutually commuting operators:

$n=3$: operators $\hat{A},\hat{B},\hat{C}$ satisfying $[\hat{A},\hat{B}]=[\hat{A},\hat{C}]=[\hat{B},\hat{C}]=0 \Rightarrow \exists$ simultaneous orthonormal eigenbasis $\{|a_i b_j c_k{}^{(l)}\rangle\}_{i,j,k,l}$ such that $\left.\begin{smallmatrix}\hat{A}\\ \hat{B}\\ \hat{C}\end{smallmatrix}\right\} |a_i b_j c_k{}^{(l)}\rangle = \left\{\begin{smallmatrix}a_i\\ b_j\\ c_k\end{smallmatrix}\right\} |a_i b_j c_k{}^{(l)}\rangle$

...and analogously for $n>3$

A set of mutually commuting operators $\overbrace{\hat{A},\hat{B},\hat{C}\ldots}^{n}$ is **complete** if eigenvalues $\underbrace{a_i, b_j, c_k \ldots}_{n}$ uniquely determine a *single* eigenvector $|a_i b_j c_k \ldots\rangle$ (no $^{(l)}$ needed)

Consider $\hat{X}$ such that $[\hat{X},\hat{A}] = [\hat{X},\hat{B}] = [\hat{X},\hat{C}] = \cdots = 0$. Then we know that $\hat{X}|a_i b_j c_k \ldots\rangle = x|a_i b_j c_k \ldots\rangle$ and the eigenvalue x is determined by $a_i, b_j, c_k, \ldots$.

$\Rightarrow\ x = f(a,b,c,\ldots) \Rightarrow\ \hat{X} = \sum_{a_i,b_j,c_k\ldots} f(a_i,b_j,c_k\ldots)\hat{P}_{a_i,b_j,c_k\ldots}\ \Rightarrow \boxed{\hat{X} = f(\hat{A},\hat{B},\hat{C},\ldots)}$

$\Rightarrow$ alternative definition of the complete set: Any $\hat{X}$ commuting with all operators from a complete set is a function of these operators.
The number n of operators in a complete set is usually identified with the number f of **quantum degrees of freedom**. Examples: Spinless and structureless particle in 3D has $f = 3 \Rightarrow$ we need 3 commuting operators, e.g. $\{\hat{x}_1, \hat{x}_2, \hat{x}_3\}$, to uniquely determine a basis in $\mathcal{H}$. Structureless particle with spin $\frac{1}{2}$ has $f = 4$, the complete set being, e.g., $\{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{S}_z\}$. $N = 2$ structureless particles with spin $\frac{1}{2}$ have $f = 8$, and so on. Note: the number f is fixed only within a certain *algebra of pre-selected operators* (otherwise any basis in $\mathcal{H}$ can always be considered as the eigenbasis of a single nondegenerate operator).

► **Combining complete sets in a product spaces**

Consider a composite system with Hilbert space $\mathcal{H} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2$

$\underbrace{\{\hat{A}_1, \hat{B}_1, \hat{C}_1 \dots\}}_{n_1} \equiv$ complete set in $\mathcal{H}_1$ $\quad \underbrace{\{\hat{A}_2, \hat{B}_2, \hat{C}_2 \dots\}}_{n_2} \equiv$ complete set in $\mathcal{H}_2$

$$\Rightarrow \underbrace{\left\{\left\{(\hat{A}_1 \otimes \hat{I}), (\hat{B}_1 \otimes \hat{I}), (\hat{C}_1 \otimes \hat{I}) \dots\right\}, \left\{(\hat{I} \otimes \hat{A}_2), (\hat{I} \otimes \hat{B}_2), (\hat{I} \otimes \hat{C}_2) \dots\right\}\right\}}_{n_1+n_2} \equiv \textbf{complete set in } \mathcal{H} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2$$

$\boxed{[\hat{X}_1 \otimes \hat{I}, \hat{I} \otimes \hat{Y}_2] = 0}\ \forall \hat{X}_1, \hat{Y}_2$ (the same eigenvalues as the original sets)

$\Rightarrow$ the total number of degrees of freedom: $f = f_1 + f_2$

■ Incompatible observables

We turn to the case $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. Such observables show mutual incompatibility: they both cannot simultaneously take exact values in any state. An increasing precision of the determination of observable $\hat{A}$ reduces the precision for observable $\hat{B}$ and vice versa. This is the celebrated quantum uncertainty relation.

► $\boxed{\boxed{[\hat{A}, \hat{B}] = i\hat{C}}} \neq 0$ with $\boxed{\hat{C} = \hat{C}^\dagger}$ for $\hat{A} = \hat{A}^\dagger$ and $\hat{B} = \hat{B}^\dagger$

$(i\hat{C})^\dagger = (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = [\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}] = -i\hat{C} \quad \Rightarrow \hat{C} = \hat{C}^\dagger$

► **Uncertainty relation**

$$\boxed{\underbrace{[\langle A^2\rangle_\psi - \langle A\rangle_\psi^2]}_{\langle\langle A^2\rangle\rangle_\psi} \underbrace{[\langle B^2\rangle_\psi - \langle B\rangle_\psi^2]}_{\langle\langle B^2\rangle\rangle_\psi} \geq \tfrac{1}{4} \underbrace{\langle\psi|\hat{C}|\psi\rangle^2}_{\langle C\rangle_\psi^2}}$$

The right-hand side, which is the lower bound of the product of dispersions, depends on $|\psi\rangle$.

Proof:

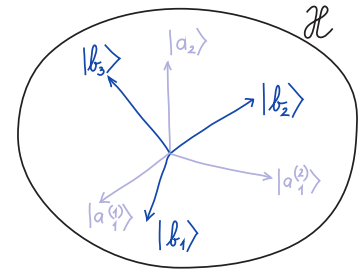
$[\langle A^2\rangle_\psi - \langle A\rangle_\psi^2] = \langle\psi|[\hat{A} - \langle A\rangle_\psi\hat{I}]^2|\psi\rangle = \langle\varphi|\varphi\rangle \quad$ with $|\varphi\rangle = [\hat{A} - \langle A\rangle_\psi\hat{I}]|\psi\rangle$

$[\langle B^2\rangle_\psi - \langle B\rangle_\psi^2] = \langle\psi|[\hat{B} - \langle B\rangle_\psi\hat{I}]^2|\psi\rangle = \langle\chi|\chi\rangle \quad$ with $|\chi\rangle = [\hat{B} - \langle B\rangle_\psi\hat{I}]|\psi\rangle$

$$\langle\langle A^2\rangle\rangle_\psi \langle\langle B^2\rangle\rangle_\psi = \langle\varphi|\varphi\rangle\langle\chi|\chi\rangle \geq |\langle\varphi|\chi\rangle|^2 = \left|\langle\psi|[\hat{A} - \langle A\rangle_\psi\hat{I}][\hat{B} - \langle B\rangle_\psi\hat{I}]|\psi\rangle\right|^2 =$$

$$\left|\langle\psi|\hat{A}\hat{B}|\psi\rangle - \langle A\rangle_\psi\langle B\rangle_\psi\right|^2 = \left|\langle\psi|\tfrac{\hat{A}\hat{B}+\hat{B}\hat{A}}{2}|\psi\rangle + \langle\psi|\underbrace{\tfrac{\hat{A}\hat{B}-\hat{B}\hat{A}}{2}}_{\frac{i}{2}\hat{C}}|\psi\rangle - \langle A\rangle_\psi\langle B\rangle_\psi\right|^2$$

$$\geq \tfrac{1}{4}\langle\psi|\hat{C}|\psi\rangle^2 \equiv \left[\tfrac{1}{2}\langle C\rangle_\psi\right]^2$$



This means that non-commuting operators $\hat{A}, \hat{B}$ cannot be diagonalized simultaneously. The more precisely we know one of the observables, the less precisely we can know the other.

■ Analogy with Poisson brackets

Although incompatible observables (with non-commuting operators) are genuinely quantum invention, there exists a surprising parallel of this behavior in classical mechanics. It is based on algebraic properties of Poisson brackets. The following paragraph may alter our perspective on quantum physics: Perhaps it is not as alien as it seemed to be, perhaps it results from a specific generalization of the mathematics involved already in the classical description. We will partially return to these issues in Sec. 8.

▸ Some properties of commutators

For arbitrary operators $\hat{A}, \hat{B}, \hat{C}, \hat{A}', ...$ and complex constants $a, b, c, a', ...$ we can easily prove the following relations:

(a) Basic $[\hat{A},\hat{B}]=-[\hat{B},\hat{A}] \quad [\hat{A},a\hat{I}]=0$

(b) Sums $\begin{matrix}[a\hat{A}+a'\hat{A}',\hat{B}]=a[\hat{A},\hat{B}]+a'[\hat{A}',\hat{B}]\\ [\hat{A},b\hat{B}+b'\hat{B}']=b[\hat{A},\hat{B}]+b'[\hat{A},\hat{B}']\end{matrix}$

(c) Products $\boxed{\begin{matrix}[\hat{A}\hat{A}',\hat{B}]=\hat{A}[\hat{A}',\hat{B}]+[\hat{A},\hat{B}]\hat{A}'\\ [\hat{A},\hat{B}\hat{B}']=\hat{B}[\hat{A},\hat{B}']+[\hat{A},\hat{B}]\hat{B}'\end{matrix}}$

(d) Jacobi identity $\boxed{[\hat{A},[\hat{B},\hat{C}]]+[\hat{B},[\hat{C},\hat{A}]]+[\hat{C},[\hat{A},\hat{B}]]=0}$

▸ **Poisson bracket** for classical observables A and B in f degrees of freedom: We have $A \equiv A(p_1...p_f, q_1...q_f)$ and $B \equiv B(p_1...p_f, q_1...q_f)$ and define

$$\boxed{\{A,B\} \equiv \sum_{i=1}^{f}\left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i}\frac{\partial A}{\partial p_i}\right)}$$

Note: alternative definition with $p_i \leftrightarrow q_i$ would yield the opposite sign of the Poisson bracket

Properties of Poisson brackets are analogous to those of commutators:

(a) Basic $\{A,B\}=-\{B,A\}, \quad \{A,a\}=0$

(b) Sums $\begin{matrix}\{aA+a'A',B\}=a\{A,B\}+a'\{A',B\}\\ \{A,bB+b'B'\}=b\{A,B\}+b'\{A,B'\}\end{matrix}$

(c) Products $\begin{matrix}\{AA',B\}=A\{A',B\}+\{A,B\}A'\\ \{A,BB'\}=B\{A,B'\}+\{A,B\}B'\end{matrix}$

(d) Jacobi ident. $\{A,\{B,C\}\}+\{B,\{C,A\}\}+\{C,\{A,B\}\}=0$

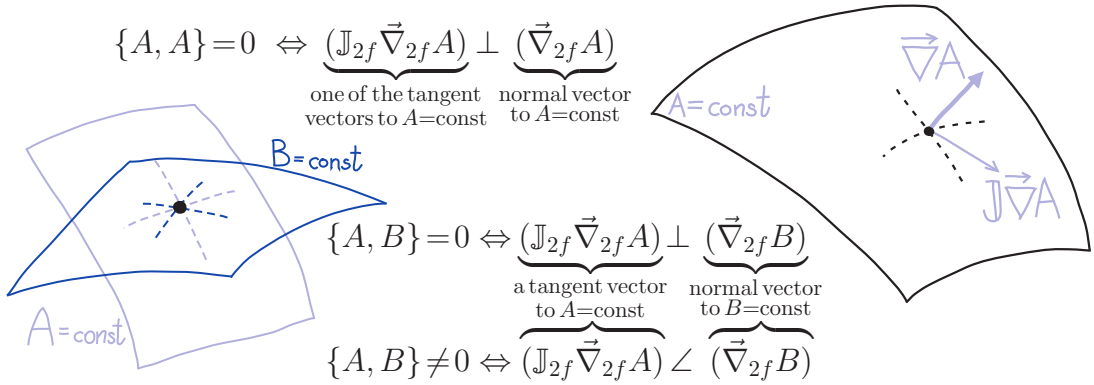
▸ **Geometrical meaning** of Poisson bracket

$$\{A,B\} = \underbrace{\left(-\frac{\partial A}{\partial p_1},...-\frac{\partial A}{\partial p_f},+\frac{\partial A}{\partial q_1},...+\frac{\partial A}{\partial q_f}\right)}_{\boxed{\mathbb{J}_{2f}\vec{\nabla}_{2f}A \text{ vector} \perp \text{to gradient}}} \cdot \underbrace{\left(\frac{\partial B}{\partial q_1},...\frac{\partial B}{\partial q_f},\frac{\partial B}{\partial p_1},...\frac{\partial B}{\partial p_f}\right)}_{\boxed{\vec{\nabla}_{2f}B \text{ gradient}}}$$

ordinary scalar product of two $2f$-dim vectors in the phase space

$\mathbb{J}_{2f} \equiv \begin{pmatrix} 0 & -I_f \\ +I_f & 0 \end{pmatrix}$ is the *symplectic matrix* in dim. $2f$ ($I_f \equiv$ unit matrix in dim. f)

$$\{A,A\}=0 \;\Leftrightarrow\; \underbrace{(\mathbb{J}_{2f}\vec{\nabla}_{2f}A)}_{\text{one of the tangent vectors to } A=\text{const}} \perp \underbrace{(\vec{\nabla}_{2f}A)}_{\text{normal vector to } A=\text{const}}$$



$$\{A,B\}=0 \Leftrightarrow \underbrace{(\mathbb{J}_{2f}\vec{\nabla}_{2f}A)}_{\text{a tangent vector to } A=\text{const}} \perp \underbrace{(\vec{\nabla}_{2f}B)}_{\text{normal vector to } B=\text{const}}$$

$$\{A,B\}\neq 0 \Leftrightarrow (\mathbb{J}_{2f}\vec{\nabla}_{2f}A) \angle (\vec{\nabla}_{2f}B)$$

$$\Rightarrow \boxed{\begin{array}{lcl} \{A,B\}=0 & \Rightarrow & \text{hypersurfaces } A\text{=const \& } B\text{=const locally coincide} \\ \{A,B\}\neq 0 & \Rightarrow & \text{hypersurfaces } A\text{=const \& } B\text{=const locally deviate} \end{array}}$$

The geometric view of Poisson brackets has consequences for classical statistical physics, when one deals with statistical ensembles of systems in different classical states, i.e., delocalized probability distributions in the phase space $(q_1...q_f, p_1...p_f) \equiv (\boldsymbol{q},\boldsymbol{p})$ instead of single points in that space. In such a statistical ensemble, any physical quantity A does not in general take a single value a, but shows a certain statistical distribution of possible a's. Assume a statistical ensemble with the phase-space probability distribution $\rho(\boldsymbol{q},\boldsymbol{p})$ spread to various directions around a point $(\boldsymbol{q}_0,\boldsymbol{p}_0)$ in the phase space. From the above geometrical considerations it follows that, in this ensemble, the quantities A and B *cannot* both take sharp values if $\{A,B\}\neq 0$ at the point $(\boldsymbol{q}_0,\boldsymbol{p}_0)$. This can be considered as a *classical analog* of quantum uncertainty, though no relations for the lower bounds of the uncertainty exist in the classical case.

▸ Dirac quantization assumption

The importance of Poisson brackets for quantum theory is codified by this essential postulate: Consider arbitrary observables A, B and C expressed by classical phase-space functions $A(\boldsymbol{q},\boldsymbol{p})$, $B(\boldsymbol{q},\boldsymbol{p})$ and $C(\boldsymbol{q},\boldsymbol{p})$ and by quantum operators $\hat{A}$, $\hat{B}$ and $\hat{C}$, respectively. These entities must satisfy the following relation between the Poisson brackets and the corresponding commutators:

$$\{A,B\}=C \quad \text{(classical)} \quad \Rightarrow \quad [\hat{A},\hat{B}]=i\hbar\hat{C} \quad \text{(quantum)}$$

Note that the $\Leftarrow$ implication does *not* in general hold as some quantum systems (e.g., spin-$\frac{1}{2}$ particles) have no classical counterparts.

■ Equivalent representations of quantum mechanics

A fascinating feature of physical description is that it can be cast in infinitely many equivalent ways. In other words, there exists a multitude of mathematical representations yielding the same observable output. In classical mechanics,

this feature is anchored in the concept of canonical transformations. In quantum mechanics, the equivalent descriptions follow from the use of various Hilbert-space bases, which may be generated by alternative complete sets of observables.

▶ Discrete representations

Any complete set of commuting operators $\{\hat{A}, \hat{B}, \dots\}$ with discrete spectra generates a countable orthonormal basis $\{|i\rangle\}_{i=1}^{d_\mathcal{H}}$ of $\mathcal{H}$.
State vectors are then represented by $\mathbb{C}^{d_\mathcal{H}}$ "columns"
and operators by $d_\mathcal{H} \times d_\mathcal{H}$ complex matrices
(both finite & infinite cases included):

$$\boxed{\sum_{i=1}^{d_\mathcal{H}} |i\rangle\langle i| = \hat{I}_\mathcal{H} \qquad \langle i|j\rangle = \delta_{ij}}$$

$$|\psi\rangle = \sum_i |i\rangle\langle i|\psi\rangle = \sum_i \underbrace{\langle i|\psi\rangle}_{\psi_i} |i\rangle \qquad \Rightarrow \qquad \boxed{|\psi\rangle \equiv \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}}$$

$$|\psi'\rangle = \hat{A}|\psi\rangle \qquad \sum_i |i\rangle \overbrace{\langle i|\psi'\rangle}^{\psi'_i} = \sum_i \sum_j |i\rangle \overbrace{\langle i|\hat{A}|j\rangle}^{A_{ij}} \overbrace{\langle j|\psi\rangle}^{\psi_j} \qquad \Rightarrow \qquad \psi'_i = \sum_j A_{ij}\psi_j$$

$$\boxed{\begin{pmatrix} \psi'_1 \\ \psi'_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}}$$

▶ Continuous representations

For a complete set $\{\hat{A}, \hat{B}, \dots\}$ with continuous spectra there exists a continuous "orthonormal basis" $\{|x\rangle\}_{x\in\mathcal{D}} \in \overline{\mathcal{H}}$ (with $\mathcal{D}$ being some relevant domain of generally a multidimensional variable x).
State vectors are then represented by wavefunctions
and operators by kernels of integral transformations:

$$\boxed{\int\limits_{x\in\mathcal{D}} |x\rangle\langle x| dx = \hat{I}_{\overline{\mathcal{H}}} \qquad \langle x|x'\rangle = \delta(x-x')}$$

$$|\psi\rangle = \int |x\rangle\langle x|\psi\rangle\, dx = \int \underbrace{\langle x|\psi\rangle}_{\psi(x)} |x\rangle\, dx \qquad \Rightarrow \qquad \boxed{|\psi\rangle \equiv \psi(x)}$$

$$|\psi'\rangle = \hat{A}|\psi\rangle \qquad \int dx\, |x\rangle \overbrace{\langle x|\psi'\rangle}^{\psi'(x)} = \int dx \int dx'\, |x\rangle \overbrace{\langle x|\hat{A}|x'\rangle}^{A(x,x')} \overbrace{\langle x'|\psi\rangle}^{\psi(x')} \qquad \Rightarrow \qquad \boxed{\psi'(x) = \int A(x,x')\,\psi(x')\,dx'}$$

▶ Mixed representations

A complete set $\{\hat{A}, \hat{B}, \dots\}$ with mixed discrete and continuous spectra generates a combined dis.-cont. "orthonormal basis"
$\{|i,x\rangle\}_{\substack{i\in\mathcal{D}_i \\ x\in\mathcal{D}_x}} \in \overline{\mathcal{H}}$ (with $\mathcal{D}_i, \mathcal{D}_x$ some domains).
State vectors are represented (finite/infinite)
"columns" of wavefunction components and operators
by kernes of matrix-integral transformations:

$$\boxed{\sum_{i\in\mathcal{D}_i} \int\limits_{\mathcal{D}_x} |i,x\rangle\langle i,x|\, dx = \hat{I}_{\overline{\mathcal{H}}} \qquad \langle i,x|i',x'\rangle = \delta_{ii'}\delta(x-x')}$$

$$|\psi\rangle = \sum_{i\in\mathcal{D}_i} \int\limits_{\mathcal{D}_x} dx\, |i,x\rangle \underbrace{\langle i,x|\psi\rangle}_{\psi_i(x)} \qquad \Rightarrow \qquad \boxed{|\psi\rangle \equiv \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \vdots \end{pmatrix}}$$

$$|\psi'\rangle = \hat{A}|\psi\rangle \qquad \sum_i \int dx\, |i,x\rangle \overbrace{\langle i,x|\psi'\rangle}^{\psi'_i(x)} = \sum_i \sum_j \int dx \int dx'\, |i,x\rangle \overbrace{\langle i,x|\hat{A}|j,x'\rangle}^{A_{ij}(x,x')} \overbrace{\langle j,x'|\psi\rangle}^{\psi_j(x')}$$

$$\Rightarrow \qquad \boxed{\begin{pmatrix} \psi_1'(x) \\ \psi_2'(x) \\ \vdots \end{pmatrix} = \int \begin{pmatrix} A_{11}(x,x') & A_{12}(x,x') & \dots \\ A_{21}(x,x') & A_{22}(x,x') & \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} \psi_1(x') \\ \psi_2(x') \\ \vdots \end{pmatrix} dx'}$$

◀ Historical remark
1925-26: M. Born, W. Heisenberg, P. Jordan write commutation relations between various observables (matrix mechanics) and introduce the concept of compatibility
1927: P. Jordan, P. Dirac attempt to introduce canonical transformations to QM
1927: John von Neumann formulates the concept of complete sets of observables and associates "canonical transformations" with different choices of this set
1927: Werner Heisenberg writes down the $\Delta x \Delta p$ uncertainty relation
1928: E.H. Kennard and H. Weyl derive the uncertainty relation from the commutator, generalization $\forall$ incompatible observables by H.P. Robertson in 1929
1930: P. Dirac relates commutators to Poisson brackets ($\Rightarrow$ canonical quantization)

3b. EXAMPLES OF OBSERVABLE SETS

We now apply the results of the previous section to the single-particle operators introduced in Sec. 2.b. In particular, the algebra of coordinate and momentum operators and that of angular momentum operators will be investigated. Representations of the single-particle Hilbert space will be built using these operators.

■ Coordinate & momentum

Coordinate and momentum operators satisfy the commonly known commutation relation—a twin of the canonical Poisson bracket of classical mechanics. It leads to the familiar form of the uncertainty relation but also to the problems of $\hat{\vec{x}}$ and $\hat{\vec{p}}$ in the ordinary Hilbert space (see Sec. 2.a). The $\hat{\vec{x}}$ & $\hat{\vec{p}}$ operators allow one to assemble a plethora of composite operators, including the oscillator ladder operators whose action depends on some specific commutation relations.

► Canonical commutation relations

From the known form of the coordinate & momentum operators we immediately get the corresponding commutators:

$\hat{x}_i \equiv x_i \cdot \qquad \hat{p}_i \equiv -i\hbar\frac{\partial}{\partial x_i} \qquad \Rightarrow \qquad \boxed{[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0, \quad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}\hat{I}}$

consistent with Poisson brackets: $\{x_i, x_j\} = \{p_i, p_j\} = 0, \quad \{x_i, p_j\} = \delta_{ij}$

These relations define general **canonically conjugate quantities**

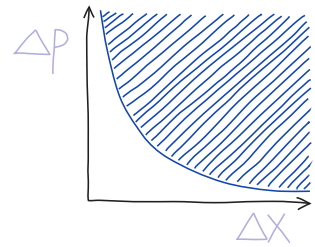
Note: The same commutation relations can also be satisfied with:

$\hat{x}_i \equiv x_i \cdot \qquad \hat{p}_i \equiv -i\hbar\frac{\partial}{\partial x_i} + f(\vec{x})$ where $f(\vec{x})$ is any differentiable function.

▸ Heisenberg uncertainty relation

From the general form $\langle\langle A^2\rangle\rangle_\psi \langle\langle B^2\rangle\rangle_\psi \geq \frac{1}{4}\langle C\rangle^2_\psi$ we obtain: $\underbrace{\langle\langle x_i^2\rangle\rangle_\psi}_{(\Delta x_i)^2}\underbrace{\langle\langle p_j^2\rangle\rangle_\psi}_{(\Delta p_j)^2} \geq \frac{1}{4}\langle\psi|\underbrace{\hbar\delta_{ij}\hat{I}}_{\hat{C}}|\psi\rangle^2 = \frac{\hbar^2}{4}\delta_{ij}$

Hence for any state $|\psi\rangle$ we can write: $\boxed{\Delta x_i \Delta p_i \geq \frac{\hbar}{2}}$



▸ Some general consequences

(a) Operators $\hat{x}_i$ and $\hat{p}_i$ *cannot* be represented in $\mathcal{H}$ of a *finite dimension* d.

To show this, we introduce the **trace of an operator**:

$$\mathrm{Tr}\,\hat{A} = \sum_{\substack{i \\ \text{arbitrary basis}}} \underbrace{\langle\phi_i|\hat{A}|\phi_i\rangle}_{A_{ii}} = \sum_i \sum_{k=1}^{d_i} \langle a_i^{(k)}|\hat{A}|a_i^{(k)}\rangle = \sum_i d_i a_i$$

The independence on the choice of basis:

$$\sum_i \langle\phi_i'|\hat{A}|\phi_i'\rangle = \sum_{i,j,k} \langle\phi_i'|\phi_j\rangle\langle\phi_j|\hat{A}|\phi_k\rangle\langle\phi_k|\phi_i'\rangle = \sum_{j,k} \overbrace{\langle\phi_k|\hat{I}|\phi_j\rangle}^{\delta_{kj}}\langle\phi_j|\hat{A}|\phi_k\rangle = \sum_j \langle\phi_j|\hat{A}|\phi_j\rangle$$

Another property:

$$\mathrm{Tr}(\hat{A}\hat{B}) = \sum_i \langle\phi_i|\hat{A}\hat{B}|\phi_i\rangle = \sum_{i,j}\langle\phi_i|\hat{A}|\phi_j\rangle\langle\phi_j|\hat{B}|\phi_i\rangle = \sum_{j,i}\langle\phi_j|\hat{B}|\phi_i\rangle\langle\phi_i|\hat{A}|\phi_j\rangle = \mathrm{Tr}(\hat{B}\hat{A})$$

For coordinate and momentum operators represented in a finite dimension d, this relation yields a contradiction: $\mathrm{Tr}[\hat{x}_i, \hat{p}_i] = 0 \neq \mathrm{Tr}(i\hbar\hat{I}_d) = i\hbar d$

However, there exist various $d = \infty$ *discrete representations* of $\hat{x}$ and $\hat{p}$, e.g., the one obtained in the basis of 1D harmonic oscillator:

$$\hat{x} = \sqrt{\tfrac{\hbar}{2M\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ \vdots & & \ddots & \ddots & \ddots & \end{pmatrix} \qquad \hat{p} = \sqrt{\tfrac{M\hbar\omega}{2}}\begin{pmatrix} 0 & -i\sqrt{1} & 0 & 0 & 0 & \dots \\ i\sqrt{1} & 0 & -i\sqrt{2} & 0 & 0 & \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & 0 & \\ 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{4} & \\ \vdots & & \ddots & \ddots & \ddots & \end{pmatrix}$$

(b) *Eigenvectors* of $\hat{x}_i$ and $\hat{p}_i$ are *out of* $\mathcal{H}$ (more precisely: $\nexists$ within $\mathcal{H}$).

Assume coordinate eigenstate $|x_i\rangle \in \mathcal{H}$ satisfying $\langle x_i|x_i\rangle = 1$. From the r.h.s. of the commutation relation we get: $\langle x_i|[\hat{x}_i, \hat{p}_i]|x_i\rangle = i\hbar$. But we simultaneously have $\langle x_i|[\hat{x}_i, \hat{p}_i]|x_i\rangle = x_i\langle x_i|\hat{p}_i|x_i\rangle - x_i\langle x_i|\hat{p}_i|x_i\rangle = 0$, which is a contradiction.

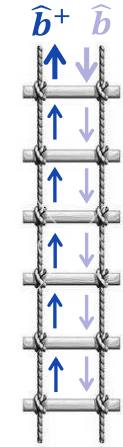
▸ Oscillator and general ladder operators

We return to the 1D harmonic oscillator: $\hat{H} = \frac{1}{2M}\hat{p}^2 + \frac{M\omega^2}{2}\hat{x}^2$. Using dimensionless coordinate $\hat{\mathrm{x}} = \frac{1}{\sqrt{2\hbar/M\omega}}\hat{x}$ and momentum $\hat{\mathrm{p}} = \frac{1}{\sqrt{2\hbar M\omega}}\hat{p}$ with the commutation relation $[\hat{\mathrm{x}}, \hat{\mathrm{p}}] = \frac{i}{2}\hat{I}$ we express the dimensionless Hamiltonian $\hat{\mathrm{H}} = \frac{1}{\hbar\omega}\hat{H}$:

$$\hat{\mathrm{H}} = \hat{\mathrm{x}}^2 + \hat{\mathrm{p}}^2 = \underbrace{(\hat{\mathrm{x}} - i\hat{\mathrm{p}})}_{\hat{b}^\dagger}\underbrace{(\hat{\mathrm{x}} + i\hat{\mathrm{p}})}_{\hat{b}} - i\underbrace{(\hat{\mathrm{x}}\hat{\mathrm{p}} - \hat{\mathrm{p}}\hat{\mathrm{x}})}_{[\hat{\mathrm{x}},\hat{\mathrm{p}}]} = \hat{b}^\dagger\hat{b} + \tfrac{1}{2}$$

The $\hat{b}$ and $\hat{b}^\dagger$ operators satisfy the mutual commutation relation $\boxed{[\hat{b},\hat{b}^\dagger]=\hat{I}}$

We also get: $\boxed{[\hat{\mathtt{H}},\hat{b}^\dagger]=+\hat{b}^\dagger,\quad [\hat{\mathtt{H}},\hat{b}]=-\hat{b}.}$



Let $|n\rangle$ be an eigenstate of $\hat{\mathtt{H}}$ with eigenvalue $\boxed{\mathtt{E}_n=n+\frac{1}{2}}$, where n is yet an unknown eigenvalue of $\hat{b}^\dagger\hat{b}$. So we have $\hat{\mathtt{H}}|n\rangle=\mathtt{E}_n|n\rangle$ and:

$$\left.\begin{aligned}\hat{\mathtt{H}}\,\hat{b}^\dagger|n\rangle&=(\hat{b}^\dagger\,\hat{\mathtt{H}}+\hat{b}^\dagger)\,|n\rangle=\overbrace{(\mathtt{E}_n+1)}^{\mathtt{E}_{n+1}}\,\hat{b}^\dagger|n\rangle\\ \hat{\mathtt{H}}\,\hat{b}\;|n\rangle&=(\hat{b}\;\hat{\mathtt{H}}-\hat{b}\;)\,|n\rangle=\underbrace{(\mathtt{E}_n-1)}_{\mathtt{E}_{n-1}}\,\hat{b}\;|n\rangle\end{aligned}\right\}\Rightarrow\left\{\begin{aligned}\hat{b}^\dagger|n\rangle&=c_\uparrow(n)|n+1\rangle\\ \hat{b}\;|n\rangle&=c_\downarrow(n)|n-1\rangle\end{aligned}\right.$$

with $c_\uparrow(n),c_\downarrow(n)\in\mathbb{R}$ some normalization constants

$$\begin{aligned}c_\uparrow(n)^2\overbrace{\langle n+1|n+1\rangle}^{1}&=\langle n|\hat{b}\hat{b}^\dagger|n\rangle=\langle n|\hat{b}^\dagger\hat{b}+1|n\rangle=n+1 &&\Rightarrow c_\uparrow(n)=\sqrt{n+1}\\ c_\downarrow(n)^2\underbrace{\langle n-1|n-1\rangle}_{1}&=\langle n|\hat{b}^\dagger\hat{b}|n\rangle=n &&\Rightarrow c_\downarrow(n)=\sqrt{n}\end{aligned}$$

Since we know that $\mathtt{E}_n\geq 0$, there must exist a value $n_{\min}$ such that $\hat{b}|n_{\min}\rangle=0$ and from the above $c_\downarrow$ we get $n_{\min}=0$. So the 1D oscillator spectrum $\mathtt{E}_n=n+\frac{1}{2}$ is given by values $n=0,1,2,3,\ldots$

The harmonic oscillator ladder operators $\hat{b}^\dagger$ and $\hat{b}$ represent a special case of more **general ladder (shift) operators**:

If $\hat{A}$ is a Hermitian operator and $\hat{T}_\Delta$ satisfies: $\boxed{\begin{aligned}[\hat{A},\hat{T}_\Delta^\dagger]&=+\Delta\hat{T}_\Delta^\dagger\\ [\hat{A},\hat{T}_\Delta]&=-\Delta\hat{T}_\Delta\end{aligned}}$ $\Delta\in\mathbb{R}$ $\Delta>0$ without loss of generality

then:

$$\hat{A}|a\rangle=a|a\rangle\quad\Rightarrow\left\{\begin{aligned}\hat{A}(\hat{T}_\Delta^\dagger|a\rangle)&=(a+\Delta)(\hat{T}_\Delta^\dagger|a\rangle)\\ \hat{A}(\hat{T}_\Delta|a\rangle)&=(a-\Delta)(\hat{T}_\Delta|a\rangle)\end{aligned}\right.$$

So the Hermitian conjugate operator $\hat{T}_\Delta^\dagger$ and $\hat{T}_\Delta$ shift eigenstates of $\hat{A}$ by values $+\Delta$ and $-\Delta$, respectively:

$$\boxed{\begin{aligned}\hat{T}_\Delta^\dagger|a\rangle&=c_\uparrow(a)|a+\Delta\rangle\quad\text{with}\quad c_\uparrow(a)=\sqrt{\langle a|\hat{T}_\Delta\hat{T}_\Delta^\dagger|a\rangle}\\ \hat{T}_\Delta|a\rangle&=c_\downarrow(a)|a-\Delta\rangle\quad\text{with}\quad c_\downarrow(a)=\sqrt{\langle a|\hat{T}_\Delta^\dagger\hat{T}_\Delta|a\rangle}\end{aligned}}$$

▶ Canonical & mechanical momentum of particle in elmg. field

Classical Hamiltonian $H=\frac{1}{2M}[\vec{p}-q\vec{A}(\vec{x})]^2+qV(\vec{x})$ with $\vec{p}\equiv$ canonical momentum

Mechanical momentum $\vec{\pi}$ defined through velocity: $\dot{\vec{x}}=\frac{\partial H}{\partial\vec{p}}=\frac{1}{M}\underbrace{[\vec{p}-q\vec{A}(\vec{x})]}_{\vec{\pi}}$

In QM, the operators of canonical & mechanical momenta can be expressed as: $\boxed{\hat{\vec{p}}=-i\hbar\vec{\nabla}}$ & $\boxed{\hat{\vec{\pi}}=-i\hbar\vec{\nabla}-q\vec{A}(\vec{x})}$

While the canonical momenta have canonical commutation relations, the commutators of mechanical momenta depend on the magnetic field:

$$[\hat{\pi}_i,\hat{\pi}_j]=\underbrace{[\hat{p}_i,\hat{p}_j]}_{0}-q[\hat{p}_i,\hat{A}_j]-q[\hat{A}_i,\hat{p}_j]+q^2\underbrace{[\hat{A}_i,\hat{A}_j]}_{0}=i\hbar q\underbrace{\left(\frac{\partial A_j}{\partial x_i}-\frac{\partial A_i}{\partial x_j}\right)}_{\varepsilon_{ijk}B_k}$$

$\boxed{[\hat{\pi}_i,\hat{\pi}_j]=i\hbar q\,\varepsilon_{ijk}B_k(\vec{x})}$ $\Rightarrow$ incompatible velocity components for $\vec{B}\neq 0$

■ Coordinate & momentum representations

Although coordinate and momentum operators are not entirely free of troubles (the corresponding eigenstates dwelling somewhere outside the ordinary Hilbert space), the most familiar representations of quantum mechanics are based on these operators. For the sake of simplicity, we restrict ourselves to the 1D case.

▸ Coordinate representation in 1D

The state vector $|\psi\rangle = \int dx\, \langle x|\psi\rangle |x\rangle$ described by wavefunction $\boxed{\psi(x) \equiv \langle x|\psi\rangle}$

Scalar product: $\langle\psi|\psi'\rangle = \int dx\, \langle\psi|x\rangle\langle x|\psi'\rangle = \int dx\, \psi(x)^*\, \psi'(x)$
Position operator: $\hat{x}\psi(x) = x\psi(x)$
Momentum operator: $\hat{p}\psi(x) = -i\hbar\frac{d}{dx}\psi(x)$
} expressions used so far

Strictly, all these relations (as well as those below) should be restricted only to $|\psi\rangle \in \underline{\mathcal{H}}$ (a dense subset of $\mathcal{H}$)

▸ Momentum representation in 1D

The state vector $|\psi\rangle = \int dp\, \langle p|\psi\rangle |p\rangle$ described by wavefunction $\boxed{\tilde{\psi}(p) \equiv \langle p|\psi\rangle}$

One gets expressions analogous (complementary) to the x-representation:

Scalar product: $\langle\psi|\psi'\rangle = \int dp\, \langle\psi|p\rangle\langle p|\psi'\rangle = \int dp\, \tilde{\psi}(p)^*\, \tilde{\psi}'(p)$

Momentum operator: $\hat{p}\tilde{\psi}(p) = \langle p|\hat{p}|\psi\rangle = p\langle p|\psi\rangle \quad \Rightarrow \quad \boxed{\hat{p}\,\tilde{\psi}(p) = p\,\tilde{\psi}(p)}$

Position operator: $\hat{x}\tilde{\psi}(p) = \langle p|\hat{x}|\psi\rangle = \int \underbrace{\langle p|\hat{x}|p'\rangle}_{X(p,p')} \underbrace{\langle p'|\psi\rangle}_{\tilde{\psi}(p')}\, dp' =$

$= \iiint \overbrace{\langle p|x\rangle}^{\frac{1}{\sqrt{2\pi\hbar}}e^{-i\frac{px}{\hbar}}} \overbrace{\langle x|\hat{x}|x'\rangle}^{x\delta(x-x')} \overbrace{\langle x'|p'\rangle}^{\frac{1}{\sqrt{2\pi\hbar}}e^{+i\frac{p'x'}{\hbar}}} \tilde{\psi}(p')\, dx\, dx'\, dp' = \frac{1}{2\pi\hbar}\iint \overbrace{xe^{i\frac{(p'-p)x}{\hbar}}}^{i\hbar\frac{d}{dp}e^{i\frac{(p'-p)x}{\hbar}}} \tilde{\psi}(p')\, dx\, dp'$

$= \frac{i}{2\pi}\frac{d}{dp}\int \underbrace{\int e^{i\frac{(p'-p)x}{\hbar}} dx}_{2\pi\hbar\delta(p'-p)} \tilde{\psi}(p')\, dp' = i\hbar\frac{d}{dp}\tilde{\psi}(p) \quad \Rightarrow \quad \boxed{\hat{x}\tilde{\psi}(p) = +i\hbar\frac{d}{dp}\tilde{\psi}(p)}$

▸ Links between x & p-representations: Fourier transformation

Relations between eigenstates:

	coordinate rep.	momentum rep.
$\|x'\rangle$	$\delta(x-x')$	$\frac{1}{\sqrt{2\pi\hbar}}\, e^{-ix'p/\hbar}$
$\|p'\rangle$	$\frac{1}{\sqrt{2\pi\hbar}}\, e^{+ip'x/\hbar}$	$\delta(p-p')$

Relations between general states:

$$\langle p|\psi\rangle = \int_{-\infty}^{+\infty} \underbrace{\langle p|x\rangle}_{\frac{1}{\sqrt{2\pi\hbar}}e^{-i\frac{px}{\hbar}}} \underbrace{\langle x|\psi\rangle}_{\psi(x)}\, dx = \boxed{\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{-i\frac{px}{\hbar}}\, \psi(x)\, dx = \tilde{\psi}(p)}$$

$$\langle x|\psi\rangle = \int_{-\infty}^{+\infty} \underbrace{\langle x|p\rangle}_{\frac{1}{\sqrt{2\pi\hbar}}e^{+i\frac{px}{\hbar}}} \underbrace{\langle p|\psi\rangle}_{\tilde{\psi}(p)}\, dp = \boxed{\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{+i\frac{px}{\hbar}}\, \tilde{\psi}(p)\, dp = \psi(x)}$$

In the **3D case**, the above expressions must be modified by the following substitutions: $\boxed{\frac{1}{\sqrt{2\pi\hbar}} \to \frac{1}{(2\pi\hbar)^{3/2}} \qquad \begin{matrix} dx \to d\vec{x} \\ dp \to d\vec{p} \end{matrix} \qquad p\,x \to \vec{p}\cdot\vec{x}}$

► Gaussian wavepackets

These represent a family of well behaved wavefunctions ($\in \mathcal{H}$) suitable for the description of particles partially localized in both coordinate & momentum spaces. They are defined as states whose probability density $\rho(p) \equiv |\tilde{\psi}(p)|^2$ in momentum space has the Gaussian form with average p_0 and width σ_p. The corresponding probability distribution $\rho(x) \equiv |\psi(x)|^2$ in the coordinate space is also a Gaussian whose width σ_x is connected to σ_p via the uncertainty relation.

$\boxed{\tilde{\psi}(p) = \frac{1}{(2\pi\sigma_p^2)^{\frac{1}{4}}} e^{-\frac{(p-p_0)^2}{4\sigma_p^2}}}$ normalization: $\int_{-\infty}^{+\infty} |\tilde{\psi}(p)|^2\, dp = 1$

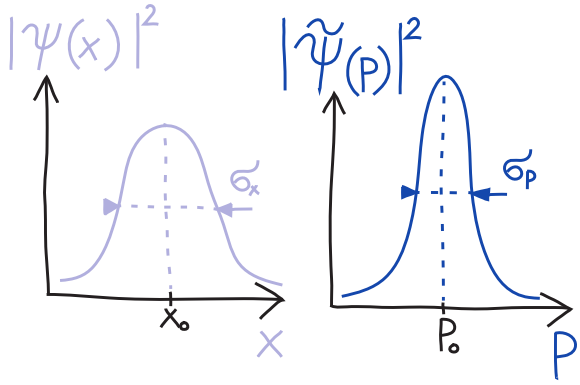
Coordinate representation:

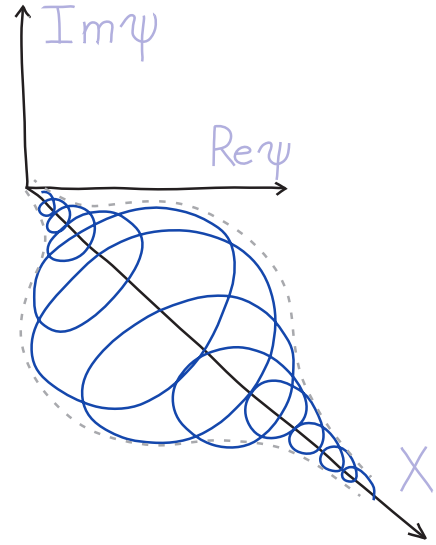
$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{+i\frac{px}{\hbar}}\, \tilde{\psi}(p)\, dp = \underbrace{\frac{1}{(8\pi^3\hbar^2\sigma_p^2)^{\frac{1}{4}}}}_{C} \int_{-\infty}^{+\infty} \underbrace{e^{+i\frac{px}{\hbar} - \frac{p^2 - pp_0 + p_0^2}{4\sigma_p^2}}}_{e^{-\frac{1}{4\sigma_p^2}p^2 + (\frac{p_0}{2\sigma_p^2} + \frac{ix}{\hbar})p - \frac{p_0^2}{4\sigma_p^2}} \equiv e^{ap^2+bp+c}} dp = C\sqrt{\frac{\pi}{|a|}}\, e^{c-\frac{b^2}{4a}} =$$

$$\boxed{\frac{1}{(2\pi\sigma_x^2)^{\frac{1}{4}}} e^{-\frac{x^2}{4\sigma_x^2}}\, e^{+i\frac{p_0 x}{\hbar}} = \psi(x)}$$

with σ_x satisfying $\boxed{\sigma_x\sigma_p = \frac{\hbar}{2}}$

$\Rightarrow$ Heisenberg relation minimized





◄ Historical remark

1926: M. Born, W. Heisenberg, P. Jordan derive commutation relations for position & momentum and for the components of angular momentum

1927-8: H. Weyl analyzes algebraic properties of position & momentum operators

1930: Paul Dirac introduces position & momentum representations and elaborates a method of solving some eigenproblems with the aid of ladder operators

1931: M. Stone & J.von Neumann prove unitary equivalence of representations conserving the canonical commutation relation

■ Angular momentum operators

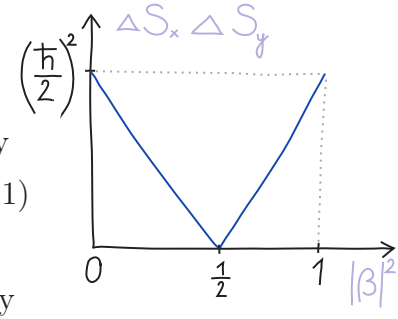
Let us analyze commutation relations of angular-momentum operators. In fact, it is these relations what allows us to recognize that a given set of operators (like Pauli matrices) represents an angular momentum. In other words: what commutes like angular momentum *is* angular momentum.

▸ Components of spin $\frac{1}{2}$

$$\left.\begin{array}{l}[\hat{S}_x,\hat{S}_y]=\frac{\hbar^2}{4}[\hat{\sigma}_x,\hat{\sigma}_y]=2i\frac{\hbar^2}{4}\hat{\sigma}_z=i\hbar\hat{S}_z\\ [\hat{S}_y,\hat{S}_z]=\frac{\hbar^2}{4}[\hat{\sigma}_y,\hat{\sigma}_z]=2i\frac{\hbar^2}{4}\hat{\sigma}_x=i\hbar\hat{S}_x\\ [\hat{S}_z,\hat{S}_x]=\frac{\hbar^2}{4}[\hat{\sigma}_z,\hat{\sigma}_x]=2i\frac{\hbar^2}{4}\hat{\sigma}_y=i\hbar\hat{S}_y\end{array}\right\} \Rightarrow \boxed{[\hat{S}_i,\hat{S}_j]=i\hbar\varepsilon_{ijk}\hat{S}_k} \text{ or } [\hat{\sigma}_i,\hat{\sigma}_j]=2i\varepsilon_{ijk}\hat{\sigma}_k$$

Uncertainty relation $\langle\langle S_x^2\rangle\rangle_\psi\langle\langle S_y^2\rangle\rangle_\psi \geq \frac{\hbar^2}{4}\langle S_z\rangle_\psi^2$

$$\Rightarrow \quad \boxed{(\Delta S_x)_\psi(\Delta S_y)_\psi \geq \tfrac{\hbar}{2}\,|\langle S_z\rangle_\psi|}$$



This is an example of state-dependent uncertainty relation. For $|\psi\rangle = \alpha|\uparrow\rangle+\beta|\downarrow\rangle$ (with $|\alpha|^2+|\beta|^2=1$) we get: $(\Delta S_x)_\psi(\Delta S_y)_\psi \geq \frac{\hbar^2}{2}\left|\frac{1}{2}-|\beta|^2\right|$

For $|\beta|^2=\frac{1}{2}$ there is no lower bound of uncertainty for the x & y components. This is because in that case the spin lies in the xy plane (see Sec. 2b), so one of the components may be sharp (dispersion equal to zero) while the dispersion of the other component must be finite.

▸ Components of orbital angular momentum

$$\left.\begin{array}{l}[\hat{L}_x,\hat{L}_y]=[\hat{y}\hat{p}_z-\hat{z}\hat{p}_y,\hat{z}\hat{p}_x-\hat{x}\hat{p}_z]=[\hat{y}\hat{p}_z,\hat{z}\hat{p}_x]+[\hat{z}\hat{p}_y,\hat{x}\hat{p}_z]=i\hbar(\hat{x}\hat{p}_y-\hat{y}\hat{p}_x)=i\hbar\hat{L}_z\\ [\hat{L}_y,\hat{L}_z]=[\hat{z}\hat{p}_x-\hat{x}\hat{p}_z,\hat{x}\hat{p}_y-\hat{y}\hat{p}_x]=[\hat{z}\hat{p}_x,\hat{x}\hat{p}_y]+[\hat{x}\hat{p}_z,\hat{y}\hat{p}_x]=i\hbar(\hat{y}\hat{p}_z-\hat{z}\hat{p}_y)=i\hbar\hat{L}_x\\ [\hat{L}_z,\hat{L}_x]=[\hat{x}\hat{p}_y-\hat{y}\hat{p}_x,\hat{y}\hat{p}_z-\hat{z}\hat{p}_y]=[\hat{x}\hat{p}_y,\hat{y}\hat{p}_z]+[\hat{y}\hat{p}_x,\hat{z}\hat{p}_y]=i\hbar(\hat{z}\hat{p}_x-\hat{x}\hat{p}_z)=i\hbar\hat{L}_y\end{array}\right\} \Rightarrow \boxed{[\hat{L}_i,\hat{L}_j]=i\hbar\varepsilon_{ijk}\hat{L}_k}$$

Poisson brackets $\{L_i,L_j\}=\varepsilon_{ijk}L_k$

▸ Components of total (orbital+spin) angular momentum

Hilbert space: $\mathcal{H}=\underbrace{\mathcal{H}_{\text{spatial}}}_{\mathcal{L}^2(\mathbb{R}3)}\otimes\underbrace{\mathcal{H}_{\text{spin}}}_{\mathbb{C}^2}$ $\qquad \boxed{\hat{J}_i=\hat{L}_i+\hat{S}_i}=\hat{L}_i\otimes\hat{I}+\hat{I}\otimes\hat{S}_i$

$$\boxed{[\hat{L}_i,\hat{S}_j]=0}=[\hat{L}_i\otimes\hat{I},\hat{I}\otimes\hat{S}_j] \quad\Rightarrow\quad [\hat{J}_i,\hat{J}_j]=[\hat{L}_i,\hat{L}_j]+[\hat{S}_i,\hat{S}_j]=i\hbar\varepsilon_{ijk}\overbrace{(\hat{L}_k+\hat{S}_k)}^{\hat{J}_k}$$

▸ Components and square of general angular momentum

We consider a general system with unspecified Hilbert space $\mathcal{H}$. Operators $\{\hat{J}_i\}_{i=1}^3$ corresponding to components of the system's angular momentum must satisfy commutation relations $\boxed{[\hat{J}_i,\hat{J}_j]=i\hbar\varepsilon_{ijk}\hat{J}_k}$ These components are incompatible, yielding e.g. this uncertainty relation: $\boxed{(\Delta J_x)_\psi(\Delta J_y)_\psi \geq \frac{\hbar}{2}\,|\langle J_z\rangle_\psi|}$

However, we construct a compatible observable:

$$\boxed{\hat{J}^2=\sum_{i=1}^{3}\hat{J}_i^2}\equiv \hat{J}_i\hat{J}_i=\delta_{ij}\hat{J}_i\hat{J}_j \qquad \textbf{squared angular momentum}$$
(summation convention is used on the r.h.s.)

The ang. momentum square $\hat{J}^2$ (its **size**) commutes with all components $\hat{J}_i$:

$$[\hat{J}_i,\hat{J}_j\hat{J}_j]=\hat{J}_j\underbrace{[\hat{J}_i,\hat{J}_j]}_{i\hbar\varepsilon_{ijk}\hat{J}_k}+\underbrace{[\hat{J}_i,\hat{J}_j]}_{i\hbar\varepsilon_{ijk}\hat{J}_k}\hat{J}_j=i\hbar\varepsilon_{ijk}(\hat{J}_j\hat{J}_k+\hat{J}_k\hat{J}_j)=\boxed{0=[\hat{J}_i,\hat{J}^2]}$$

$\Rightarrow \hat{J}^2$ can be diagonalized simultaneously with any component $\hat{J}_i$

The conventional pair of compatible ang. momentum observables: $\boxed{\hat{J}^2,\hat{J}_3\equiv\hat{J}_z}$

► **Simultaneous eigenfunctions** of $\hat{J}^2$ & $\hat{J}_z$ for a single particle

Orbital momentum:
$$\boxed{\begin{array}{l}\hat{L}^2R(r)Y_{lm}(\vartheta,\varphi)=l(l+1)\hbar^2\,R(r)Y_{lm}(\vartheta,\varphi)\\ \hat{L}_z\,R(r)Y_{lm}(\vartheta,\varphi)=m\hbar\,R(r)Y_{lm}(\vartheta,\varphi)\end{array}}\ \forall R(r)$$
$$l=0,1,2,...,\quad m=-l,(-l{+}1),\ldots,(+l{-}1),+l.$$

Spin $\frac{1}{2}$: $\hat{S}^2=\frac{\hbar^2}{4}[\underbrace{\hat{\sigma}_x^2}_{\hat{I}}+\underbrace{\hat{\sigma}_y^2}_{\hat{I}}+\underbrace{\hat{\sigma}_z^2}_{\hat{I}}]=\underbrace{\frac{3}{4}}_{\frac{1}{2}(\frac{1}{2}+1)=s(s+1)}\hbar^2\hat{I}$

$$\hat{S}^2\binom{\alpha}{\beta}=\tfrac{1}{2}(\tfrac{1}{2}{+}1)\hbar^2\binom{\alpha}{\beta}\quad\forall\binom{\alpha}{\beta}\in\mathbb{C}^2,$$
$$\hat{S}_z\binom{\alpha}{0}=+\tfrac{1}{2}\hbar\binom{\alpha}{0},\quad \hat{S}_z\binom{0}{\beta}=-\tfrac{1}{2}\hbar\binom{0}{\beta}\quad\forall\alpha,\beta\in\mathbb{C}$$

So the spinors $\boldsymbol{\psi}(\vec{x})=\left\{\begin{matrix}R(r)Y_{lm}(\vartheta,\varphi)\binom{1}{0}\\ R(r)Y_{lm}(\vartheta,\varphi)\binom{0}{1}\end{matrix}\right\}$ are simultaneous eigenvectors of operators $\left[\hat{L}^2,\hat{L}_z,\hat{S}^2,\hat{S}_z\right]$ with these eigenvalues: $\left[\hbar^2l(l{+}1),\hbar m,\hbar\tfrac{1}{2}(\tfrac{1}{2}{+}1),\pm\tfrac{1}{2}\hbar\right]$

General spin: These considerations can be extended to particles with arbitrary spins, both bosons & fermions (the theory will be gradually elaborated below in this Sec. and in Sec. 4b). The spin size is determined by quantum number $\boxed{s=\tfrac{1}{2},1,\tfrac{3}{2},2,\tfrac{5}{2},\ldots}$ and we set $\hat{S}^2{=}s(s{+}1)\hbar^2\hat{I}$ in the spin Hilbert space $\mathcal{H}_{\text{spin}}{=}\mathbb{C}^{2s+1}\equiv\mathbb{C}^2,\mathbb{C}^3,\mathbb{C}^4,\ldots$. The spin projection operator $\hat{S}_z$ has eigenvalues $\hbar m_s$, which take $2s{+}1$ values given by $m_s=-s,(-s{+}1),\ldots,(+s{-}1),+s$; this operator can be represented by a diagonal matrix.

$$\boxed{\hat{S}^2\begin{pmatrix}\alpha_{+s}\\ \vdots\\ \alpha_{-s}\end{pmatrix}=s(s{+}1)\hbar^2\begin{pmatrix}\alpha_{+s}\\ \vdots\\ \alpha_{-s}\end{pmatrix}}\ \forall\ \begin{pmatrix}\alpha_{+s}\\ \vdots\\ \alpha_{-s}\end{pmatrix}\in\mathbb{C}^{2s+1},\qquad \boxed{\hat{S}_z\begin{pmatrix}0\\ \vdots\\ \alpha_{m_s}\\ \vdots\\ 0\end{pmatrix}=m_s\hbar\begin{pmatrix}0\\ \vdots\\ \alpha_{m_s}\\ \vdots\\ 0\end{pmatrix}}$$

$$\begin{pmatrix}1\\0\\0\\ \vdots\\0\end{pmatrix},\begin{pmatrix}0\\1\\0\\ \vdots\\0\end{pmatrix},\ldots,\begin{pmatrix}0\\0\\ \vdots\\0\\1\end{pmatrix}\equiv\left\{\begin{array}{r}\text{simultaneous eigenvectors}\\ \text{of }\hat{S}^2\text{ and }\hat{S}_z\end{array}\right.$$

In Sec. 4b, we will describe how s is related to rotational transformations of wavefunctions and give another representation of $s{=}1$ states.

Note: Although spin represents a kind of "internal rotation" of a particle, it cannot be interpreted as a classical-like rotational motion of a massive "corpuscle". To explain in this way the spin size $S \approx s\hbar$ would require a diameter of the particle $R \gtrsim \frac{\hbar}{Mc}$, which is too large (for electron $\gtrsim 10^2$ larger than nuclei).

► Angular-momentum ladder operators

From the above commutation relations we derive ladder operators which help to derive the most relevant properties of general angular momentum observables.

Let $|jm,...\rangle \equiv |jm\rangle$ stand for the angular momentum eigenvectors (we skip the other quantum numbers "...")

$$\boxed{\begin{array}{l}\hat{J}^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle \\ \hat{J}_3|jm\rangle = \hbar m|jm\rangle\end{array}}$$

We introduce operators $\boxed{\hat{J}_\pm = \hat{J}_1 \pm i\hat{J}_2}$ satisfying $\hat{J}_-^\dagger = \hat{J}_+$

$\boxed{[\hat{J}^2, \hat{J}_\pm] = 0}$ $\Rightarrow$ $\hat{J}_\pm$ do not affect j

$$[\hat{J}_3, \hat{J}_\pm] = \underbrace{[\hat{J}_3, \hat{J}_1]}_{i\hbar\varepsilon_{312}\hat{J}_2} \pm i\underbrace{[\hat{J}_3, \hat{J}_2]}_{i\hbar\varepsilon_{321}\hat{J}_1} = i\hbar(\hat{J}_2 \mp i\hat{J}_1) = \pm\hbar\underbrace{(\hat{J}_1 \pm i\hat{J}_2)}_{\hat{J}_\pm} \quad \Rightarrow \quad \text{general}$$

ladder-operator relations $\left\{\begin{array}{l}[\hat{A},\hat{T}_\Delta^\dagger]=+\Delta\,\hat{T}_\Delta \\ [\hat{A},\hat{T}_\Delta]=-\Delta\,\hat{T}_\Delta\end{array}\right\}$ are satisfied: $\boxed{[\hat{J}_3, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm}$

Hence we get: $\hat{J}_\pm|jm\rangle = \sqrt{\langle jm|\hat{J}_\mp\hat{J}_\pm|jm\rangle}\,|j(m\pm1)\rangle$

$$\hat{J}_\mp\hat{J}_\pm = (\hat{J}_1 \mp i\hat{J}_2)(\hat{J}_1 \pm i\hat{J}_2) = \hat{J}_1^2 + \hat{J}_2^2 \pm i\overbrace{[\hat{J}_1, \hat{J}_2]}^{i\hbar\hat{J}_3} = \hat{J}^2 - \hat{J}_3^2 \mp \hbar\hat{J}_3$$

$$\boxed{\hat{J}_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}\;|j(m\pm1)\rangle}$$

► Possible values of j and m quantum numbers

From the finite value of $\hat{J}^2$ in state $|jm\rangle$ we expect that any projection of $\hat{\vec{J}}$ is bounded, so there must be some limiting values $m_{\min}$ & $m_{\max}$ such that

$$\boxed{\begin{array}{l}\hat{J}_-|jm_{\max}\rangle = 0 \\ \hat{J}_+|jm_{\min}\rangle = 0\end{array}} \quad \text{with} \quad \boxed{\begin{array}{l}m_{\max} = +j \\ m_{\min} = -j\end{array}}$$

as follows from the above relation $\hat{J}_\pm|j(m=\pm j)\rangle = 0$

We can also use positive definiteness of operator $\hat{J}_1^2 + \hat{J}_2^2 = \hat{J}^2 - \hat{J}_3^2$, that is $(\hat{J}_1^2 + \hat{J}_2^2)|jm\rangle = \hbar^2[j(j+1) - m^2]|jm\rangle$ $\Rightarrow$ $-\sqrt{j(j+1)} \le m \le +\sqrt{j(j+1)}$,

and solve:

$$\begin{array}{lll} \underbrace{\hat{J}_+\hat{J}_-}_{\hat{J}^2-\hat{J}_3^2+\hbar\hat{J}_3}|jm_{\min}\rangle & = 0 = & \underbrace{\hat{J}_-\hat{J}_+}_{\hat{J}^2-\hat{J}_3^2-\hbar\hat{J}_3}|jm_{\max}\rangle \\ j(j+1)-m_{\min}^2+m_{\min} & = 0 = & j(j+1)-m_{\max}^2-m_{\max} \end{array} \quad \Rightarrow \quad \Downarrow \text{ the above values } m_{\min} \text{ and } m_{\max}$$

Therefore, the action of $\hat{J}_\pm$ on $|jm\rangle$ proceeds according to the scheme:

$$\boxed{0 \underset{\hat{J}_-}{\overset{\times}{\leftarrow}} |j\underbrace{m_{\min}}_{-j}\rangle \underset{\hat{J}_-}{\overset{\hat{J}_+}{\rightleftharpoons}} |j\underbrace{(m_{\min}+1)}_{-j+1}\rangle \underset{\hat{J}_-}{\overset{\hat{J}_+}{\rightleftharpoons}} \cdots\cdots \underset{\hat{J}_-}{\overset{\hat{J}_+}{\rightleftharpoons}} |j\underbrace{(m_{\max}-1)}_{+j-1}\rangle \underset{\hat{J}_-}{\overset{\hat{J}_+}{\rightleftharpoons}} |j\underbrace{m_{\max}}_{+j}\rangle \underset{\times}{\overset{\hat{J}_+}{\rightarrow}} 0}$$

This chain is closed *iff* $\boxed{j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots}$ $\Rightarrow$ general angular momentum can have only an **integer** or **half-integer** squared-size quantum number. The half-integer values appear only in connection with the spin of fermionic particles, including the size of the total angular momentum of a system that contains such particles.

■ Addition of two angular momenta

Consider an angular momentum vector which is a sum of two partial angular momenta (like the total angular momentum obtained from spin and orbital momenta of a single particle). The system can be characterized by the eigenvectors of both partial angular momenta, as well as by the eigenvectors of the total angular momentum. In general, we consider a product Hilbert space $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$ with spaces $\mathcal{H}^{(1)}$ and $\mathcal{H}^{(2)}$ associated, respectively, with two different sets of angular momentum operators $\hat{\vec{J}}^{(1)}$ and $\hat{\vec{J}}^{(2)}$. Individual components satisfy commutation relations $[\hat{J}_i^{(m)}, \hat{J}_j^{(n)}] = i\hbar\varepsilon_{ijk}\delta_{mn}\hat{J}_k^{(m)}$, where $m, n = 1, 2$. Below we again consider only the angular-momentum quantum numbers j and m and skip the remaining quantum numbers, which depend on the system of interest and can be easily included in the description.

▶ Uncoupled angular-momentum basis

First, we consider a trivial complete set of commuting operators formed by the square and z-component of both partial angular momenta. This yields a factorized (unenangled) basis in the full space $\mathcal{H}$:

$$\left\{\hat{J}^{(1)2}, \hat{J}_3^{(1)}, \hat{J}^{(2)2}, \hat{J}_3^{(2)}\right\} \equiv \text{complete set I} \Rightarrow \boxed{\left\{\underbrace{|j_1 m_1\rangle|j_2 m_2\rangle}_{|j_1 m_1 j_2 m_2\rangle}\right\} \equiv \text{basis I}}$$

▶ Coupled angular-momentum basis

Second, we construct a complete set of commuting operators which includes summed (total) angular momentum operators. This set generates a coupled (entangled) basis in $\mathcal{H}$:

Total angular-momentum $\boxed{\hat{\vec{J}} = \hat{\vec{J}}^{(1)} + \hat{\vec{J}}^{(2)}}$ $\quad \hat{J}_i = \hat{J}_i^{(1)} \otimes \hat{I}^{(2)} + \hat{I}^{(1)} \otimes \hat{J}_i^{(2)}$

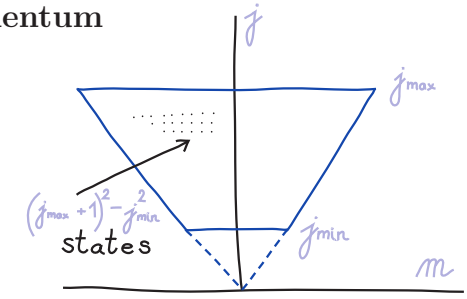
$$[\hat{J}_i, \hat{J}_j] = \overbrace{[\hat{J}_i^{(1)}, \hat{J}_j^{(1)}]}^{i\hbar\varepsilon_{ijk}\hat{J}_k^{(1)}} + \overbrace{[\hat{J}_i^{(2)}, \hat{J}_j^{(2)}]}^{i\hbar\varepsilon_{ijk}\hat{J}_k^{(2)}} = i\hbar\varepsilon_{ijk}\overbrace{(\hat{J}_k^{(1)} + \hat{J}_k^{(2)})}^{\hat{J}_k}$$

standard commutation relations

$$\Rightarrow \qquad [\hat{J}^2, \hat{J}_3] = 0 = \left\{ \begin{matrix} [\hat{J}^2, \hat{J}^{(1)2}] = [\hat{J}_3, \hat{J}^{(1)2}] \\ [\hat{J}^2, \hat{J}^{(2)2}] = [\hat{J}_3, \hat{J}^{(2)2}] \end{matrix} \quad \text{but} \quad \begin{matrix} [\hat{J}^2, \hat{J}_3^{(1)}] \\ [\hat{J}^2, \hat{J}_3^{(2)}] \end{matrix} \right\} \neq 0$$

$$\left\{\hat{J}^{(1)2}, \hat{J}^{(2)2}, \hat{J}^2, \hat{J}_3\right\} \equiv \text{complete set II} \Rightarrow \boxed{\left\{|j_1 j_2 j m\rangle\right\} \equiv \text{basis II}}$$

▶ Possible values of total angular momentum



The allowed values of j obtained partly from dimension considerations: basis I has dimension $\boxed{d=(2j_1+1)(2j_2+1)}$ and the same d is required for basis II. This helps to determine the bounds for the size quantum number of the total angular momentum $j \in [j_{\min}, j_{\max}]$:

(a) $\hat{J}_3 = \hat{J}_3^{(1)} + \hat{J}_3^{(2)} \Rightarrow m_{\max} = m_{\max 1} + m_{\max 2} = j_1 + j_2 \Rightarrow$ $\boxed{j_{\max} = j_1 + j_2}$

(b) The determination of minimal j from the dimension criterion:

Number of states for $j = \left\{ \begin{smallmatrix} 0,1,\ldots \\ \frac{1}{2},\frac{3}{2},\ldots \end{smallmatrix} \right.$ $j_{\max}$ is $d_> = \lfloor (j_{\max}+1)^2 \rfloor \geq d$, with the surplus: $d_> - d = \lfloor (j_1+j_2+1)^2 \rfloor - (2j_1+1)(2j_2+1) = \lfloor (j_1-j_2)^2 \rfloor \geq 0$

Number of states for $j = j_{\min}, \ldots, j_{\max}$ is $d = \lfloor (j_{\max}+1)^2 \rfloor - \lfloor j_{\min}^2 \rfloor$

$\Rightarrow$ $\boxed{j_{\min} = |j_1 - j_2|}$

▶ Transformation between bases I and II

$$\boxed{|j_1 j_2 j m\rangle = \sum_{m_1=-j_1}^{+j_1} \sum_{m_2=-j_2}^{+j_2} C^{jm}_{j_1 m_1 j_2 m_2} |j_1 m_1\rangle |j_2 m_2\rangle}$$

Clebsch-Gordan (CG) **coefficients**

$$\boxed{\begin{array}{c} C^{jm}_{j_1 m_1 j_2 m_2} \\ \equiv (j_1 m_1 j_2 m_2 | jm) \\ \equiv \langle j_1 m_1 j_2 m_2 | j_1 j_2 j m \rangle \end{array}}$$

$$\left. \begin{array}{l} m \neq m_1 + m_2 \quad \text{or} \\ j \notin [|j_1 - j_2|, j_1 + j_2] \end{array} \right\} \Rightarrow C^{jm}_{j_1 m_1 j_2 m_2} = 0$$

Note: The symbol $C^{jm}_{j_1 m_1 j_2 m_2}$ (alternative notations used in the literature given above) looks a bit too "indexy", but it is easy to get used to it. Just remember that the lower 4 indices specify the two partial angular momenta and the 2 upper indices denote the resulting total angular momentum.

▶ Some properties of Clebsch-Gordan coefficients

(a) $\boxed{C^{jm}_{j_1 m_1 j_2 m_2} \in \mathbb{R}}$ (by convention)

(b) From reality we get: $\langle j_1 m_1 j_2 m_2 | j_1 j_2 j m \rangle = \langle j_1 j_2 j m | j_1 m_1 j_2 m_2 \rangle$, hence:

$$\boxed{|j_1 m_1\rangle |j_2 m_2\rangle = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m=-j}^{+j} C^{jm}_{j_1 m_1 j_2 m_2} |j_1 j_2 j m\rangle}$$ **inverse relation**

(c) Multiply $|j_1 j_2 j m\rangle = \sum_{m_1, m_2} C^{jm}_{j_1 m_1 j_2 m_2} |j_1 m_1\rangle |j_2 m_2\rangle$

$\langle j_1 j_2 j' m'| = \sum_{m_1', m_2'} C^{j'm'}_{j_1 m_1' j_2 m_2'} \langle j_1 m_1'| \langle j_2 m_2'|$

$$\Rightarrow \quad \boxed{\sum_{m_1, m_2} C^{jm}_{j_1 m_1 j_2 m_2} C^{j'm'}_{j_1 m_1 j_2 m_2} = \delta_{jj'} \delta_{mm'}}$$ **orthogonality relation I**

(d) Multiply $|j_1m_1\rangle|j_2m_2\rangle = \sum_{j,m} C^{jm}_{j_1m_1j_2m_2}|j_1j_2jm\rangle$

$\langle j_1m_1'|\langle j_2m_2'| = \sum_{j',m'} C^{j'm'}_{j_1m_1'j_2m_2'}\langle j_1j_2j'm'|$

$$\Rightarrow \quad \boxed{\sum_{j,m} C^{jm}_{j_1m_1j_2m_2}C^{jm}_{j_1m_1'j_2m_2'} = \delta_{m_1m_1'}\delta_{m_2m_2'}} \qquad \textbf{orthogonality relation II}$$

The following relations we give here without the proofs:

(e) $C^{jm}_{j_1m_1j_2m_2} = \underbrace{(-)^{j-j_1-j_2}}_{\pm} C^{jm}_{j_2m_2j_1m_1}$ **exchange of indices I**

Special case: $C^{jm}_{j_1m_1j_1m_1} = 0$ for $(j-2j_1)$=odd

(f) $C^{jm}_{j_1m_1j_2m_2} = \underbrace{(-)^{j_1-m_1}}_{\pm}\sqrt{\frac{2j+1}{2j_2+1}}C^{j_2(-m_2)}_{j_1m_1j(-m)}$ **exchange of indices II**

(g) $C^{jm}_{j_1m_1j_2m_2} = \underbrace{(-)^{j-j_1-j_2}}_{\pm} C^{j(-m)}_{j_1(-m_1)j_2(-m_2)}$ **sign inversion**

Special case: $C^{j0}_{j_10j_20} = 0$ for $(j-j_1-j_2)$=odd

▶ 3j symbols

Definition: $\boxed{\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \equiv \frac{(-)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} C^{j_3(-m_3)}_{j_1m_1j_2m_2}}$

These coefficients represent just a more symmetric form of CG coefficients:

$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \varepsilon \begin{pmatrix} j_k & j_l & j_n \\ m_k & m_l & m_n \end{pmatrix}$ with $\varepsilon = \begin{cases} +1 & \text{for even permutation} \\ (-)^{j_1+j_2+j_3} & \text{for odd permutation} \end{cases}$

$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$

▶ Construction of Clebsch-Gordan coefficients

The CG coefficients can be calculated with the aid of the angular momentum ladder operators, which in the $\mathcal{H}^{(1)}\otimes\mathcal{H}^{(2)}$ space have the form $\hat{J}_\pm = \hat{J}^{(1)}_\pm + \hat{J}^{(2)}_\pm \equiv \hat{J}^{(1)}_\pm \otimes \hat{I}^{(2)} + \hat{I}^{(1)} \otimes \hat{J}^{(2)}_\pm$. The calculation proceeds as follows:

$$\hat{J}_\pm|j_1j_2jm\rangle = [\hat{J}^{(1)}_\pm \otimes \hat{I}^{(2)} + \hat{I}^{(1)} \otimes \hat{J}^{(2)}_\pm] \sum_{m_1,m_2} C^{jm}_{j_1m_1j_2m_2}|j_1m_1\rangle|j_2m_2\rangle$$

$$\hbar\sqrt{j(j+1)-m(m\pm1)}|j_1j_2j(m\pm1)\rangle = \hbar \sum_{m_1,m_2} \sqrt{j_1(j_1+1)-m_1(m_1\pm1)}C^{jm}_{j_1m_1j_2m_2}|j_1(m_1\pm1)\rangle|j_2m_2\rangle + \hbar \sum_{m_1,m_2} \sqrt{j_2(j_2+1)-m_2(m_2\pm1)}C^{jm}_{j_1m_1j_2m_2}|j_1m_1\rangle|j_2(m_2\pm1)\rangle$$

Multiply by $\langle j_1m_1'|\langle j_2m_2'| \quad \Rightarrow$

$$\sqrt{j(j+1)-m(m\pm1)}C^{j(m\pm1)}_{j_1m_1'j_2m_2'} = \sum_{m_1,m_2}\sqrt{j_1(j_1+1)-m_1(m_1\pm1)}C^{jm}_{j_1m_1j_2m_2}\delta_{m_1'(m_1\pm1)}\delta_{m_2'm_2} + \sum_{m_1,m_2}\sqrt{j_2(j_2+1)-m_2(m_2\pm1)}C^{jm}_{j_1m_1j_2m_2}\delta_{m_1'm_1}\delta_{m_2'(m_2\pm1)}$$

After $\begin{matrix} m_1' \\ m_2' \end{matrix}\Big\} \mapsto \Big\{ \begin{matrix} m_1 \\ m_2 \end{matrix}$ substitution we obtain the following **recursive relation**

$$C^{j(m\pm1)}_{j_1m_1j_2m_2} = \sqrt{\frac{j_1(j_1+1)-m_1(m_1\mp1)}{j(j+1)-m(m\pm1)}}C^{jm}_{j_1(m_1\mp1)j_2m_2} + \sqrt{\frac{j_2(j_2+1)-m_2(m_2\mp1)}{j(j+1)-m(m\pm1)}}C^{jm}_{j_1m_1j_2(m_2\mp1)} \Rightarrow$$

$$\boxed{C^{jm}_{j_1m_1j_2m_2} = \sqrt{\frac{j_1(j_1+1)-m_1(m_1\mp1)}{j(j+1)-m(m\mp1)}}C^{j(m\mp1)}_{j_1(m_1\mp1)j_2m_2} + \sqrt{\frac{j_2(j_2+1)-m_2(m_2\mp1)}{j(j+1)-m(m\mp1)}}C^{j(m\mp1)}_{j_1m_1j_2(m_2\mp1)}}$$

This relation enables one to construct the CG coefficients using the fact that

$$|j_1 j_2 j_{\max} \underbrace{(\pm j_{\max})}_{m}\rangle = |j_1 \underbrace{(\pm j_1)}_{m_1}\rangle |j_2 \underbrace{(\pm j_2)}_{m_2}\rangle \quad \Rightarrow \quad \boxed{C^{j_{\max}(\pm j_{\max})}_{j_1(\pm j_1) j_2(\pm j_2)} = 1}$$

► **Example: coupling two spins $\frac{1}{2}$**

$\boxed{j_1 = j_2 = \frac{1}{2} \quad \Rightarrow \quad j_{\max} = 1, j_{\min} = 0}$

From $|\frac{1}{2}\frac{1}{2}11\rangle = |\frac{1}{2}\frac{1}{2}\rangle_1 |\frac{1}{2}\frac{1}{2}\rangle_2$

we calculate: $\overbrace{\hat{J}_-|\frac{1}{2}\frac{1}{2}11\rangle}^{\sqrt{2}|\frac{1}{2}\frac{1}{2}10\rangle} = \overbrace{(\hat{J}^{(1)}_-|\frac{1}{2}\frac{1}{2}\rangle_1)}^{|\frac{1}{2}(-\frac{1}{2})\rangle_1} |\frac{1}{2}\frac{1}{2}\rangle_2 + |\frac{1}{2}\frac{1}{2}\rangle_1 \overbrace{(\hat{J}^{(2)}_-|\frac{1}{2}\frac{1}{2}\rangle_2)}^{|\frac{1}{2}(-\frac{1}{2})\rangle_2}$

$\Rightarrow \quad |\frac{1}{2}\frac{1}{2}10\rangle = \frac{1}{\sqrt{2}}|\frac{1}{2}(-\frac{1}{2})\rangle_1 |\frac{1}{2}\frac{1}{2}\rangle_2 + \frac{1}{\sqrt{2}}|\frac{1}{2}\frac{1}{2}\rangle_1 |\frac{1}{2}(-\frac{1}{2})\rangle_2$

Then $|\frac{1}{2}\frac{1}{2}1(-1)\rangle = |\frac{1}{2}(-\frac{1}{2})\rangle_1 |\frac{1}{2}(-\frac{1}{2})\rangle_2$

and $|\frac{1}{2}\frac{1}{2}00\rangle$ is obtained from orthogonality to $|\frac{1}{2}\frac{1}{2}10\rangle$

$\Rightarrow \quad |\frac{1}{2}\frac{1}{2}00\rangle = \frac{1}{\sqrt{2}}|\frac{1}{2}(-\frac{1}{2})\rangle_1 |\frac{1}{2}\frac{1}{2}\rangle_2 - \frac{1}{\sqrt{2}}|\frac{1}{2}\frac{1}{2}\rangle_1 |\frac{1}{2}(-\frac{1}{2})\rangle_2$ (up to phase convention)

So we obtain the following CG coefficients:

$$\begin{array}{lll} C^{1(+1)}_{\frac{1}{2}(+\frac{1}{2})\frac{1}{2}(+\frac{1}{2})} & =1= & C^{1(-1)}_{\frac{1}{2}(-\frac{1}{2})\frac{1}{2}(-\frac{1}{2})} \\ C^{10}_{\frac{1}{2}(-\frac{1}{2})\frac{1}{2}(+\frac{1}{2})} & =\frac{1}{\sqrt{2}}= & C^{10}_{\frac{1}{2}(+\frac{1}{2})\frac{1}{2}(-\frac{1}{2})} \\ C^{00}_{\frac{1}{2}(-\frac{1}{2})\frac{1}{2}(+\frac{1}{2})} & =\frac{1}{\sqrt{2}}= & -C^{00}_{\frac{1}{2}(+\frac{1}{2})\frac{1}{2}(-\frac{1}{2})} \end{array}$$

Using a simplified notation:

$$\begin{array}{lcll} |\frac{1}{2}\frac{1}{2}11\rangle & = & |\uparrow\rangle_1|\uparrow\rangle_2 & \\ |\frac{1}{2}\frac{1}{2}10\rangle & = & \frac{1}{\sqrt{2}}|\downarrow\rangle_1|\uparrow\rangle_2 + \frac{1}{\sqrt{2}}|\uparrow\rangle_1|\downarrow\rangle_2 & \text{triplet} \\ |\frac{1}{2}\frac{1}{2}1(-1)\rangle & = & |\downarrow\rangle_1|\downarrow\rangle_2 & \\ |\frac{1}{2}\frac{1}{2}00\rangle & = & \frac{1}{\sqrt{2}}|\downarrow\rangle_1|\uparrow\rangle_2 - \frac{1}{\sqrt{2}}|\uparrow\rangle_1|\downarrow\rangle_2 & \text{singlet} \end{array}$$

We will remember that the triplet is formed by three states which are all **symmetric** under the exchange of spins, while the unique singlet state is **antisymmetric** under the exchange of spins. As particles with spin $\frac{1}{2}$ are fermions, whose overall wave function must be antisymmetric under the particle exchange, the above spin-exchange relations impose opposite coordinate-exchange relations for the spatial wavefunction.

■ Addition of three and more angular momenta

Coupling of $k > 2$ angular momenta is not just an academic issue. Already the system of two particles with spins and mutual orbital momentum leads to the $k = 3$ problem $\hat{\vec{J}} = \hat{\vec{S}}^{(1)} + \hat{\vec{S}}^{(2)} + \hat{\vec{L}}$. The $k > 2$ coupling is trickier than the $k = 2$ case as the summed angular momentum operators $\hat{J}^2$ and $\hat{J}_3$ must be supplemented by $(2k-2)$ additional commuting operators to form a complete set. While for $k = 2$, as seen above, the two additional operators are just the $\hat{J}^{(1)2}$ and $\hat{J}^{(2)2}$ squares, for $k > 2$ one has to find more than k additional operators—hence the squares of partial momenta do not suffice. It turns out that the choice of these extra operators is not unique...

▶ $k = 3$: total & paired angular momenta

The triple product of Hilbert spaces, in which the three partial ang. momenta live, and the standard commutation relations for these partial momenta:

$$\mathcal{H} = \underbrace{\mathcal{H}^{(1)}}_{\vec{J}^{(1)}} \otimes \underbrace{\mathcal{H}^{(2)}}_{\vec{J}^{(2)}} \otimes \underbrace{\mathcal{H}^{(3)}}_{\vec{J}^{(3)}} \quad \text{with} \quad [\hat{J}_i^{(m)}, \hat{J}_j^{(n)}] = i\hbar\varepsilon_{ijk}\delta_{mn}\hat{J}_k^{(m)}$$

Total angular momentum: $\hat{\vec{J}} = \hat{\vec{J}}^{(1)} + \hat{\vec{J}}^{(2)} + \hat{\vec{J}}^{(3)}$

Paired angular momenta: $\hat{\vec{J}}^{(nl)} = \hat{\vec{J}}^{(n)} + \hat{\vec{J}}^{(l)} \quad \Rightarrow \quad \hat{\vec{J}}^{(12)}, \hat{\vec{J}}^{(13)}, \hat{\vec{J}}^{(23)}$

$$[\hat{J}_i^{(nl)}, \hat{J}_j^{(n'l')}] = i\hbar\varepsilon_{ijk}(\delta_{nn'}\hat{J}_k^{(n)} + \delta_{ll'}\hat{J}_k^{(l)})$$

Compatibility:

$$[\hat{J}^2, \hat{J}_3] = 0 = \left\{ \begin{matrix} [\hat{J}^2,\hat{J}^{(1)2}] = [\hat{J}_3,\hat{J}^{(1)2}] = [\hat{J}^2,\hat{J}^{(23)2}] = [\hat{J}_3,\hat{J}^{(23)2}] \\ [\hat{J}^2,\hat{J}^{(2)2}] = [\hat{J}_3,\hat{J}^{(2)2}] = [\hat{J}^2,\hat{J}^{(13)2}] = [\hat{J}_3,\hat{J}^{(13)2}] \\ [\hat{J}^2,\hat{J}^{(3)2}] = [\hat{J}_3,\hat{J}^{(3)2}] = [\hat{J}^2,\hat{J}^{(12)2}] = [\hat{J}_3,\hat{J}^{(12)2}] \end{matrix} \right\} \begin{matrix} [\hat{J}^2,\hat{J}_3^{(1)}] \\ [\hat{J}^2,\hat{J}_3^{(2)}] \\ [\hat{J}^2,\hat{J}_3^{(3)}] \end{matrix} \neq 0 \neq \left\{ \begin{matrix} [\hat{J}^2,\hat{J}_3^{(23)}] \\ [\hat{J}^2,\hat{J}_3^{(13)}] \\ [\hat{J}^2,\hat{J}_3^{(12)}] \end{matrix} \right.$$

▶ $k = 3$: different coupling schemes

Several complete sets of commuting operators & associated bases:

$\hat{J}^{(1)2}, \hat{J}_3^{(1)}, \hat{J}^{(2)2}, \hat{J}_3^{(2)}, \hat{J}^{(3)2}, \hat{J}_3^{(3)}$	$\Rightarrow$	$\lvert j_1 m_1\rangle \lvert j_2 m_2\rangle \lvert j_3 m_3\rangle$	... basis I
$\hat{J}^{(1)2}, \hat{J}^{(2)2}, \hat{J}^{(3)2}, \hat{J}^{(23)2}, \hat{J}^2, \hat{J}_3$	$\Rightarrow$	$\lvert j_1 j_2 j_3 j_{23} j m\rangle$	... basis II
$\hat{J}^{(1)2}, \hat{J}^{(2)2}, \hat{J}^{(3)2}, \hat{J}^{(13)2}, \hat{J}^2, \hat{J}_3$	$\Rightarrow$	$\lvert j_1 j_2 j_3 j_{13} j m\rangle$	... basis III
$\hat{J}^{(1)2}, \hat{J}^{(2)2}, \hat{J}^{(3)2}, \hat{J}^{(12)2}, \hat{J}^2, \hat{J}_3$	$\Rightarrow$	$\lvert j_1 j_2 j_3 j_{12} j m\rangle$	... basis IV

Generation of the coupled bases (II,III,IV) from the uncoupled one (I):

$$\begin{aligned} |j_1 j_2 j_3 j_{23} j m\rangle &= \sum_{m_1, m_{23}} C^{jm}_{j_1 m_1 j_{23} m_{23}} |j_1 m_1\rangle \sum_{m_2, m_3} C^{j_{23} m_{23}}_{j_2 m_2 j_3 m_3} |j_2 m_2\rangle |j_3 m_3\rangle \\ &= \sum_{\substack{m_1, m_2, m_3 \\ m_{23}}} C^{jm}_{j_1 m_1 j_{23} m_{23}} C^{j_{23} m_{23}}_{j_2 m_2 j_3 m_3} |j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle \qquad \ldots \text{II} \end{aligned}$$

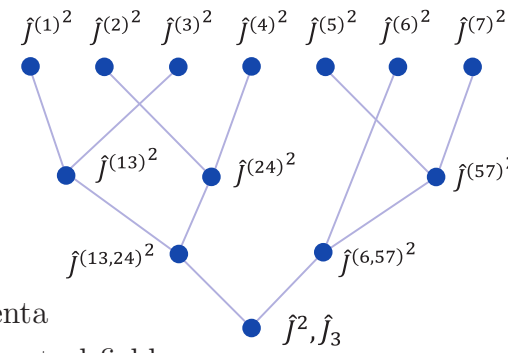
... similarly III & IV

Relation between coupled bases:

$$|j_1 j_2 j_3 j_{23} j m\rangle = (-)^{j_1+j_2+j_3+j} \sum_{j_{12}} \sqrt{(2j_{23}+1)(2j_{12}+1)} \underbrace{\left\{ \begin{matrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{matrix} \right\}}_{\textbf{6j symbol}} |j_1 j_2 j_3 j_{12} j m\rangle$$

▶ General k

The way how to obtain coupling schemes for higher k is analogous and can be captured graphically. Here is an example of a specific coupling of $k = 7$ angular momenta with 14 commuting operators:



An important case is the $k = 4$ coupling of orbital & spin angular momenta $\hat{\vec{L}}^{(1)}, \hat{\vec{L}}^{(2)}$ & $\hat{\vec{S}}^{(1)}, \hat{\vec{S}}^{(2)}$ for 2 particles in a central field. Two physically meaningful coupling schemes with the respective commut-

ing operator sets are as follows:

(a) **J-J coupling** $\{\hat{L}^{(1)2}, \hat{L}^{(2)2}, \hat{S}^{(1)2}, \hat{S}^{(2)2}, \overbrace{(\hat{\vec{L}}^{(1)}+\hat{\vec{S}}^{(1)})^2}^{\hat{J}^{(1)2}}, \overbrace{(\hat{\vec{L}}^{(2)}+\hat{\vec{S}}^{(2)})^2}^{\hat{J}^{(2)2}}, \hat{J}^2, \hat{J}_3\}$

(b) **L-S coupling** $\{\hat{L}^{(1)2}, \hat{L}^{(2)2}, \hat{S}^{(1)2}, \hat{S}^{(2)2}, \underbrace{(\hat{\vec{L}}^{(1)}+\hat{\vec{L}}^{(2)})^2}_{\hat{L}^2}, \underbrace{(\hat{\vec{S}}^{(1)}+\hat{\vec{S}}^{(2)})^2}_{\hat{S}^2}, \hat{J}^2, \hat{J}_3\}$

◂ Historical remark

1866: A. Clebsch & P. Gordan introduce CG coefficients for spherical harmonics
1925: Discussions about the physical interpretation of electron spin
1925: H.N. Russel and F.A. Saunders outline the L-S coupling scheme
1930: P. Dirac presents the algebraic treatment of angular momentum operators
1940-42: E. Wigner & G. Racah analyze general coupling of >2 angular momenta

■ Complete sets of commuting operators for a structureless particle

Below we give several examples of the complete set of observables characterizing a single spinless particle in 3D. This system has $f=3$ classical degrees of freedom, and also its quantum state is determined by eigenvalues of 3 commuting operators. These operators can be chosen in different ways, forming possible continuous, discrete and mixed representations of the problem. A nonzero spin of the particle extends this set by additional commuting operators.

▸ Cartesian coordinates $\hat{\vec{x}} \equiv (\hat{x}_1, \hat{x}_2, \hat{x}_3)$

Eigenbasis $\boxed{\Phi_{\vec{x}'}(\vec{x}) = \delta(\vec{x}-\vec{x}')}$ with $\langle \Phi_{\vec{x}'} | \Phi_{\vec{x}''} \rangle = \delta(\vec{x}'-\vec{x}'')$

General wavefunction: $\psi(\vec{x}) = \int d\vec{x}' \psi(\vec{x}')\, \Phi_{\vec{x}'}(\vec{x})$

Note: the physical dimension of $\Phi_{\vec{x}'}(\vec{x})$ is $[\text{length}]^{-3}$ because it represents an amplitude density in a *joint space* $\vec{x} \times \vec{x}'$ (while a normal wavefunction is an amplitude density only in $\vec{x}$)

▸ Cartesian momenta $\hat{\vec{p}} \equiv (\hat{p}_1, \hat{p}_2, \hat{p}_3)$

Eigenbasis $\boxed{\Phi_{\vec{p}}(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\frac{\vec{p}\cdot\vec{x}}{\hbar}}}$ with $\langle \Phi_{\vec{p}} | \Phi_{\vec{p}'} \rangle = \frac{1}{(2\pi\hbar)^3} \underbrace{\int e^{-i\frac{(\vec{p}-\vec{p}')\cdot\vec{x}}{\hbar}} d\vec{x}}_{(2\pi\hbar)^3 \delta(\vec{p}-\vec{p}')} = \delta(\vec{p}-\vec{p}')$

General wavefunction: $\psi(\vec{x}) = \int d\vec{p}\, \tilde{\psi}(\vec{p})\, \Phi_{\vec{p}}(\vec{x})$

Note: the phasical dimension of $\Phi_{\vec{p}}(\vec{x})$ is $[\text{length}]^{-\frac{3}{2}}[\text{momentum}]^{-\frac{3}{2}}$ because it represents an amplitude density in a *joint space* $\vec{x} \times \vec{p}$

▸ Radial momentum and orbital angular momentum $(\hat{p}_r, \hat{\boldsymbol{L}}^2, \hat{L}_z)$

Eigenbasis $\boxed{\Phi_{p_r lm}(\vec{x}) = \underbrace{\frac{1}{(\pi\hbar)^{1/2}} \frac{e^{i\frac{p_r r}{\hbar}}}{r}}_{R_{p_r}(r)} Y_{lm}(\vartheta, \varphi)}$ with $\underbrace{\langle \Phi_{p_r lm} | \Phi_{p_r' l' m'} \rangle = \delta(p_r - p_r')\delta_{ll'}\delta_{mm'}}_{\frac{1}{\pi\hbar}\int_0^\infty \frac{e^{-i\frac{(p_r-p_r')r}{\hbar}}}{r^2} \left[\int_0^{2\pi}\int_0^{\pi} Y_{lm}^*(\vartheta,\varphi) Y_{l'm'}(\vartheta,\varphi) \sin\vartheta\, d\vartheta\, d\varphi\right] r^2 dr}$

General wavefunction: $\psi(\vec{x}) = \sum_{l,m} \int dp_r\, \alpha_{p_r lm} \Phi_{p_r lm}(\vec{x})$

▶ Isotropic Hamiltonian and orbital ang. momentum ($\hat{H}_{\rm rot}, \hat{L}^2, \hat{L}_z$)

Instead of radial momentum of the last example we can use a Hamiltonian $\hat{H}_{\rm rot}$ corresponding to a spherically symmetric *infinite* potential well $V(r)$ (an isotropic harmonic oscillator, Coulomb potential, an infinite square well etc.) with a discrete infinite spectrum of bound states enumerated by $n = 1, 2, ...$

Eigenbasis $\boxed{\Phi_{nlm}(\vec{x}) = \underbrace{R_{nl}(r)}_{\frac{1}{r}u_{nl}(r)}\, Y_{lm}(\vartheta,\varphi)}$ with $\langle\Phi_{nlm}|\Phi_{n'l'm'}\rangle = \delta_{nn'}\delta_{ll'}\delta_{mm'}$

$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2Mr^2}+V\right] u_{nl} = E_{nl}u_{nl}$

General wavefunction: $\psi(\vec{x}) = \sum_{n,l,m} \alpha_{nlm}\Phi_{nlm}(\vec{x})$

▶ Harmonic oscillator Hamiltonian components ($\hat{H}_1, \hat{H}_2, \hat{H}_3$)

Eigenbasis $\boxed{\Phi_{n_1n_2n_3}(\vec{x}) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3)}$ $\langle\Phi_{n_1n_2n_3}|\Phi_{n_1'n_2'n_3'}\rangle = \delta_{n_1n_1'}\delta_{n_2n_2'}\delta_{n_3n_3'}$, where $\psi_{n_k}(x_k)$ for k=1,2,3 is the egenstate of $\hat{H}_k$ with energy $E_{n_k} = \hbar\omega_k(n_k+\frac{1}{2})$.

Infinitely many other complete sets can be found. The complete set is enriched if the particle has **spin** with arbitrary nonzero size quantum number s. This yields the following types of complete sets:

▶ Sets containing spin projection ($\hat{A}_1, \hat{A}_2, \hat{A}_3, \hat{S}^2, \hat{S}_z$)

Here $(\hat{A}_1, \hat{A}_2, \hat{A}_3)$ stands for any of the above complete sets of a spinless particle. The squared spin operator is trivial, $\hat{S}^2 = \hbar^2 s(s+1)\hat{I}$, so there is effectively just one additional commuting operator, the spin projection $\hat{S}_z$ with quantum number $m_s = -s, \ldots, +s$. This means that the Hilbert space is expanded $(2s+1)$ times relative to the spinless case.

▶ Sets containing total angular momentum ($\hat{A}_{\rm rot}, \hat{L}^2, \hat{S}^2, \hat{J}^2, \hat{J}_z$)

Here $\hat{A}_{\rm rot}$ is an operator invariant under rotations (isotropic Hamiltonian, radial momentum etc.) and $\hat{J}^2, \hat{J}_z$ correspond to $\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$. The eigenvalues of $\hat{J}^2$ are $\hbar^2 j(j+1)$ with $|l-s| \le j \le l+s$ (so j is integer or half-integer for s integer or half-integer, respectively), and the eigenvalues of $\hat{J}_z$ are $m_j = -j, \ldots, +j$.

4a. REPRESENTATION OF PHYSICAL TRANSFORMATIONS

To represent physical observables is not the only role of operators in quantum theory. A specific type of operators, namely the unitary ones, is used to express various kinds of transformations that lead to equivalent descriptions of the same physics. These transformations are applied when switching from one representation to another, or when expressing the action of symmetry operations, such as translations or rotations, on the system.

■ Unitary operators

At first, we explore basic mathematical properties of unitary operators. In a separable Hilbert space, these operators can be introduced as transformations between different orthonormal bases.

▶ Transformations between orthonormal bases

Basis I: $\{|i\rangle\}_i \equiv \{|1\rangle, |2\rangle, \dots\}$ $\quad \langle i|j\rangle = \delta_{ij}$

Basis II: $\{|i'\rangle\}_i \equiv \{|1'\rangle, |2'\rangle, \dots\}$ $\quad \langle i'|j'\rangle = \delta_{ij}$

$|i'\rangle = \hat{U}|i\rangle$ where $\hat{U} \equiv \sum_i |i'\rangle\langle i|$ is an **unitary operator**: $\quad \hat{U}^\dagger = \sum_i |i\rangle\langle i'| = \hat{U}^{-1}$

▶ 3 equivalent definitions of unitary operators

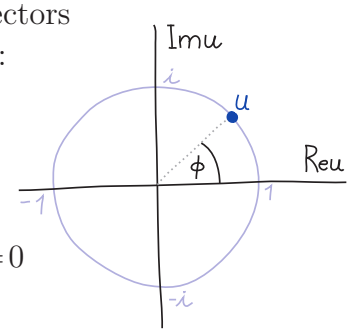
(1) $\hat{U}$ transforms an orthonormal basis to another orthonormal basis: $\boxed{\{|i\rangle\}_i \underset{\hat{U}^{-1}}{\overset{\hat{U}}{\rightleftarrows}} \{|i'\rangle\}_i}$

(2) $\hat{U}$ is invertible such that: $\boxed{\hat{U}^{-1} = \hat{U}^\dagger}$

(3) $\hat{U}$ conserves all scalar products: $\boxed{\langle \hat{U}\psi_1 | \hat{U}\psi_2\rangle = \langle \psi_1|\psi_2\rangle}$

▶ Eigenvalues & eigenvectors of unitary operators

Eigenvalues of $\hat{U}$ lie on a unit circle in $\mathbb{C}$ and eigenvectors corresponding to different eigenvalues are orthogonal:



Consider $\quad \hat{U}|u\rangle = u|u\rangle \quad \Leftrightarrow \quad \langle u|\hat{U}^\dagger = \langle u|u^*$

$$\Rightarrow \langle u|\underbrace{\hat{U}^\dagger\hat{U}}_{\hat{I}}|u\rangle = uu^*\underbrace{\langle u|u\rangle}_{1} \Rightarrow uu^* = 1 \Rightarrow \boxed{u = e^{i\phi}}$$

$$\Rightarrow \langle u|\overbrace{\hat{U}^\dagger\hat{U}}|u'\rangle = u'u^*\langle u|u'\rangle \quad \Rightarrow \quad \underbrace{u'u^*}_{e^{i(\phi'-\phi)}} = 1 \text{ or } \langle u|u'\rangle = 0$$

$$\Rightarrow \text{for } \phi' \neq \phi (\text{mod} 2\pi): \boxed{\langle u|u'\rangle = 0}$$

▶ Spectral decomposition

$$\boxed{\hat{U} = \sum_i \underbrace{e^{i\phi_i}}_{u_i} \underbrace{\hat{P}_{\phi_i}}_{\sum_k |u_i^{(k)}\rangle\langle u_i^{(k)}|}} \text{ with } \boxed{\hat{P}_{\phi_i}\hat{P}_{\phi_j} = \delta_{ij}\hat{P}_{\phi_i}}$$

$k \equiv$ degeneracy index

▶ Expression via exponential of a Hermitian operator

$\boxed{\hat{U} = e^{i\hat{G}}}$ with $\hat{G} = \hat{G}^\dagger$ and $\boxed{e^{\hat{X}} \equiv \sum_{k=0}^{\infty} \frac{\hat{X}^k}{k!}}$ exponential of an operator defined through the Taylor series of e^x

(a) exponential $\Rightarrow$ unitary: $\hat{U}^\dagger = \sum_{k=0}^{\infty} \frac{(-i\hat{G})^k}{k!} = e^{-i\hat{G}} = \hat{U}^{-1}$

(b) exponential $\Leftarrow$ unitary: $\forall\, \hat{U} \equiv \sum_i e^{i\phi_i}\hat{P}_{\phi_i}$ define $\boxed{\hat{G} \equiv \sum_i \phi_i \hat{P}_{\phi_i}} = \hat{G}^\dagger \Rightarrow \hat{U} = e^{i\hat{G}}$

► **Example**: $\hat{U} = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$

Eigenvalues $u_1 = 1 = e^{i0}$ and $u_2 = -1 = e^{i\pi}$

Eigenvectors $|+1\rangle \equiv \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right)$ and $|-1\rangle \equiv \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} +1 \\ -1 \end{smallmatrix}\right)$ (orthonormal)

$\hat{G} = 0|+1\rangle\langle+1| + \pi|-1\rangle\langle-1| = \frac{\pi}{2}\left(\begin{smallmatrix} +1 & -1 \\ -1 & +1 \end{smallmatrix}\right)$ with $\left(\begin{smallmatrix} +1 & -1 \\ -1 & +1 \end{smallmatrix}\right)^k = 2^{k-1}\left(\begin{smallmatrix} +1 & -1 \\ -1 & +1 \end{smallmatrix}\right)$ for $k \geq 1$

$$e^{i\hat{G}} = \hat{I} + \underbrace{\sum_{k=1}^{\infty} \frac{(i\pi)^k}{k!}}_{e^{i\pi}-1=-2} \underbrace{\left[\tfrac{1}{2}\left(\begin{smallmatrix} +1 & -1 \\ -1 & +1 \end{smallmatrix}\right)\right]^k}_{\frac{1}{2}\left(\begin{smallmatrix} +1 & -1 \\ -1 & +1 \end{smallmatrix}\right)} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) - \left(\begin{smallmatrix} +1 & -1 \\ -1 & +1 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right) = \hat{U}$$

► **Commutation relation for exponentials**

$e^{\hat{X}}e^{\hat{Y}} = e^{\hat{Y}}e^{\hat{X}} = e^{\hat{X}+\hat{Y}}$ for $[\hat{X},\hat{Y}] = 0$, $\boxed{e^{\hat{X}}e^{\hat{Y}} \neq e^{\hat{Y}}e^{\hat{X}} \neq e^{\hat{X}+\hat{Y}}}$ for $[\hat{X},\hat{Y}] \neq 0$

Baker-Campbell-Hausdorff (BCH) formula (one of its forms):

$$e^{\hat{X}}\hat{A}e^{-\hat{X}} = \underbrace{\hat{A}}_{[\hat{X},\hat{A}]_0} + \tfrac{1}{1!}\underbrace{[\hat{X},\hat{A}]}_{[\hat{X},\hat{A}]_1} + \tfrac{1}{2!}\underbrace{[\hat{X},[\hat{X},\hat{A}]]}_{[\hat{X},\hat{A}]_2} + \tfrac{1}{3!}\underbrace{[\hat{X},[\hat{X},[\hat{X},\hat{A}]]]}_{[\hat{X},\hat{A}]_3} \ldots + \tfrac{1}{k!}\,[\hat{X},\hat{A}]_k + \ldots$$

This means that $e^{\hat{X}}e^{\hat{Y}} = \left(e^{\hat{Y}} + \sum_{k=1}^{\infty} \frac{1}{k!}\,[\hat{X},e^{\hat{Y}}]_k\right) e^{\hat{X}}$, or in another form:

$e^{\hat{X}}e^{\hat{Y}} = e^{\hat{Z}}$ with $\hat{Z} = \hat{X}+\hat{Y}+\frac{1}{2}[\hat{X},\hat{Y}]+\frac{1}{12}([\hat{X},\hat{Y}]_2+[\hat{Y},\hat{X}]_2)-\frac{1}{24}[\hat{Y},[\hat{X}\hat{Y}]_2]+\ldots$

Special case: $[\hat{X},[\hat{X},\hat{Y}]] = [\hat{Y},[\hat{X},\hat{Y}]] = \cdots = 0 \quad \Rightarrow \quad \boxed{e^{\hat{X}}e^{\hat{Y}} = e^{\hat{X}+\hat{Y}}e^{\frac{1}{2}[\hat{X},\hat{Y}]}}$

■ Unitary transformations as "quantum canonical transformations"

Unitary operators materialize transitions between alternative QM representations, defined by distinct bases in the system's Hilbert space (see Sec. 3a). They also express transformations between state vectors of the same system as seen from various reference frames, differing, e.g., by translations, rotations, or Galilean boosts. Physical descriptions in all these representations or reference frames must be fully equivalent. In this sense, the unitary transformations are analogues of classical canonical transformations.

► **Diagonalization of an operator**

The transformation from a general basis $\{|i\rangle\}_i$ to an eigenbasis $\{|a_j^{(k)}\rangle\}_{j,k}$ of any Hermitian operator $\hat{A}$ is of course a unitary transformation. We assume for a moment a nondegenerate spectrum $\{a_i\}_i$ of $\hat{A}$. The degenerate case would be expressed analogously but in a clumsier notation.

$$\underbrace{\begin{pmatrix} U_{11} & U_{12} & \ldots \\ U_{21} & U_{22} & \\ \vdots & & \ddots \end{pmatrix}}_{\hat{U}} \underbrace{\begin{pmatrix} A_{11} & A_{12} & \ldots \\ A_{21} & A_{22} & \\ \vdots & & \ddots \end{pmatrix}}_{\hat{A}} \underbrace{\begin{pmatrix} U_{11}^* & U_{21}^* & \ldots \\ U_{12}^* & U_{22}^* & \\ \vdots & & \ddots \end{pmatrix}}_{\hat{U}^\dagger} = \underbrace{\begin{pmatrix} a_1 & 0 & \ldots \\ 0 & a_2 & \\ \vdots & & \ddots \end{pmatrix}}_{\hat{A}_{\rm diag}} \Rightarrow \boxed{\hat{A}_{\rm diag} = \hat{U}\hat{A}\,\hat{U}^\dagger}$$

eigenvectors $\boxed{|a_i\rangle \equiv \begin{pmatrix} U_{i1}^* \\ U_{i2}^* \\ \vdots \end{pmatrix}}$

▶ Link between equivalent representations

Postulate: Various representations of quantum state vectors & operators are equivalent *iff* they are connected by a unitary transformation

We assume a general transformation of bases $\{|i\rangle\}_i \xrightarrow{\hat{U}} \{|i'\rangle\}_i$. This implies:

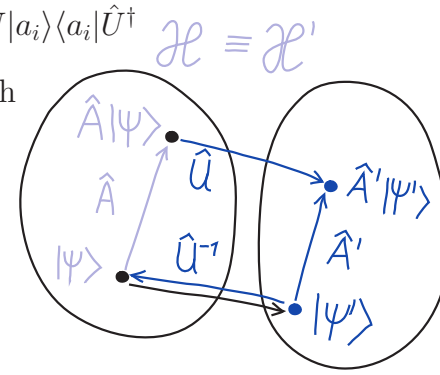
Transformation of vectors: $\boxed{|\psi'\rangle = \hat{U}|\psi\rangle}$

$$|\psi\rangle = \sum_i \alpha_i |i\rangle \quad \mapsto \quad |\psi'\rangle = \sum_i \alpha_i |i'\rangle$$

Transformation of operators: $\boxed{\hat{A}' = \hat{U}\hat{A}\,\hat{U}^\dagger} = \hat{U}\hat{A}\,\hat{U}^{-1}$

$$\hat{A} = \sum_i a_i \hat{P}_{a_i} \quad \mapsto \quad \hat{A}' = \sum_i a_i \hat{U}\hat{P}_{a_i}\hat{U}^\dagger = \sum_i a_i \hat{U}|a_i\rangle\langle a_i|\hat{U}^\dagger$$

Interpretation of the operator relation through the identity $\hat{A}'|\psi'\rangle = \hat{U}\big(\hat{A}\underbrace{|\psi\rangle}_{\hat{U}^{-1}|\psi'\rangle}\big)$, with $\hat{A}'|\psi'\rangle$ defined via the "detour path" $\hat{U}\hat{A}\hat{U}^{-1}|\psi'\rangle$ (see the sketch where the target space of $\hat{U}$ is formally denoted as $\mathcal{H}'$)



◀ Historical remark

1897-1906: Independent derivations of the Baker-Campbell-Hausdorff formula
1900-10: David Hilbert elaborates the theory of (unitary) operators in $\mathcal{H}$
1927-32: Unitary operators and representation theory appear in the mathematical formulation of QM (P. Dirac, J.von Neumann)

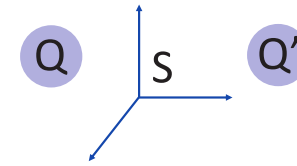
■ Symmetry in quantum mechanics

It is often repeated that symmetry represents the most powerful concept in physics. The famous Weyl's definition "*A thing is symmetrical if there is something you can do to it so that after you have finished doing it it looks the same as before*" can be always applied (in fact, this is Feynman's informal transcription of Weyl's original formulation). For us, the *thing* means either a given physical system (its most essential attributes) or a general form of its quantum description. *To do something to it* then means to look at the system from another reference frame or through a different representation.

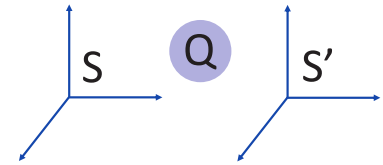
▶ Active and passive transformations

Let us consider two frameworks S and S', which correspond to alternative reference frames (coordinate systems) or alternative ways of description (representations). Transformations between these frames can be realized in the "active" or "passive" way:

Active transformation:
Operators $\hat{A}$ unchanged
State vectors transformed $|\psi\rangle \mapsto |\psi'\rangle = \hat{U}|\psi\rangle$
Example: an atom that has moved from the Earth to Mars is watched from the same motionless reference frame



Passive transformation:
State vectors $|\psi\rangle$ unchanged
Operators transformed $\hat{A} \mapsto \hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$
Example: a motionless atom is watched from a reference frame that has been moved from the Earth to Mars



▶ Symmetry in a wider sense (sensu lato)

The simultaneous active and passive transformation ("a moved atom observed from a moved frame") yields identity. More precisely, a simultaneous transformation of state vectors $|\psi\rangle \mapsto |\psi'\rangle = \hat{U}|\psi\rangle$ and operators $\hat{A} \mapsto \hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$ preserves the structure and all predictions of quantum theory:

$\langle\psi_1'|\psi_2'\rangle = \langle\hat{U}\psi_1|\hat{U}\psi_2\rangle = \langle\psi_1|\underbrace{\hat{U}^\dagger\hat{U}}_{\hat{I}}|\psi_2\rangle = \langle\psi_1|\psi_2\rangle$ ...scalar products

$\langle i'|\hat{A}'|j'\rangle = \langle i|\overbrace{\hat{U}^\dagger\hat{U}}^{\hat{I}}\,\hat{A}\,\overbrace{\hat{U}^\dagger\hat{U}}^{\hat{I}}|j\rangle = \langle i|\hat{A}|j\rangle$ ...matrix elements

$\hat{A}|a\rangle = a|a\rangle \Rightarrow \underbrace{\hat{U}\hat{A}\hat{U}^\dagger}_{\hat{A}'}\underbrace{\hat{U}|a\rangle}_{|a'\rangle} = a\underbrace{\hat{U}|a\rangle}_{|a'\rangle}$ ...eigenvalues

$\overbrace{[\hat{A}',\hat{B}']}^{i\hat{C}} = \hat{A}'\hat{B}' - \hat{B}'\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger\hat{U}\hat{B}\hat{U}^\dagger - \hat{U}\hat{B}\hat{U}^\dagger\hat{U}\hat{A}\hat{U}^\dagger = \overbrace{\hat{U}[\hat{A},\hat{B}]\hat{U}^\dagger}^{i\hat{C}'}$ ...commutators

$\Rightarrow$ $\boxed{\mathrm{QM}_{S'} = \mathrm{QM}_S}$ The QM description is the same for both S & S'. This only means that quantum theory by its very nature includes the notion of symmetry.

▶ Symmetry in a narrower sense (sensu stricto)

This kind of symmetry concerns *specific systems* rather than the whole theory. We say that a particular system is invariant under the S → S' transformation *iff* its Hamiltonian does not change under that transformation: $\boxed{\hat{H}' = \hat{H}}$
This is because for any system the Hamiltonian represents the most important physical operator (describing also the dynamics, see Sec. 5a).

$\hat{H}' = \hat{U}\hat{H}\,\hat{U}^\dagger = \hat{H} \;\Rightarrow \hat{U}\hat{H} = \hat{H}\hat{U} \;\Rightarrow$ $\boxed{[\hat{H},\hat{U}] = 0 \;\Leftrightarrow\; [\hat{H},\hat{G}] = 0}$ (with $\hat{U} = e^{i\hat{G}}$)

This has strong consequences:

(a) **degeneracy** of energy levels: $\hat{H}|\psi\rangle = E|\psi\rangle \quad \Rightarrow$ $\boxed{\hat{H}(\hat{U}|\psi\rangle) = E(\hat{U}|\psi\rangle)}$
$\Rightarrow$ if $\hat{U}|\psi\rangle \neq |\psi\rangle$, the level E is degenerate

(b) **conservation laws** (the existence of integrals of motions, see Sec. 5a)

■ One flight over the group theory

Unitary transformations describing symmetries of physical systems do most typically come in some specific sets, which are called groups. A clear example can be the infinite group of rotations by different angles around various axes. Group theory represents a superb case of "the unreasonable effectiveness of mathematics in the natural sciences" (as pointed out by E. Wigner). Initiated as a purely theoretical discipline, it grew into one of the most commonly applied branches of mathematics today. Here we just summarize (from a bird's eye view) the very basic concepts that are of immediate importance for QM.

► Basic definitions

Group $\mathcal{G}$ is a set of elements $\{g\}$ which is closed with respect to a binary operation $\circ$ (group multiplication) $\boxed{g_1, g_2 \in \mathcal{G} \Rightarrow \underbrace{(g_1 \circ g_2)}_{\equiv g_1 g_2} \in \mathcal{G}}$ satisfying the following properties:

(1) $(g_1 g_2) g_3 = g_1 (g_2 g_3)$ associativity
(2) $\exists\ e \in \mathcal{G} :\ ge = eg = g\ \forall g \in \mathcal{G}$ unit element
(3) $\forall\ g \in \mathcal{G}\ \exists\ g^{-1} :\ gg^{-1} = g^{-1}g = e$ inverse elements

Note: Commutativity is not required! If it is also satisfied, so if $g_1 g_2 = g_2 g_1$ $\forall\ g_1, g_2 \in \mathcal{G}$, the group is called **Abelian**.

► Unitary representation of group $\mathcal{G}$

Mapping to unitary operators: $\boxed{g \ \mapsto\ \hat{U}_g}$, $\boxed{g_1 g_2 \ \mapsto\ \hat{U}_{g_2}\hat{U}_{g_1} \ \equiv\ \hat{U}_2\hat{U}_1}$

Group properties naturally satisfied: $(\hat{U}_2\hat{U}_1)^\dagger = \hat{U}_1^{-1}\hat{U}_2^{-1} = (\hat{U}_2\hat{U}_1)^{-1}$ closure
(1) $(\hat{U}_3\hat{U}_2)\hat{U}_1 = \hat{U}_3(\hat{U}_2\hat{U}_1)$ associativity
(2) $e \ \mapsto\ \hat{I} = \hat{I}^\dagger = \hat{I}^{-1}$ unit element
(3) $\hat{U} = e^{i\hat{A}} \Rightarrow \hat{U}^{-1} = e^{-i\hat{A}}$ inverse elements

Hilbert space $\mathcal{H}$ where operators $\hat{U}_g$ act $\equiv$ **carrier space** of $\mathcal{G}$
Since QM works with $\mathcal{H}$, it provides a direct physical "arena" for group theory.

Invariant subspace: a subspace $\mathcal{H}_\mathcal{G} \subset \mathcal{H}$ is invariant under $\mathcal{G}$ if $\hat{U}_g|\psi\rangle \in \mathcal{H}_\mathcal{G}$ $\forall\, \hat{U}_g \in \mathcal{G}$ and $\forall\, |\psi\rangle \in \mathcal{H}_\mathcal{G}$

Matrix representation: $\hat{U}_g \equiv \begin{pmatrix} \ddots & 0 & \cdots & & \\ 0 & \boxed{\in \mathcal{H}_\mathcal{G}^{(1)}} & 0 & & \\ \vdots & 0 & \ddots & 0 & \\ & & 0 & \boxed{\in \mathcal{H}_\mathcal{G}^{(2)}} & \\ & & & & \ddots \end{pmatrix}$ block diagonal structure of all $\hat{U}_g \in \mathcal{H}_\mathcal{G}$

Any invariant subspace $\mathcal{H}_\mathcal{G}^{(i)}$ and the corresponding submatrices of group operators $\hat{U}_g$ can serve as a complete representation of $\mathcal{G}$.
Irreducible representation (irrep) of group $\mathcal{G}$: representation for which there are no invariant subspaces $\mathcal{H}_\mathcal{G} \subset \mathcal{H}$.

▶ Finite (discrete) groups

Groups with a finite (or at least discrete) number of elements (describe, e.g., spatial symmetries of crystals or reflection transformations): $\boxed{\mathcal{G} \equiv \{g_i\}_{i\in\mathbb{N}}}$

Example: **cyclic group** $\boxed{\mathcal{Z}_2 \equiv \{\hat{P}, \hat{I}\}}$ with $\hat{I} \equiv$ unit operator and $\hat{P} \equiv$ generalized **parity transformation** satisfying $\hat{P} = \hat{P}^{-1} = \hat{P}^\dagger$ $(\Rightarrow \hat{P}^2 = \hat{I})$ that can represent the spatial inversion, 2-particle exchange, particle-antiparticle or particle-hole transformation etc.

▶ Continuous (Lie) groups

Groups with elements parametrized by a n-dimensional real vector $\vec{s} \Rightarrow$ the group elements (e.g., spatial translations) form a continuum: $\boxed{\mathcal{G} \equiv \{g(\vec{s})\}_{\vec{s}\in\mathbb{R}^n}}$

The group operations between various pairs of elements and the inversion of various single elements define some $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ and $\mathbb{R}^n \to \mathbb{R}^n$ functions:

$$\begin{array}{lll} g(\vec{s}_1)g(\vec{s}_2)=g(\vec{s}_3) & \Rightarrow & \vec{s}_3 = \vec{f}(\vec{s}_1, \vec{s}_2) \\ g(\vec{s})^{-1} = g(\vec{s}\,') & \Rightarrow & \vec{s}\,' = \vec{h}(\vec{s}) \end{array} \qquad \begin{array}{l} \text{If both functions } \vec{f} \;\&\; \vec{h} \text{ are fully} \\ \text{differentiable, then } \mathcal{G} \text{ is a } \textbf{Lie group} \end{array}$$

Unitary representation of a given Lie group is a mapping to a continuous family of unitary operators acting in a suitable Hilbert space: $\boxed{\boxed{g(\vec{s}) \mapsto \hat{U}(\vec{s})}}$

▶ One-parameter Lie group $\quad \boxed{\boxed{\mathcal{G} \equiv \{\hat{U}(s)\}_{s\in\mathbb{R}}}}$

Requirements: $\begin{cases} \hat{U}(0) = \hat{I} & \text{choice of origin} \qquad \overset{!}{=} 1 \\ \hat{U}(s+ds) = \hat{U}(s)\hat{U}(ds) & \text{local additivity} \Leftarrow f(s,ds) = s + \overbrace{\frac{\partial f}{\partial s_2}}^{\overset{!}{=}1} ds \end{cases}$

$$\left.\begin{array}{l} \hat{U}(s) = \hat{I} + \left(\frac{d\hat{U}}{ds}\right)_0 s + \frac{1}{2}\left(\frac{d^2\hat{U}}{ds^2}\right)_0 s^2 + \ldots \\ \hat{U}(s)\hat{U}(s)^\dagger = \hat{I} + \underbrace{\left[\left(\frac{d\hat{U}}{ds}\right)_0 + \left(\frac{d\hat{U}}{ds}\right)_0^\dagger\right]}_{0} s + \underbrace{[\ldots]}_{0} s^2 + \ldots \end{array}\right\} \Rightarrow \begin{array}{l} \left(\frac{d\hat{U}}{ds}\right)_0 = i\hat{G} \\ \text{with } \boxed{\hat{G} = \hat{G}^\dagger} \end{array}$$

$$\Rightarrow \text{condition} \quad \left(\frac{d\hat{U}}{ds}\right)_s = \lim_{ds\to 0} \frac{\hat{U}(s+ds) - \hat{U}(s)}{ds} = \hat{U}(s)\left(\frac{d\hat{U}}{ds}\right)_0 = i\hat{U}(s)\hat{G}$$

$\boxed{\boxed{\hat{U}(s) = e^{i\hat{G}s}}}$ is the most general solution, where $\hat{G} \equiv$ **generator** of $\mathcal{G}$

$\Rightarrow$ the group is **Abelian**: $\hat{U}(s_1)\hat{U}(s_2) = \hat{U}(s_1+s_2) = \hat{U}(s_2)\hat{U}(s_1)$

▶ Multiparameter Lie group $\quad \boxed{\boxed{\mathcal{G} \equiv \{\hat{U}(\vec{s})\}_{\vec{s}\in\mathbb{R}^n} \quad n \geq 2}}$

$\boxed{\boxed{\hat{U}(\vec{s}) = e^{i\vec{\hat{G}}\cdot\vec{s}}}} = e^{i\sum_{k=1}^{n} \hat{G}_k s_k}$ with $\vec{\hat{G}} \equiv \left\{\hat{G}_k = \frac{1}{i}\left(\frac{\partial U(\vec{s})}{\partial s_k}\right)_{\vec{s}=0}\right\}_{k=1}^{n} \equiv$ set of generators

$$\neq \prod_{k=1}^{n} e^{i\hat{G}_k s_k} \qquad \text{in the } \textbf{non-Abelian} \text{ case: } [\hat{G}_k, \hat{G}_l] \neq 0$$

$$\hat{U}(\vec{s}_1)\hat{U}(\vec{s}_2) \neq \hat{U}(\vec{s}_1+\vec{s}_2) \neq \hat{U}(\vec{s}_2)\hat{U}(\vec{s}_1)$$

Taylor expansion: $\overbrace{\hat{I}+i\hat{G}_i s_i-\frac{1}{2}\hat{G}_i\hat{G}_{i'}s_i s_{i'}-\frac{i}{6}\hat{G}_i\hat{G}_{i'}\hat{G}_{i''}s_i s_{i'}s_{i''}+\ldots}^{\text{summation conv.}}$

$$\hat{U}(\vec{s}) \approx \hat{I}+\frac{i}{1!}\sum_i \hat{G}_i s_i-\frac{1}{2!}\sum_{i,i'}\hat{G}_i\hat{G}_{i'}s_i s_{i'}-\frac{i}{3!}\sum_{i,i',i''}\hat{G}_i\hat{G}_{i'}\hat{G}_{i''}s_i s_{i'}s_{i''}+\ldots$$

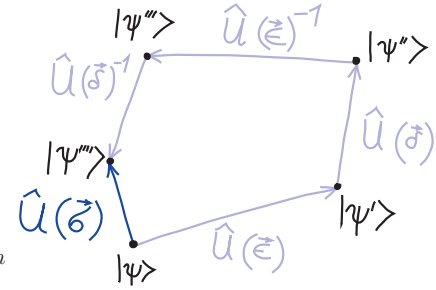
▶ Algebra of generators

Products of infinitesimal unitary transformations $\hat{U}(\delta\vec{s})$ form again some infinitesimal unitary transformations (closure property of $\mathcal{G}$). This turns out to imply that the generators must form a closed set (so called algebra) with respect to commutation relations. We show this by the following product of 4 infinitesimal transformations:

$$\underbrace{\hat{U}(\vec{\delta})^{-1}\hat{U}(\vec{\epsilon})^{-1}\hat{U}(\vec{\delta})\hat{U}(\vec{\epsilon})}_{\approx} = \underbrace{\hat{U}(\vec{\sigma})}_{\approx} \qquad \text{with } \boxed{\sigma_l \approx \sum_{mn} S_{mnl}\epsilon_m\delta_n} \text{ for } \vec{\epsilon},\vec{\delta}\to 0$$

$$\underbrace{\begin{array}{c}(\hat{I}-i\hat{G}_i\delta_i-\frac{1}{2}\hat{G}_i\hat{G}_{i'}\delta_i\delta_{i'})\\ \times(\hat{I}-i\hat{G}_j\epsilon_j-\frac{1}{2}\hat{G}_j\hat{G}_{j'}\epsilon_j\epsilon_{j'})\\ \times(\hat{I}+i\hat{G}_k\delta_k-\frac{1}{2}\hat{G}_k\hat{G}_{k'}\delta_k\delta_{k'})\\ \times(\hat{I}+i\hat{G}_l\epsilon_l-\frac{1}{2}\hat{G}_l\hat{G}_{l'}\epsilon_l\epsilon_{l'})\end{array}}_{\approx \text{ (up to 2nd order)}} \qquad \hat{I}+i\hat{G}_l\sigma_l$$

$$\hat{I}+\underbrace{(\hat{G}_m\hat{G}_n-\hat{G}_n\hat{G}_m)}_{[\hat{G}_m,\hat{G}_n]}\epsilon_m\delta_n = \hat{I}+iS_{mnl}\hat{G}_l\epsilon_m\delta_n$$



$$\Rightarrow \boxed{[\hat{G}_m,\hat{G}_n]=i\sum_l S_{mnl}\hat{G}_l}$$

closure relation for algebra of generators

$S_{mnl} \equiv$ **structure constants**

So instead of studying the infinite set $\hat{U}(\vec{s}) \in \mathcal{G}$, we can focus on the finite algebra of generators $\{\hat{G}_i\}_{i=1}^n$, whose structure constants characterize the group $\mathcal{G}$. However, in some cases, the generator algebra alone does not distinguish some subtle differences between groups, see the $\mathrm{O}(n)$ and $\mathrm{SO}(n)$ examples below.

▶ Invariant (Casimir) operator

An operator $\hat{C}_\mathcal{G} \equiv \hat{C}(\hat{\vec{G}})$ associated with group $\mathcal{G}$ such that $\boxed{[\hat{C}_\mathcal{G},\hat{G}_i]=0}$ $\forall i$

Eigenspaces of $\hat{C}_\mathcal{G}$ within the space $\mathcal{H}$ are invariant under the action of all generators $\{\hat{G}_i\} \Rightarrow$ these subspaces often carry irreducible representations of $\mathcal{G}$

▶ Examples: orthogonal and unitary groups in finite dimensions

Unitary group U(d): group of unitary matrices $\hat{U}$ of dimension d

It has $\boxed{n=d^2}$ Hermitian generators: $i=1,2,\ldots,d^2$

$$\hat{G}_i = \underbrace{\begin{pmatrix}1&0&0&\ldots&0\\0&0&0&\ldots&0\\0&0&0&\ldots&0\\\vdots&&&&\vdots\\0&0&0&\ldots&0\end{pmatrix},\ldots}_{d \text{ diagonal}},\ \underbrace{\begin{pmatrix}0&1&0&\ldots&0\\1&0&0&\ldots&0\\0&0&0&\ldots&0\\\vdots&&&&\vdots\\0&0&0&\ldots&0\end{pmatrix},\ldots}_{\frac{d(d-1)}{2} \text{ offdiag. real}},\ \underbrace{\begin{pmatrix}0&-i&0&\ldots&0\\i&0&0&\ldots&0\\0&0&0&\ldots&0\\\vdots&&&&\vdots\\0&0&0&\ldots&0\end{pmatrix},\ldots}_{\frac{d(d-1)}{2} \text{ offdiag. imaginary}}$$

Casimir operator must be proportional to the unit matrix $\hat{I}$. There are two independent ways how to build such an operator from the generators, which yields linear and quadratic invariants $\hat{C}^{(1)}$ and $\hat{C}^{(2)}$:

$$\boxed{\begin{aligned}\hat{C}^{(1)}_{\mathrm{U}(d)} &= \sum_{i=1}^{d} \hat{G}_i = \hat{I} \\ \hat{C}^{(2)}_{\mathrm{U}(d)} &= \sum_{i=1}^{d^2} \hat{G}_i^2 = (2d-1)\hat{I}\end{aligned}}$$

In fact, 3 independent quadratic invariants exist with i running separately over the diagonal, offdiagonal real and offdiagonal imaginary generators.

Special unitary group SU(d): subgroup of U(d) including unitary matrices $\hat{U}$ of dimension d with $\mathrm{Det}\,\hat{U}=1$ (property conserved in multiplications)

From $\mathrm{Det}\, e^{\hat{A}} = e^{\mathrm{Tr}\,\hat{A}}$ it follows that SU(d) has $\boxed{n=d^2-1}$ generators: $d(d-1)$ of them coincide with the offdiagonal generators of U(d) and the remaining $d-1$ ones with independent traceless linear combinations $\hat{G}'_i$ of the diagonal U(n) generators, e.g. $\hat{G}'_i = \hat{G}_i - \frac{1}{d}\hat{I}$ for $i=1,..,d-1$. Only quadratic (& higher) Casimir operators: $\hat{C}^{(2)}_{\mathrm{SU}(d)} = \sum_{i=d+1}^{d^2} \hat{G}_i^2 = (2d-2)\hat{I}$, $\hat{C}^{(2)'}_{\mathrm{SU}(d)} = \sum_{i=1}^{d-1} \hat{G}_i'^2 + \sum_{i,j=1}^{d-1} \hat{G}'_i\hat{G}'_j \propto \hat{I}$

Special orthogonal group SO(d): subgroup of SU(d) including orthogonal matrices $\hat{O}$ of dimension d with $\mathrm{Det}\,\hat{O}=1$ (conserved in multiplications)

Because of reality of $\hat{O}$, the generators coincide with the $\boxed{n=\frac{1}{2}d(d-1)}$ imaginary offdiagonal generators of U(d), which automatically leads to the unit determinant. Unique quadratic Casimir invariant:

$$\boxed{\hat{C}^{(2)}_{\mathrm{SO}(d)} = \sum_{i=\frac{d(d+1)}{2}+1}^{d^2} \hat{G}_i^2 = (d-1)\hat{I}}$$

Orthogonal group O(d): subgroup of U(d) including orthogonal matrices $\hat{O}$ of dimension d with $\mathrm{Det}\,\hat{O} = \pm 1$. This group is richer than SO(d) (containing it as a subgroup), but has the same set of generators. It arises from SO(d) by adding a single orthogonal matrix (or a discrete set) whose action on any $\hat{O} \in \mathrm{SO}(d)$ yields matrices with determinant $= -1$. It can be, e.g., any of the $i = 1, \ldots, d$ operators $e^{i\pi\hat{G}_i}$. The quadratic Casimir invariant: $\hat{C}^{(2)}_{\mathrm{O}(d)} = \hat{C}^{(2)}_{\mathrm{SO}(d)}$

◀ Historical remark

1830 (approx.): dawn of the group theory (the name given by É. Galois)
1873: Sophus Lie introduces continuous groups (later work of W. Killing, E. Cartan)
1928-32: M.H. Stone and J.von Neumann obtain QM-related results on Lie groups
1928: Hermann Weyl: *Gruppentheorie und Quantenmechanik*—book placing the group theory to the foundations of QM
1927-37: Eugene Wigner elaborates group techniques in the classification of atomic and later nuclear spectra; the 1931 book *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra*
1929: Hans Bethe applies point groups in polyatomic molecules
1931: Hendrik Casimir introduces the invariant operator
1940's-50's: Giulio Racah refines group methods in the theory of complex spectra

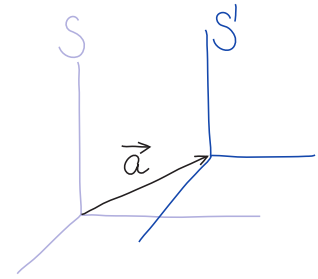
4b. EXAMPLES OF SYMMETRY TRANFORMATIONS

We will now describe basic spatial and spatio-temporal transformations of non-relativistic quantum systems. We will see that quantum operators of elementary physical observables can be naturally introduced as generators of the corresponding Lie groups. This may tempt us to think about quantum Hilbert spaces and sets of observables in terms of representations of the fundamental symmetries of nature, seeking the origin of quantum uncertainty relations in the non-Abelian character of the corresponding groups. We will also introduce a very powerful calculus of spherical tensors that have specific transformation properties under spatial rotations.

■ Space translation

We start with the most trivial transformations, namely translations in the coordinate space. These form an Abelian group generated by momentum operators. We will also shortly visit crystals with their band energy spectra.

▶ Coordinate translation operator



We consider a translation of the coordinate system by a fixed vector $\vec{a}$. From the analogy with classical relation $\vec{x}\,' = \vec{x} - \vec{a}$ we require that the unitary operator $\hat{T}_{\vec{a}}$ that describes the translation must satisfy the following relation: $\boxed{\hat{T}_{\vec{a}}\,\hat{\vec{x}}\,\hat{T}_{\vec{a}}^{-1} = \hat{\vec{x}} - \vec{a}\hat{I}}$

$\Rightarrow$ commutation relations $[\hat{x}_i, \hat{T}_{\vec{a}}] = a_i \hat{T}_{\vec{a}}$

coincide with the relations of general shift operators $\begin{cases} [\hat{A},\hat{T}_\Delta^\dagger]=+\Delta\hat{T}_\Delta^\dagger \\ [\hat{A},\hat{T}_\Delta]=-\Delta\hat{T}_\Delta \end{cases}$

$\Rightarrow \quad \hat{T}_{\vec{a}}^{-1} = \hat{T}_{\vec{a}}^\dagger = \hat{T}_{-\vec{a}}$

$\Rightarrow \quad \hat{x}_i|\vec{x}\rangle = x_i|\vec{x}\rangle \quad \Rightarrow \quad \hat{x}_i(\hat{T}_{\vec{a}}|\vec{x}\rangle) = (x_i + a_i)(\hat{T}_{\vec{a}}|\vec{x}\rangle) \quad \Rightarrow \quad \boxed{\hat{T}_{\vec{a}}|\vec{x}\rangle = |\vec{x}+\vec{a}\rangle}$

proportionality coefficient $\sqrt{\langle\vec{x}|\hat{T}_{\vec{a}}^{-1}\hat{T}_{\vec{a}}|\vec{x}\rangle} = 1$

$\Rightarrow \quad \langle\vec{x}|\hat{T}_{\vec{a}}\,\psi\rangle = \langle\hat{T}_{\vec{a}}^{-1}\vec{x}|\psi\rangle = \langle\vec{x}-\vec{a}|\psi\rangle = \boxed{\psi(\vec{x}-\vec{a}) = \hat{T}_{\vec{a}}\,\psi(\vec{x})}$ transformation of wavefunctions

▶ Generators of translations along coordinate axes

Translation $\vec{a} = a\vec{n}_j$ along $j = 1, 2, 3$ axes: $[\hat{x}_i, \hat{T}_{a\vec{n}_j}] = \delta_{ij} a \hat{T}_{a\vec{n}_j}$

Infinitesimal translations: $\hat{T}_{(\delta a)\vec{n}_j} \approx \hat{I} + i\hat{G}_j(\delta a) \quad \Rightarrow \quad \boxed{[\hat{x}_i, \hat{G}_j] = -i\delta_{ij}\hat{I}}$

This is essentially the commutation relation of the momentum operator and we can set: $\boxed{\hat{G}_j = -\frac{1}{\hbar}\hat{p}_j}$ i.e., generators of translations are proportional to momentum component operators

$[\hat{G}_i, \hat{G}_j] = 0 \quad \Rightarrow$ **Abelian group** $\qquad [\hat{G}_i, \hat{p}_j] = 0 \quad \Rightarrow \quad \boxed{\hat{T}_{\vec{a}}\,\hat{\vec{p}}\,\hat{T}_{\vec{a}}^{-1} = \hat{\vec{p}}}$

▶ Finite translations in any direction

Finite translation along the j^{th}axis is obtained by repetitions of many small translations: $\hat{T}_{a\vec{n}_j} = \lim\limits_{n\to\infty}\left(\hat{I} - \frac{i}{\hbar}\hat{p}_j\frac{a}{n}\right)^n = e^{-i\frac{a\hat{p}_j}{\hbar}}$

Finite translation along a general direction: $\boxed{\hat{T}_{\vec{a}} = e^{-i\frac{\vec{a}\cdot\hat{\vec{p}}}{\hbar}}}$

Direct verification for the wavefunction transformation:
$\hat{T}_{\vec{a}}\,\psi(\vec{x}) = \sum\limits_{k=0}^{\infty}\frac{1}{k!}(-\vec{a}\cdot\vec{\nabla})^k\psi(\vec{x}) = \psi(\vec{x}-\vec{a})$

▶ Translation for many-particle systems

The spatial translation operator for $N \geq 2$ systems is generated by the total momentum operator $\hat{\vec{P}} = \sum\limits_{k=1}^{N}\hat{\vec{p}}_k \quad \Rightarrow \quad \hat{T}_{\vec{a}} = e^{-i\frac{\vec{a}\cdot\hat{\vec{P}}}{\hbar}} = \bigotimes\limits_{k=1}^{N}\hat{T}_{\vec{a},k}$

$$\Rightarrow \ (\hat{T}_{\vec{a}}\Psi)(\vec{x}_1,\ldots,\vec{x}_N) = \Psi(\vec{x}_1-\vec{a},\ldots,\vec{x}_N-\vec{a})$$

Translation does not affect the spin variables (if any) of individual particles.

▶ Translational invariance sensu stricto

A system is invariant under spatial translations *iff* $[\hat{T}_{\vec{a}}, \hat{H}] = 0$. This means that the Hamiltonian must commute with all the generators — the components of the (total) momentum operator $\hat{\vec{P}}$.

For $N = 1$ particle this means that $\hat{H} = H(\hat{\vec{p}}, \hat{\vec{S}})$ ⇒ Hamiltonian does not depend on spatial coordinates, only on momentum and spin components

For $N \geq 2$ particles: $\boxed{\hat{H} = H\left(\{\hat{\vec{p}}_k\}, \{\hat{\vec{x}}_k - \hat{\vec{x}}_l\}, \{\hat{\vec{S}}_k\}\right)}$ ⇒ Hamiltonian depends only on *relative coordinates*, for instance: $\hat{H} = \sum\limits_k \frac{1}{2M_k}\hat{\vec{p}}_k^{\,2} + \sum\limits_{k\geq l} V\left(\{\hat{\vec{x}}_k - \hat{\vec{x}}_l\}\right)$

▶ Discrete translations (invariance of a crystal lattice)

We consider the simplest cubic crystal lattice whose elementary cell has sides $\vec{L} \equiv (L_x, L_y, L_z)$. The Hamiltonian of a single particle moving in such an infinite periodic structure is symmetric (sensu stricto) under a discrete set of translation transformations $\hat{T}_{\vec{a}_{\vec{n}}} = e^{-i\frac{\vec{a}_{\vec{n}}\cdot\hat{\vec{p}}}{\hbar}}$ with translation vectors $\vec{a}_{\vec{n}} = (n_x L_x, n_y L_y, n_z L_z) = \vec{n}\cdot\vec{L}$, where $n_i = 0, \pm1, \pm2, \ldots$ It can be the Hamiltonian of the standard form $\hat{H} = \frac{\hat{\vec{p}}^2}{2M} + V(\hat{\vec{x}})$ with a periodic potential $V(\vec{x})$.

Symmetry: $[\hat{T}_{\vec{a}_{\vec{n}}}, \hat{H}] = 0 \quad \Rightarrow \quad \hat{T}_{\vec{a}_{\vec{n}}}$ and $\hat{H}$ have a common set of eigenfunctions

A general eigenfunction has the form: $\boxed{\psi(\vec{x}) = u(\vec{x})\ e^{i\frac{\vec{\Pi}\cdot\vec{x}}{\hbar}}}$ **Bloch theorem**

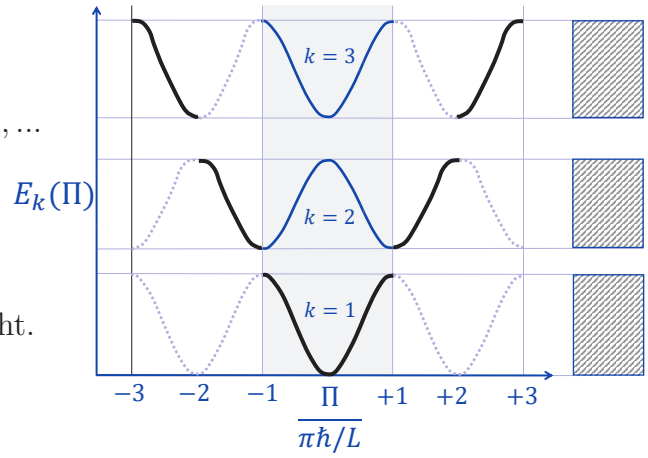
Here $u(\vec{x})$ is any $\vec{L}$-periodic function, $u(\vec{x} + \vec{a}_{\vec{n}}) = u(\vec{x})$
and $\vec{\Pi}$ is a vector called **quasimomentum**

$$\hat{T}_{\vec{a}_{\vec{n}}}\psi(\vec{x}) = e^{-i\frac{\hat{\vec{p}}\cdot\vec{a}_{\vec{n}}}{\hbar}}u(\vec{x})e^{i\frac{\vec{\Pi}\cdot\vec{x}}{\hbar}} = u(\vec{x}-\vec{a}_{\vec{n}})e^{i\frac{\vec{\Pi}\cdot(\vec{x}-\vec{a}_{\vec{n}})}{\hbar}} = e^{-i\frac{\vec{\Pi}\cdot\vec{a}_{\vec{n}}}{\hbar}}u(\vec{x})e^{i\frac{\vec{\Pi}\cdot\vec{x}}{\hbar}} = \underbrace{e^{-i\frac{\vec{\Pi}\cdot\vec{a}_{\vec{n}}}{\hbar}}}_{\text{eigenvalue}}\psi(\vec{x})$$

In this form of $\psi(\vec{x})$ we search for the eigenfunctions of $\hat{H}$.

Assume the **1D case** of a particle in potential $V(x)$ with period L:
$\hat{H}\psi(x) = E\psi(x) \quad \Rightarrow \quad \left[\frac{1}{2M}\left(-i\hbar\frac{d}{dx}+\Pi\right)^2 + V(x) - E\right]u(x) = 0$
This equation solved for a fixed Π and $x \in [0, L]$ with the boundary condition $u(0) = u(L)$ gives a discrete energy spectrum $E = E_k(\Pi)$ with $k = 1, 2, ...$

The quasimomentum Π can be restricted to the first **Brillouin zone** with $\Pi \in [-\frac{\pi\hbar}{L}, +\frac{\pi\hbar}{L}]$. For $\Pi \mapsto \Pi' = \Pi \pm n\frac{2\pi\hbar}{L}$ with $n = 1, 2, ...$ the transformation $u(x) \mapsto u'(x) = u(x)e^{\mp i(2\pi n x/L)}$ ensures that $E_k(\Pi) = E_k(\Pi + n\frac{2\pi\hbar}{L})$. The picture for $\Pi \in (-\infty, +\infty)$ can look e.g. like the one on the right. We obtain a **band spectrum** of energies. The dependence $E_k(\Pi)$ with $k = \left\lceil \left|\frac{\Pi}{\pi\hbar/L}\right| \right\rceil = 1, 2, ...$ (the black curves), called the **dispersion relation**, represents is an analog of the trival free-particle quadratic dispersion relation $E(p) = \frac{1}{2M}p^2$.



◄ Historical remark
1928: Felix Bloch develops the theory of electrons in crystal lattices; the underlying mathematics was previously studied by G. W. Hill (1877) and G. Floquet (1883)

■ Space rotation

We come to another kind of fundamental spatial transformations, namely the rotations. It turns out that generators of the rotation group coincide with components of the total angular momentum, which makes the group non-Abelian. While the orbital angular momentum generates rotations of scalar single-particle wavefunctions, rotations of more complicated wavefunctions, like vectors or spinors, require an additional angular momentum of the particle — the spin. We will therefore complete the theory of spin by defining its transformation properties under rotations. We will also introduce quantities called spherical tensors, whose specific transformation properties will allow us to develop a powerful tensor calculus with far reaching consequences.

► Coordinate transformation

Rotation about axis $\vec{n}$ by angle ϕ in ordinary space expressed by: $\vec{x}\,' = \overbrace{\mathbf{R}^{-1}_{\vec{n}\phi}}^{\substack{3\times3 \text{ rotation} \\ \text{matrix}}}\vec{x}$

Note: we assume (consistently with translations) that matrix $\mathbf{R}_{\vec{n}\phi}$ represents passive rotation of the coordinate frame, so coordinates transform by its inverse.

Radius conserved $\Rightarrow$ orthogonality: $\boxed{\mathbf{R}^{\mathrm{T}}_{\vec{n}\phi}\mathbf{R}_{\vec{n}\phi}=\mathbf{I}} \Rightarrow \sum_i r_{ij}r_{ik}=\delta_{jk}$

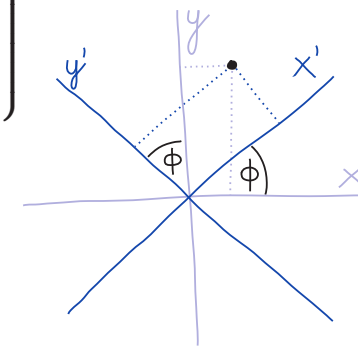
$$\mathbf{R}^{-1}_{\vec{n}_z\phi}=\begin{pmatrix}\cos\phi & \sin\phi & 0\\ -\sin\phi & \cos\phi & 0\\ 0 & 0 & 1\end{pmatrix} \Rightarrow \mathbf{R}^{-1}_{\vec{n}_z\delta\phi}\approx \mathbf{I}+\underbrace{\begin{pmatrix}0 & 1 & 0\\ -1 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}}_{i\mathbf{G}_3}\delta\phi$$

$$\mathbf{R}^{-1}_{\vec{n}_y\phi}=\begin{pmatrix}\cos\phi & 0 & -\sin\phi\\ 0 & 1 & 0\\ \sin\phi & 0 & \cos\phi\end{pmatrix} \Rightarrow \mathbf{R}^{-1}_{\vec{n}_y\delta\phi}\approx \mathbf{I}+\underbrace{\begin{pmatrix}0 & 0 & -1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix}}_{i\mathbf{G}_2}\delta\phi$$

$$\mathbf{R}^{-1}_{\vec{n}_x\phi}=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\phi & \sin\phi\\ 0 & -\sin\phi & \cos\phi\end{pmatrix} \Rightarrow \mathbf{R}^{-1}_{\vec{n}_x\delta\phi}\approx \mathbf{I}+\underbrace{\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 0\end{pmatrix}}_{i\mathbf{G}_1}\delta\phi$$

Any finite rotation is expressed via generators of infinitesimal rotations:

$$\boxed{\mathbf{R}^{-1}_{\vec{n}\phi}=e^{i(\vec{\mathbf{G}}\cdot\vec{n})\phi}}$$



Commutators of the generator matrices:

$$\boxed{[\mathbf{G}_i,\mathbf{G}_j]=i\varepsilon_{ijk}\mathbf{G}_k}$$

These are essentially the commutation relations of angular-momentum components.

Hence for the operator $\hat{R}_{\vec{n}\phi}$ and generators $\hat{G}_i$ of rotations in quantum Hilbert spaces we assume:

Postulate: Generators of rotation of an arbitrary quantum system $= \frac{1}{\hbar}\times$ operators of the total angular momentum components

▶ Quantum rotation operator $\boxed{\hat{R}_{\vec{n}\phi}=e^{-i(\hat{\vec{G}}\cdot\vec{n})\phi}}$ with $\boxed{\hat{\vec{G}}=\frac{1}{\hbar}\hat{\vec{J}}}$

This assumption holds for all systems, i.e. N-particle systems (with $N=1,2,3,...$) as well as systems of a non-particle nature, with $\hat{J}$ expressing the total angular momentum of the system, e.g., the summed orbital and spin angular momentum of all particles. Thus the form of angular momentum operators fully defines the system's transformation properties under rotations. Below we will work within the Hilbert space of a single particle, so: $\boxed{\hat{\vec{G}}=\frac{1}{\hbar}(\hat{\vec{L}}+\hat{\vec{S}})}$

▶ Transformation of coordinates & momenta

(a) rotation around z:

$$\hat{x}'_i\equiv\hat{R}_{\vec{n}_z\phi}\hat{x}_i\hat{R}^{-1}_{\vec{n}_z\phi}=\underbrace{e^{-i(\hat{L}_3+\hat{S}_3)\phi/\hbar}}_{e^{-i\hat{L}_3\phi/\hbar}e^{-i\hat{S}_3\phi/\hbar}}\hat{x}_i\underbrace{e^{+i(\hat{L}_3+\hat{S}_3)\phi/\hbar}}_{e^{+i\hat{S}_3\phi/\hbar}e^{+i\hat{L}_3\phi/\hbar}}=e^{-i\hat{L}_3\phi/\hbar}\hat{x}_ie^{+i\hat{L}_3\phi/\hbar}$$

Infinitesimal rotation:

$$\hat{x}'_i\approx\left(\hat{I}-\tfrac{i}{\hbar}\hat{L}_3\delta\phi\right)\hat{x}_i\left(\hat{I}+\tfrac{i}{\hbar}\hat{L}_3\delta\phi\right)\approx\hat{x}_i-\tfrac{i}{\hbar}\underbrace{[\hat{L}_3,\hat{x}_i]}_{-i\hbar(\delta_{i2}\hat{x}_1-\delta_{i1}\hat{x}_2)}\delta\phi=\begin{cases}\hat{x}_1+\hat{x}_2\delta\phi\\ \hat{x}_2-\hat{x}_1\delta\phi\\ \hat{x}_3\end{cases}$$

The same for momentum:

$$\hat{p}'_i\approx\left(\hat{I}-\tfrac{i}{\hbar}\hat{L}_3\delta\phi\right)\hat{p}_i\left(\hat{I}+\tfrac{i}{\hbar}\hat{L}_3\delta\phi\right)\approx\hat{p}_i-\tfrac{i}{\hbar}\underbrace{[\hat{L}_3,\hat{p}_i]}_{+i\hbar(\delta_{i1}\hat{p}_2-\delta_{i2}\hat{p}_1)}\delta\phi=\begin{cases}\hat{p}_1+\hat{p}_2\delta\phi\\ \hat{p}_2-\hat{p}_1\delta\phi\\ \hat{p}_3\end{cases}$$

(b) general rotation:

$$\underbrace{\hat{\vec{x}}'}_{\begin{pmatrix}\hat{x}_1'\\ \hat{x}_2'\\ \hat{x}_3'\end{pmatrix}} \equiv \hat{R}_{\vec{n}\phi}\ \hat{\vec{x}}\ \hat{R}^{-1}_{\vec{n}\phi} = \underbrace{\mathbf{R}^{-1}_{\vec{n}\phi}\ \hat{\vec{x}}}_{\begin{pmatrix} r_{11} & r_{12} & r_{13}\\ r_{21} & r_{22} & r_{23}\\ r_{31} & r_{32} & r_{33}\end{pmatrix}^{-1}\begin{pmatrix}\hat{x}_1\\ \hat{x}_2\\ \hat{x}_3\end{pmatrix}} \quad \Rightarrow \quad \hat{\vec{x}}\hat{R}_{\vec{n}\phi} = \mathbf{R}_{\vec{n}\phi}\hat{R}_{\vec{n}\phi}\hat{\vec{x}}$$

$$\hat{\vec{p}}' \equiv \hat{R}_{\vec{n}\phi}\ \hat{\vec{p}}\ \hat{R}^{-1}_{\vec{n}\phi} = \mathbf{R}^{-1}_{\vec{n}\phi}\ \hat{\vec{p}}$$

* this form of the defining relation will be useful below

▶ **Transformation of angular momentum**

(a) z-rotation: $\hat{J}_i' \approx \left(\hat{I} - \frac{i}{\hbar}\hat{J}_3\delta\phi\right)\hat{J}_i\left(\hat{I} + \frac{i}{\hbar}\hat{J}_3\delta\phi\right) \approx \hat{J}_i - \frac{i}{\hbar}\underbrace{[\hat{J}_3, \hat{J}_i]}_{i\hbar\varepsilon_{3ij}\hat{J}_j}\delta\phi = \begin{cases}\hat{J}_1 + \hat{J}_2\delta\phi\\ \hat{J}_2 - \hat{J}_1\delta\phi\\ \hat{J}_3\end{cases}$

(b) general rotation: $\hat{\vec{J}}' \equiv \hat{R}_{\vec{n}\phi}\hat{\vec{J}}\hat{R}^{-1}_{\vec{n}\phi} = \mathbf{R}^{-1}_{\vec{n}\phi}\hat{\vec{J}}$ $\quad \hat{\vec{S}}' = \mathbf{R}^{-1}_{\vec{n}\phi}\hat{\vec{S}}$ $\quad \hat{\vec{L}}' = \mathbf{R}^{-1}_{\vec{n}\phi}\hat{\vec{L}}$

▶ **Action on wavefunctions** (coordinate & momentum representation)

$$\underbrace{\hat{\vec{x}}\ (\hat{R}_{\vec{n}\phi}}_{\mathbf{R}_{\vec{n}\phi}\hat{R}_{\vec{n}\phi}\hat{\vec{x}}\ \text{see formula}\ *\ \text{above}}\ |\vec{x}\rangle) = (\mathbf{R}_{\vec{n}\phi}\vec{x})(\hat{R}_{\vec{n}\phi}|\vec{x}\rangle) \quad \Rightarrow \quad \hat{R}_{\vec{n}\phi}|\vec{x}\rangle = |\mathbf{R}_{\vec{n}\phi}\vec{x}\rangle$$

$$\left.\begin{aligned}\langle\vec{x}|\hat{R}_{\vec{n}\phi}\psi\rangle &= \langle\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x}|\psi\rangle\\ \langle\vec{p}|\hat{R}_{\vec{n}\phi}\psi\rangle &= \langle\mathbf{R}^{-1}_{\vec{n}\phi}\vec{p}|\psi\rangle\end{aligned}\right\} \Rightarrow \boxed{\begin{aligned}\hat{R}_{\vec{n}\phi}\psi(\vec{x}) &= \psi(\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x})\\ \hat{R}_{\vec{n}\phi}\tilde{\psi}(\vec{p}) &= \tilde{\psi}(\mathbf{R}^{-1}_{\vec{n}\phi}\vec{p})\end{aligned}}$$

▶ **Transformation of scalar wavefunction** $\psi(\vec{x})$

A scalar wavefunction was used above to describe a spinless quantum particle. It is a 1-component function assigning to each point of space a single complex number which is invariant under all spatial transformations. Only the argument of $\psi(\vec{x})$ is affected by the transformation:

$$\hat{R}_{\vec{n}\phi}\psi(\vec{x}) = \psi(\underbrace{\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x}}_{\vec{x}'}) \quad \Rightarrow \quad \hat{\vec{J}} \equiv \hat{\vec{L}} \quad \Rightarrow \quad \textbf{spin 0}$$

Example: $\underbrace{\hat{R}_{\vec{n}_3\delta\phi}}_{e^{-i\hat{L}_3\delta\phi/\hbar}}\psi(\vec{x}) \approx \left[\hat{I} - \left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)\delta\phi\right]\psi(\vec{x}) = \psi\left[\overbrace{\begin{pmatrix}1 & +\delta\phi & 0\\ -\delta\phi & 1 & 0\\ 0 & 0 & 1\end{pmatrix}}^{\mathbf{R}^{-1}_{\vec{n}_3\delta\phi}}\begin{pmatrix}x_1\\ x_2\\ x_3\end{pmatrix}\right]$

▶ **Transformation of vector wavefunction** $\boldsymbol{\psi}(\vec{x}) \equiv \begin{pmatrix}\psi_1(\vec{x})\\ \psi_2(\vec{x})\\ \psi_3(\vec{x})\end{pmatrix}$

Now we assume that a given quantum particle is described by a 3-component wavefunction which transforms under rotations like a vector function. Besides the argument $\vec{x}$, also the direction of the vector $\boldsymbol{\psi}$ is affected by the rotation. The defining transformation property reads as:

$$\hat{R}_{\vec{n}\phi}\boldsymbol{\psi}(\vec{x}) = \underbrace{\begin{pmatrix} r_{11} & r_{12} & r_{13}\\ r_{21} & r_{22} & r_{23}\\ r_{31} & r_{32} & r_{33}\end{pmatrix}_{\vec{n}\phi}}_{\hat{\mathbf{R}}_{\vec{n}\phi}\equiv\mathbf{R}_{\vec{n}\phi}}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}(\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x}) = \underbrace{e^{-i\frac{\hat{\vec{S}}\cdot\vec{n}}{\hbar}\phi}\boldsymbol{\psi}}_{\boldsymbol{\psi}'}(\underbrace{\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x}}_{\vec{x}'})$$

Generators of $\hat{\mathbf{R}}^{-1}_{\vec{n}\phi}$: $\quad \hat{S}_1 = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix} \quad \hat{S}_2 = \hbar \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad \hat{S}_3 = \hbar \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Example (z-rotation): $\underbrace{\hat{R}_{\vec{n}_3\delta\phi}}_{e^{-i[\hat{S}_3+\hat{L}_3]\delta\phi/\hbar}} \begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \\ \psi_3(\vec{x}) \end{pmatrix} \approx \underbrace{\left[\hat{I} - \begin{pmatrix} 0 & +1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \delta\phi\right]}_{\begin{pmatrix} 1 & -\delta\phi & 0 \\ +\delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}} \underbrace{e^{-i\frac{\hat{L}_3\delta\phi}{\hbar}} \begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \\ \psi_3(\vec{x}) \end{pmatrix}}_{\begin{pmatrix} \psi_1(\mathbf{R}^{-1}_{\vec{n}_3\delta\phi}\vec{x}) \\ \psi_2(\mathbf{R}^{-1}_{\vec{n}_3\delta\phi}\vec{x}) \\ \psi_3(\mathbf{R}^{-1}_{\vec{n}_3\delta\phi}\vec{x}) \end{pmatrix}}$

$\hat{S}_1^2+\hat{S}_2^2+\hat{S}_3^2 = \overbrace{s(s+1)}^{2}\hbar^2\hat{I} \;\Rightarrow\; \boxed{s=1}$

$\hbar\,\mathrm{Det}(\hat{S}_i-\lambda\hat{I})=0 \;\Rightarrow \lambda=\pm1,0 \;\Rightarrow\; \boxed{s_i = \hbar\begin{Bmatrix} -1 \\ 0 \\ +1 \end{Bmatrix}} \quad\Rightarrow\quad \textbf{spin 1}$

So, 3-component wavefuctions $\boldsymbol{\psi}(\vec{x})$ with vector transformation properties describe particles with spin 1. We now find the link of Cartesian components $\psi_i(\vec{x})$ with i=1,2,3 to the probability amplitudes $\psi_{m_s}(\vec{x})$ for individual spin projections $m_s=0,\pm1$ to the z-axis direction:

Eigenvectors of $\hat{S}_3$: $\quad \xi_{+1} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ -i \\ 0 \end{pmatrix} \quad \xi_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \xi_{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} +1 \\ -i \\ 0 \end{pmatrix}$

$$\overbrace{\begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \\ \psi_3(\vec{x}) \end{pmatrix}}^{\psi_{+1}(\vec{x})\xi_{+1}+\psi_0(\vec{x})\xi_0+\psi_{-1}(\vec{x})\xi_{-1}} = \begin{pmatrix} \frac{1}{\sqrt{2}}[\psi_{-1}(\vec{x})-\psi_{+1}(\vec{x})] \\ -\frac{i}{\sqrt{2}}[\psi_{-1}(\vec{x})+\psi_{+1}(\vec{x})] \\ \psi_0(\vec{x}) \end{pmatrix} \Rightarrow \boxed{\begin{pmatrix} \psi_{+1}(\vec{x}) \\ \psi_0(\vec{x}) \\ \psi_{-1}(\vec{x}) \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}}[\psi_1(\vec{x})-i\psi_2(\vec{x})] \\ \psi_3(\vec{x}) \\ +\frac{1}{\sqrt{2}}[\psi_1(\vec{x})+i\psi_2(\vec{x})] \end{pmatrix}}$$

▶ Transformation of spinor wavefunction $\boldsymbol{\psi}(\vec{x}) \equiv \begin{pmatrix} \psi_\uparrow(\vec{x}) \\ \psi_\downarrow(\vec{x}) \end{pmatrix}$ spin $\frac{1}{2}$

At last we come to the spin-$\frac{1}{2}$ wavefunction introduced in Sec. 1b. We know that in this case the components $\psi_\uparrow(\vec{x})$ and $\psi_\downarrow(\vec{x})$ express directly the amplitudes of finding the $\uparrow$ and $\downarrow$ spin z-projections of the particle at the position $\vec{x}$. But how the spinor wavefunction $\boldsymbol{\psi}(\vec{x})$ transforms under rotations? Because in this case the spin matrices are known to be the Pauli matrices, the spinor transformation can be easily determined from

$$\boxed{\hat{R}_{\vec{n}\phi}\boldsymbol{\psi}(\vec{x}) = \underbrace{e^{-i\frac{\hat{\vec{S}}\cdot\vec{n}}{\hbar}\phi}\boldsymbol{\psi}}_{\boldsymbol{\psi}'}(\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x}) = \underbrace{[\hat{\mathbf{S}}_{\vec{n}\phi}\boldsymbol{\psi}]}_{\boldsymbol{\psi}'}(\mathbf{R}^{-1}_{\vec{n}\phi}\vec{x})}$$

We now find the unknown 2×2 matrix $\hat{\mathbf{S}}_{\vec{n}\phi}$:

$$\hat{\mathbf{S}}_{\vec{n}\phi} = e^{-i\frac{\hat{\vec{S}}\cdot\vec{n}}{\hbar}\phi} = \sum_{k=0}^{\infty}\frac{1}{k!}\left(-\frac{i\phi}{2}\right)^k(\hat{\vec{\sigma}}\cdot\vec{n})^k = \ldots \qquad \text{with } (\hat{\vec{\sigma}}\cdot\vec{n})^k = \begin{cases} \hat{I} & \text{for } k\text{=even} \\ \hat{\vec{\sigma}}\cdot\vec{n} & \text{for } k\text{=odd} \end{cases}$$

$$(\hat{\vec{\sigma}}\cdot\vec{n})^2 = \sum_{i,j=1}^{3} n_i n_j \hat{\sigma}_i\hat{\sigma}_j = \frac{1}{2}\sum_{i,j=1}^{3} n_i n_j \underbrace{(\hat{\sigma}_i\hat{\sigma}_j+\hat{\sigma}_j\hat{\sigma}_i)}_{2\delta_{ij}\hat{I}} + \frac{1}{2}\underbrace{\sum_{i,j=1}^{3} n_i n_j(\hat{\sigma}_i\hat{\sigma}_j-\hat{\sigma}_j\hat{\sigma}_i)}_{0} = \underbrace{\sum_{i=1}^{3} n_i^2}_{1}\hat{I}$$

$$\cdots = \underbrace{\sum_{k=0,2,4,\ldots}\frac{1}{k!}\left(-\frac{i\phi}{2}\right)^k}_{\cos\frac{\phi}{2}}\hat{I} + \underbrace{\sum_{k=1,3,5,\ldots}\frac{1}{k!}\left(-\frac{i\phi}{2}\right)^k}_{-i\sin\frac{\phi}{2}}(\hat{\vec{\sigma}}\cdot\vec{n}) = \boxed{\left(\cos\tfrac{\phi}{2}\right)\hat{I} - i\left(\sin\tfrac{\phi}{2}\right)(\hat{\vec{\sigma}}\cdot\vec{n}) = \hat{\mathbf{S}}_{\vec{n}\phi}}$$

spinor transformation

$$\Rightarrow \boxed{\hat{\mathbf{S}}_{\vec{n}(2\pi)} = -\hat{I}, \quad \hat{\mathbf{S}}_{\vec{n}(4\pi)} = +\hat{I}}$$

Special case: $\hat{\mathbf{S}}_{\vec{n}_z\phi} = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{+i\phi/2} \end{pmatrix}$

Only now the definition of spinor is complete. It does not mean just any two-component wavefunction. The spinor is an object which transforms under rotations in the specific way given above. Note the surprising property of spinors that only rotations by 720°, and not those by 360°, yield identity!

◄ Historical remark

1913: Élie Cartan discovered complex "tensors" with spinor transform. properties
1927: Wolfgang Pauli introduces spinors to QM

► Rotational invariance sensu stricto

Hamiltonian $\hat{H}$ satisfying $[\hat{H}, \hat{R}_{\vec{n}\phi}]=0$ for any $\vec{n}, \phi$ must satisfy $[\hat{H}, \hat{J}_i]=0\ \forall i$. For a single-particle Hamiltonian of the form $\hat{H} = \frac{\hat{p}^2}{2M} + \hat{V}$ this means that the potential is isotropic: $\hat{V} \equiv V(r)$. An N-particle Hamiltonian with $N \geq 1$ may depend only on rotational invariants such as: $\hat{\vec{x}}_k \cdot \hat{\vec{x}}_l$, $\hat{\vec{p}}_k \cdot \hat{\vec{p}}_l$, $\hat{\vec{x}}_k \cdot \hat{\vec{p}}_l$, $|\hat{\vec{x}}_k - \hat{\vec{x}}_l| = \sqrt{(\hat{\vec{x}}_k - \hat{\vec{x}}_l)\cdot(\hat{\vec{x}}_k - \hat{\vec{x}}_l)}$, $\hat{\vec{S}}_k \cdot \hat{\vec{S}}_l$, $\hat{\vec{x}}_k \cdot \hat{\vec{S}}_l$ $\hat{\vec{p}}_k \cdot \hat{\vec{S}}_l$ etc. $(k, l = 1, ..., N)$.
In combination with the symmetry under translations this reduces to combinations containing scalar products of quantities $(\hat{\vec{x}}_k - \hat{\vec{x}}_l)$, $\hat{\vec{p}}_k$ and $\hat{\vec{S}}_k$.
Both rotational and translational symmetries sensu stricto are strictly required when dealing with Hamiltonians describing fundamental physics!

■ Irreducible representations of the rotation group

Since the square $\hat{J}^2$ of the total angular momentum commutes with all its components $\hat{J}_i$, the subspaces of the entire Hilbert space $\mathcal{H}$ spanned by the total angular-momentum eigenvectors $|ajm\rangle$ with any fixed j (and a standing for arbitrary remaining quantum numbers) are invariant under the action of all rotation operators $\hat{R}_{\vec{n}\phi}$. In these subspaces, the rotations are described by a hierarchy of Wigner matrices, which for each j form an irreducible representation of the rotation group. Quantum theory thus provides a fundamental platform for the realization of this group.

► Factorization of rotation operators

Any rotation expressed by a 3D matrix $\mathbf{R}$ can be equivalently characterized by axis $\vec{n}$ and angle ϕ of the rotation or by 3 Euler angles α, β, γ. Quantum rotation operator in $\mathcal{H}$ will be now interchangeably denoted by symbols $\hat{R}_{\mathbf{R}} \equiv \hat{R}_{\vec{n}\phi} \equiv \hat{R}(\alpha\beta\gamma)$.

Rotation around $\vec{n}$ by ϕ: operator $\boxed{\hat{R}_{\mathbf{R}} \equiv \hat{R}_{\vec{n}\phi} = e^{-\frac{i}{\hbar}\left(\hat{\vec{J}}\cdot\vec{n}\right)\phi}} \neq \hat{R}_z \hat{R}_y \hat{R}_x$

Expression of a general rotation via **Euler angles**: 3 successive rotations

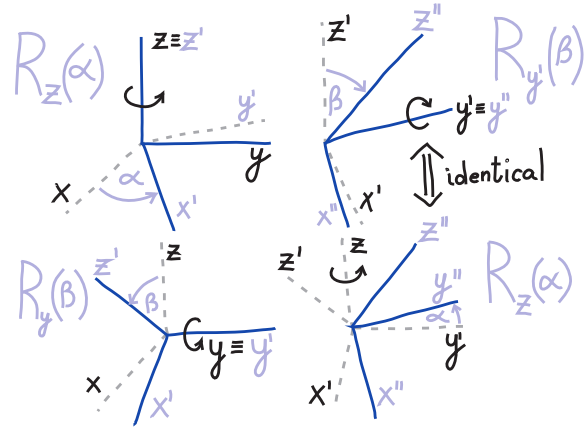
(1) around $\vec{n}_z$ by α
(2) around $\vec{n}'_y \equiv \mathbf{R}_{\vec{n}_z\alpha}\vec{n}_y$ by β
(3) around $\vec{n}'_z \equiv \mathbf{R}_{\vec{n}'_y\beta}\vec{n}_z$ by γ

$$\Rightarrow \quad \boxed{\underbrace{\hat{R}_{\vec{n}\phi}}_{\hat{R}(\alpha\beta\gamma)} = \underbrace{\hat{R}_{\vec{n}'_z\gamma}}_{\hat{R}_{z'}(\gamma)} \underbrace{\hat{R}_{\vec{n}'_y\beta}}_{\hat{R}_{y'}(\beta)} \underbrace{\hat{R}_{\vec{n}_z\alpha}}_{\hat{R}_z(\alpha)}}$$

Using identities

$$\left\{\begin{array}{l}\hat{R}_{z'}(\gamma)=\hat{R}_{y'}(\beta)\hat{R}_z(\gamma)\hat{R}^{-1}_{y'}(\beta)\\ \hat{R}_{y'}(\beta)=\hat{R}_z(\alpha)\hat{R}_y(\beta)\hat{R}^{-1}_z(\alpha)\end{array}\right\}$$

i.e., e.g., $\hat{R}_{y'}(\beta)\hat{R}_z(\alpha)=\hat{R}_z(\alpha)\hat{R}_y(\beta)$, as shown on the right:



we obtain a **factorized formula** in the fixed coordinate system xyz:

$$\boxed{\hat{R}(\alpha\beta\gamma)=\hat{R}_z(\alpha)\hat{R}_y(\beta)\hat{R}_z(\gamma)}$$

▶ Wigner matrices

Based on the above formulas, we can evaluate the form of the rotation operators in the space spanned by angular-momentum eigenvectors $|jm\rangle$.

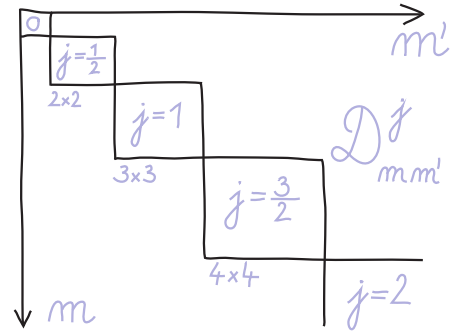
$$\hat{R}(\alpha\beta\gamma)|jm\rangle=\sum_{j'm'}\underbrace{\langle j'm'|\hat{R}(\alpha\beta\gamma)|jm\rangle}_{\delta_{jj'}D^j_{m'm}(\alpha\beta\gamma)}|j'm'\rangle=\sum_{m'}\underbrace{D^j_{m'm}(\alpha\beta\gamma)}_{\text{Wigner matrix}}|jm'\rangle$$

$D^j_{m'm}(\alpha\beta\gamma)\equiv D^j_{m'm}(\vec{n}\phi)\equiv D^j_{m'm}(\mathbf{R})$ matrix of dimension $2j+1$

$$=\langle jm'|\hat{R}_z(\alpha)\hat{R}_y(\beta)\hat{R}_z(\gamma)|jm\rangle=e^{-i(m'\alpha+m\gamma)}\overbrace{\langle jm'|\hat{R}_y(\beta)|jm\rangle}^{d^j_{m'm}(\beta)}$$

Wigner matrices (D-functions) form an **irrep** of the rotational group for any fixed value $\boxed{j=0,\frac{1}{2},1,\frac{3}{2},2,\frac{5}{2},3,\ldots}$

(a) identity $\phi=0$, (b) inverse $\phi=-\phi$,
(d) group $\equiv$ matrix multiplications
$D^j_{m'm}(\mathbf{R}_2\mathbf{R}_1)=\sum_{m''}D^j_{m'm''}(\mathbf{R}_2)D^j_{m''m}(\mathbf{R}_1)$



▶ Transformation of general-spin wavefucntion

The $(2s+1)$-component wavefunction $\boldsymbol{\psi}(\vec{x})\equiv\{\psi_{m_s}(\vec{x})\}^{+s}_{m_s=-s}$ of a particle with an arbitrary spin s in the $\hat{S}_z$ representation is transformed by means of the Wigner matrices:

$$\begin{pmatrix}\psi'_{+s}(\vec{x})\\ \vdots\\ \psi'_{-s}(\vec{x})\end{pmatrix}=\begin{pmatrix}D^s_{ss}(\mathbf{R}) & \ldots & D^s_{(-s)s}(\mathbf{R})\\ \vdots & \ddots & \vdots\\ D^s_{s(-s)}(\mathbf{R}) & \ldots & D^s_{(-s)(-s)}(\mathbf{R})\end{pmatrix}\begin{pmatrix}\psi_{+s}(\mathbf{R}^{-1}\vec{x})\\ \vdots\\ \psi_{-s}(\mathbf{R}^{-1}\vec{x})\end{pmatrix}$$

▶ Clebsch-Gordan series for Wigner matrices

Rotation operators in the Hilbert space of coupled angular momenta:

$$\mathcal{H}=\underbrace{\mathcal{H}_1}_{\text{irrep }j_1}\otimes\underbrace{\mathcal{H}_2}_{\text{irrep }j_2}\quad\Rightarrow\quad\hat{R}(\alpha\beta\gamma)=\hat{R}_1(\alpha\beta\gamma)\otimes\hat{R}_2(\alpha\beta\gamma)$$

Operator $\hat{R}$ can be expressed in both (a) separable basis $|j_1 m_1\rangle|j_2 m_2\rangle \equiv |j_1 m_1 j_2 m_2\rangle$ and (b) coupled basis $|j_1 j_2 j m\rangle$:

$$\langle j_1 m_1 j_2 m_2|\hat{R}|j_1 m_1' j_2 m_2'\rangle = \underbrace{\langle j_1 m_1|\hat{R}_1|j_1 m_1'\rangle}\,\underbrace{\langle j_2 m_2|\hat{R}_2|j_2 m_2'\rangle}$$

$$= \sum_{jm}\sum_{j'm'} \overbrace{\langle j_1 m_1 j_2 m_2|j_1 j_2 j m\rangle}^{C^{jm}_{j_1 m_1 j_2 m_2}} \overbrace{\langle j_1 j_2 j m|\hat{R}|j_1 j_2 j' m'\rangle}^{D^{j_1}_{m_1 m_1'}\ \delta_{jj'} D^{j}_{mm'}\ D^{j_2}_{m_2 m_2'}} \overbrace{\langle j_1 j_2 j' m'|j_1 m_1' j_2 m_2'\rangle}^{C^{j'm'}_{j_1 m_1' j_2 m_2'}}$$

$$\Rightarrow \boxed{D^{j_1}_{m_1 m_1'}(\mathbf{R})\ D^{j_2}_{m_2 m_2'}(\mathbf{R}) = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{\substack{m\\ m'=-j}}^{+j} C^{jm}_{j_1 m_1 j_2 m_2} C^{jm'}_{j_1 m_1' j_2 m_2'}\ D^{j}_{mm'}(\mathbf{R})}$$

This relation determines the decomposition of the **reducible product representation** of the rotation group (given by coupling of the j_1 & j_2 irreps) into a direct **sum of irreducible representations**:

$$D^{j_1} \otimes D^{j_2} = D^{|j_1-j_2|} \oplus \cdots\cdots \oplus D^{(j_1+j_2)}$$

■ Spherical tensor operators

We are ready now to understand and appreciate the introduction of spherical tensors, i.e., objects (in our case operators) which transform according to a single irreducible representation of the rotation group. Spherical tensors have some favorable properties that make them mathematically more convenient than the familiar Cartesian tensors.

▶ Cartesian tensors ⇔ Cartesian transformations under rotations

n^{th} rank tensor: $\underbrace{T_{ijk\ldots}}_{\substack{n \text{ indices}\\ i,j,k\cdots=1,2,3}} \mapsto \boxed{T'_{ijk\ldots} = \sum_{i'j'k'\ldots} \underbrace{\mathbf{R}^{-1}_{ii'}\mathbf{R}^{-1}_{jj'}\mathbf{R}^{-1}_{kk'}\ldots}_{\text{Cartesian rot. matrices}} T_{i'j'k'\ldots}}$

Representation of the rotation group on Cartesian tensors is **reducible**

Example: 2nd rank tensor

$$T_{ij} = \overbrace{\tfrac{1}{3}\mathrm{Tr}\,T\,\delta_{ij}}^{\text{scalar}} + \overbrace{\tfrac{1}{2}[T_{ij}-T_{ji}]}^{\text{antisymmetric tensor}} + \overbrace{\tfrac{1}{2}[T_{ij}+T_{ji}] - \tfrac{1}{3}\mathrm{Tr}T\,\delta_{ij}}^{\text{traceless symmetric tensor}}$$

Each part of the decomposition constitutes an irrep of the rotation group

▶ Irreducible (spherical) tensors

These tensor quantities are transformed by irreducible Wigner matrices:

λ^{th} rank spherical tensor

$$\boxed{(T')^{\lambda}_{\mu} = \sum_{\mu'} D^{\lambda}_{\mu'\mu}(\mathbf{R})\ T^{\lambda}_{\mu'}}$$

λ^{th} rank **spherical tensor operator**

$$\boxed{\hat{R}_{\mathbf{R}}\,\hat{T}^{\lambda}_{\mu}\,\hat{R}^{-1}_{\mathbf{R}} = \sum_{\mu'} D^{\lambda}_{\mu'\mu}(\mathbf{R})\,\hat{T}^{\lambda}_{\mu'}}$$

An alternative (equivalent) definition of spherical tensor operators is given by the commutation relations of $\hat{T}^{\lambda}_{\mu}$ with angular momentum operators. These relations can be obtained by considering an infinitesimal rotation:

$$\overbrace{[\hat{I}-\tfrac{i}{\hbar}(\hat{\vec{J}}\cdot\vec{n})\delta\phi]}^{\delta\hat{R}}\hat{T}^\lambda_\mu\overbrace{[\hat{I}+\tfrac{i}{\hbar}(\hat{\vec{J}}\cdot\vec{n})\delta\phi]}^{\delta\hat{R}^{-1}}=\sum_{\mu'}\overbrace{\langle\lambda\mu'|[\hat{I}-\tfrac{i}{\hbar}(\hat{\vec{J}}\cdot\vec{n})\delta\phi]|\lambda\mu\rangle}^{D^\lambda_{\mu'\mu}(\delta\mathbf{R})}\hat{T}^\lambda_{\mu'}$$

$$\Rightarrow\quad\left[(\hat{\vec{J}}\cdot\vec{n}),\hat{T}^\lambda_\mu\right]=\sum_{\mu'}\langle\lambda\mu'|(\hat{\vec{J}}\cdot\vec{n})|\lambda\mu\rangle\hat{T}^\lambda_{\mu'}$$

$$\Rightarrow\quad\boxed{\left[\hat{J}_3,\hat{T}^\lambda_\mu\right]=\hbar\mu\hat{T}^\lambda_\mu}\qquad\boxed{\left[\hat{J}_\pm,\hat{T}^\lambda_\mu\right]=\hbar\sqrt{\lambda(\lambda+1)-\mu(\mu\pm1)}\hat{T}^\lambda_{\mu\pm1}}$$

These commutation relations are actually much simpler to check than the transformation formulas with Wigner matrices.

► **Examples: First & second rank tensors**

(1) $\boldsymbol{\lambda=1}$ **tensor (vector)**:

Cartesian vector operator $\quad\hat{\vec{V}}\equiv(\hat{V}_1,\hat{V}_2,\hat{V}_3)\quad\Rightarrow\quad\hat{R}_\mathbf{R}\hat{V}_i\hat{R}^{-1}_\mathbf{R}=\sum_{i'=1}^{3}\mathbf{R}^{-1}_{ii'}\hat{V}_{i'}$

Infinitesimal rotation around axis $\vec{n}$ (sum. convention used):

$\hat{V}_i-\frac{i}{\hbar}\delta\phi[\hat{J}_k,\hat{V}_i]n_k=\hat{V}_i+\delta\phi\varepsilon_{ijk}\hat{V}_jn_k\ \Rightarrow\boxed{[\hat{J}_k,\hat{V}_i]=i\hbar\varepsilon_{kij}\hat{V}_j}$

Spherical components of the vector operator:

$$\boxed{\begin{array}{rcl}\hat{V}^1_{+1}&=&-\frac{1}{\sqrt{2}}(\hat{V}_1+i\hat{V}_2)\\ \hat{V}^1_0&=&\hat{V}_3\\ \hat{V}^1_{-1}&=&+\frac{1}{\sqrt{2}}(\hat{V}_1-i\hat{V}_2)\end{array}}$$

satisfy spherical tensor commut. relations

$$\left[\hat{J}_3,\hat{V}^1_0\right]=\left[\hat{J}_\pm,\hat{V}^1_{\pm1}\right]=0$$

$$\left[\hat{J}_\pm,\hat{V}^1_{\mp1}\right]=\sqrt{2}\hbar\hat{V}^1_0,\quad\left[\hat{J}_\pm,\hat{V}^1_0\right]=\sqrt{2}\hbar\hat{V}^1_{\pm1}$$

Note: This reminds us the relations between (ψ_1,ψ_2,ψ_3) and $(\psi_{-1},\psi_0,\psi_{+1})$ components of a vector wavefunction $\boldsymbol{\psi}$ (spin-1 particle). The $\pm i$ terms differ because $\boldsymbol{\psi}$ transforms as $\mathbf{R}\boldsymbol{\psi}(\mathbf{R}^{-1}\vec{x})$ and not as $\mathbf{R}^{-1}\boldsymbol{\psi}$.

(2) $\boldsymbol{\lambda=2}$ **tensor** (relations without proofs):

Cartesian tensor operator

$$\hat{T}_{ij}\equiv\begin{pmatrix}\hat{T}_{11}&\hat{T}_{12}&\hat{T}_{13}\\ \hat{T}_{21}&\hat{T}_{22}&\hat{T}_{23}\\ \hat{T}_{31}&\hat{T}_{32}&\hat{T}_{33}\end{pmatrix}\text{ satisfying }\hat{T}_{ij}=\hat{T}_{ji}\text{ and }\textstyle\sum_i\hat{T}_{ii}=0$$

Spherical components

$$\hat{R}_\mathbf{R}\hat{T}_{ij}\hat{R}^{-1}_\mathbf{R}=\sum_{i',j'=1}^{3}\mathbf{R}^{-1}_{ii'}\mathbf{R}^{-1}_{jj'}\hat{T}_{i'j'}$$

$$\boxed{\begin{array}{rcl}\hat{T}^2_0&=&-\sqrt{\frac{3}{2}}\,(\hat{T}_{11}+\hat{T}_{22})\\ \hat{T}^2_{\pm1}&=&\mp(\hat{T}_{31}\pm i\hat{T}_{32})\\ \hat{T}^2_{\pm2}&=&\frac{1}{2}(\hat{T}_{11}-\hat{T}_{22}\pm2i\hat{T}_{21})\end{array}}\qquad\begin{array}{l}=\sqrt{\frac{3}{2}}\,\hat{T}_{33}\\ =\mp(\hat{T}_{13}\pm i\hat{T}_{23})\\ =\hat{T}_{11}+\frac{1}{2}\hat{T}_{33}\pm i\hat{T}_{12}=-\hat{T}_{22}-\frac{1}{2}\hat{T}_{33}\pm i\hat{T}_{12}\end{array}$$

► **Coupling of spherical tensors**

Let $\hat{A}^{\lambda_1}_{\mu_1}$ and $\hat{B}^{\lambda_2}_{\mu_2}$ be spherical tensors of ranks λ_1 and λ_2. Then

$$\boxed{\hat{T}^\lambda_\mu=\sum_{\mu_1,\mu_2}C^{\lambda\mu}_{\lambda_1\mu_1\lambda_2\mu_2}\hat{A}^{\lambda_1}_{\mu_1}\hat{B}^{\lambda_2}_{\mu_2}\equiv[\hat{A}^{\lambda_1}\times\hat{B}^{\lambda_2}]^\lambda_\mu}$$ is spherical tensor of rank λ

Proof:

$$\hat{R}\,\hat{T}^{\lambda}_{\mu}\hat{R}^{-1} = \sum_{\mu_1,\mu_2} C^{\lambda\mu}_{\lambda_1\mu_1\lambda_2\mu_2} \overbrace{\hat{R}\,\hat{A}^{\lambda_1}_{\mu_1}\hat{R}^{-1}}^{\sum_{\mu'_1} D^{\lambda_1}_{\mu'_1\mu_1}\hat{A}^{\lambda_1}_{\mu'_1}} \overbrace{\hat{R}\,\hat{B}^{\lambda_2}_{\mu_2}\hat{R}^{-1}}^{\sum_{\mu'_2} D^{\lambda_2}_{\mu'_2\mu_2}\hat{B}^{\lambda_2}_{\mu'_2}} = \sum_{\mu_1,\mu_2}\sum_{\mu'_1,\mu'_2} C^{\lambda\mu}_{\lambda_1\mu_1\lambda_2\mu_2} \overbrace{D^{\lambda_1}_{\mu'_1\mu_1} D^{\lambda_2}_{\mu'_2\mu_2}}^{\sum_{\lambda'}\sum_{\mu',\mu''} C^{\lambda'\mu'}_{\lambda_1\mu'_1\lambda_2\mu'_2} C^{\lambda'\mu''}_{\lambda_1\mu_1\lambda_2\mu_2} D^{\lambda'}_{\mu'\mu''}} \hat{A}^{\lambda_1}_{\mu'_1}\hat{B}^{\lambda_2}_{\mu'_2}$$

$$= \sum_{\lambda'}\sum_{\mu',\mu''}\sum_{\mu'_1,\mu'_2} \underbrace{\sum_{\mu_1,\mu_2} C^{\lambda\mu}_{\lambda_1\mu_1\lambda_2\mu_2} C^{\lambda'\mu''}_{\lambda_1\mu_1\lambda_2\mu_2}}_{\delta_{\lambda\lambda'}\delta_{\mu\mu''}} C^{\lambda'\mu'}_{\lambda_1\mu'_1\lambda_2\mu'_2} D^{\lambda'}_{\mu'\mu''} \hat{A}^{\lambda_1}_{\mu'_1}\hat{B}^{\lambda_2}_{\mu'_2}$$

What a beatiful flyspeckful derivation!

$$= \sum_{\mu'} D^{\lambda}_{\mu'\mu} \overbrace{\sum_{\mu'_1,\mu'_2} C^{\lambda\mu'}_{\lambda_1\mu'_1\lambda_2\mu'_2} \hat{A}^{\lambda_1}_{\mu'_1}\hat{B}^{\lambda_2}_{\mu'_2}}^{\hat{T}^{\lambda}_{\mu'}} = \sum_{\mu'} D^{\lambda}_{\mu'\mu}\hat{T}^{\lambda}_{\mu'}$$

Conclusion: coupling of spherical tensors creates other spherical tensors with ranks given by the usual angular-momentum coupling relations.

Special case: **scalar coupling**

$$[\hat{A}^{\lambda}\times\hat{B}^{\lambda}]^0_0 = \sum_{\mu} \underbrace{C^{00}_{\lambda\mu\lambda(-\mu)}}_{\frac{(-)^{\lambda-\mu}}{\sqrt{2\lambda+1}}} \hat{A}^{\lambda}_{\mu}\hat{B}^{\lambda}_{-\mu} = \boxed{\frac{(-)^{-\lambda}}{\sqrt{2\lambda+1}} \underbrace{\sum_{\mu}(-)^{\mu}\hat{A}^{\lambda}_{+\mu}\hat{B}^{\lambda}_{-\mu}}_{(\hat{A}^{\lambda}\cdot\hat{B}^{\lambda})}}$$

scalar product of tensor operators

▶ Properties of matrix elements of spherical tensors

If spherical tensor operators are written in the angular-momentum eigenbasis, the corresponding matrix elements exhibit interesting properties: many of them vanishe, the remaining ones satisfy some simple relations. The rules behind this behavior come from the coupling of angular momenta.

$\{|ajm\rangle\} \equiv$ angular-momentum basis with a denoting other quant. numbers

$\langle a'j'm'|\hat{T}^{\lambda}_{\mu}|ajm\rangle \equiv$ matrix elements of a general spherical tensor

Application of the definition properties of spherical tensors:

(a) $\langle a'j'm'|\underbrace{[\hat{J}_3,\hat{T}^{\lambda}_{\mu}]-\hbar\mu\hat{T}^{\lambda}_{\mu}}_{=0}|ajm\rangle = \hbar\underbrace{[(m'-m)-\mu)]}_{=0}\underbrace{\langle a'j'm'|\hat{T}^{\lambda}_{\mu}|ajm\rangle}_{\neq 0}$

$\Rightarrow m+\mu=m'$

(b) $\langle a'j'm'|\underbrace{[\hat{J}_{\pm},\hat{T}^{\lambda}_{\mu}]-\hbar\sqrt{\lambda(\lambda+1)-\mu(\mu\pm1)}\,\hat{T}^{\lambda}_{\mu\pm1}}_{=0}|ajm\rangle = 0$

$$\Rightarrow \quad \sqrt{j'(j'+1)-m'(m'\mp1)}\langle a'j'(m'\mp1)|\hat{T}^{\lambda}_{\mu}|ajm\rangle - \sqrt{j(j+1)-m(m\pm1)}\langle a'j'm'|\hat{T}^{\lambda}_{\mu}|aj(m\pm1)\rangle = \sqrt{\lambda(\lambda+1)-\mu(\mu\pm1)}\langle a'j'm'|\hat{T}^{\lambda}_{\mu\pm1}|ajm\rangle$$

$$\Rightarrow \langle a'j'(m'\mp1)|\hat{T}^{\lambda}_{\mu}|ajm\rangle = \sqrt{\tfrac{j(j+1)-m(m\pm1)}{j'(j'+1)-m'(m'\mp1)}}\langle a'j'm'|\hat{T}^{\lambda}_{\mu}|aj(m\pm1)\rangle + \sqrt{\tfrac{\lambda(\lambda+1)-\mu(\mu\pm1)}{j'(j'+1)-m'(m'\mp1)}}\langle a'j'm'|\hat{T}^{\lambda}_{\mu\pm1}|ajm\rangle$$

The last relation is compared with the above-derived recursive relation for the Clebsch-Gordan coefficients with substitutions (see the r.h.s.) after which it reads:

$$\left.\begin{matrix} j_1,m_1 \\ j_2,m_2 \\ j,m \end{matrix}\right\} \mapsto \left\{\begin{matrix} j,m \\ \lambda,\mu \\ j',m' \end{matrix}\right.$$

$$\pm \;\mapsto\; \mp$$

$$C^{j'(m'\mp1)}_{jm\lambda\mu} = \sqrt{\frac{j(j+1)-m(m\pm1)}{j'(j'+1)-m'(m'\mp1)}}\,C^{j'm'}_{j(m\pm1)\lambda\mu} + \sqrt{\frac{\lambda(\lambda+1)-\mu(\mu\pm1)}{j'(j'+1)-m'(m'\mp1)}}\,C^{j'm'}_{jm\lambda(\mu\pm1)}$$

Indeed, with mapping $\langle a'j'm'|\hat{T}^\lambda_\mu|ajm\rangle \leftrightarrow C^{j'm'}_{jm\lambda\mu}$ both relations are the same.
$\Rightarrow$ matrix elements $\langle a'j'm'|\hat{T}^\lambda_\mu|ajm\rangle$ for fixed j, λ, j' can be constructed from the same recursive relations as Clebsch-Gordan coefficients $C^{j'm'}_{jm\lambda\mu}$
$\Rightarrow$ $\langle a'j'm'|\hat{T}^\lambda_\mu|ajm\rangle \propto C^{j'm'}_{jm\lambda\mu}$ This is the content of the following theorem:

► Wigner-Eckart theorem

$$\langle a'j'm'|\hat{T}^\lambda_\mu|ajm\rangle = \underbrace{\langle a'j'||\hat{T}^\lambda||aj\rangle}_{\substack{\textbf{reduced}\\ \textbf{matrix element}}}\; C^{j'm'}_{jm\lambda\mu}$$

The meaning:
(a) The dependence on m, m', μ is just that of the CG coefficient.
(b) The dependence on j, j', λ is involved in both the CG coefficient and the quantity $\langle a'j'||\hat{T}^\lambda||aj\rangle$, called the reduced matrix element. It can be understood as a proportionality constant (for fixed m, m', μ) which cannot be determined from the algebraic properties of angular-momentum operators, but needs to be evaluated for each particular case.
(c) Overall, the theorem implies **selection rules** for tensor operators:

$$\langle a'j'm'|\hat{T}^\lambda_\mu|ajm\rangle \neq 0 \;\Rightarrow\; \begin{cases} |j-\lambda| \le j' \le (j+\lambda) \\ m+\mu = m' \end{cases}$$

other equivalent forms of the **triangle inequality**
$|j'-\lambda| \le j \le (j+\lambda)$
$|j-j'| \le \lambda \le (j+j')$

These rules are essential e.g. for electromagnetic transitions between discrete energy eigenstates of various bound systems (atoms, nuclei...). Quantum amplitude of such a transition (per time unit) between states $|ajm\rangle$ and $|a'j'm'\rangle$ for multipolarity λ (total angular momentum of the absorbed or emitted photon) is given by a matrix element of the above type. So, e.g., a $j \xrightarrow{\lambda} j'$ transition requires j, j', λ satisfying the triangle inequality.

◄ Historical remark
1927: E. Wigner introduces D-matrices and applies the rotation group in QM
1930: C. Eckart publishes and applies his formulation of the W.-E. theorem
1942: G. Racah further extends the use of spherical tensors in spectroscopy

■ Space inversion

Spatial inversion (taking mirror images of all 3 spatial axes, therefore replacing "right" by "left" and vice versa) is just a discrete transformation. Nevertheless, there exists an observable associated with it—the spatial parity. In contrast to the above cases, space inversion is not a valid symmetry of this world.

► Coordinate, momentum & angular momentum transformation

The unitary space inversion operator $\hat{P}$ is defined by relations:

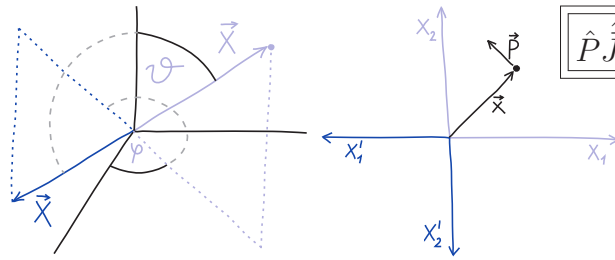
$\boxed{\hat{P}\,\hat{\vec{x}}\,\hat{P}^{-1} = -\hat{\vec{x}}}$ $\qquad$ $\boxed{\hat{P}\,\hat{\vec{p}}\,\hat{P}^{-1} = -\hat{\vec{p}}}$ $\quad\Rightarrow\quad \hat{P}\hat{\vec{L}}\hat{P}^{-1} = \hat{P}(\hat{\vec{x}}\times\hat{\vec{p}})\hat{P}^{-1} = +\hat{\vec{L}}$

$\hat{P}\hat{\vec{S}}\hat{P}^{-1} = +\hat{\vec{S}}$

$\boxed{\hat{P}\hat{\vec{J}}\hat{P}^{-1} = +\hat{\vec{J}}}$

Cartesian coordinates:
$x_i \to -x_i \quad (i{=}1,2,3)$

Spherical coordinates:
$r \to r$
$\vartheta \to (\pi - \vartheta)$
$\varphi \to (\varphi + \pi)$



▶ Classification of observables with respect to space inversion

So far, we classified observables according to their transformation under rotations. The space inversion enriches this classification.

$\hat{P}\hat{\vec{V}}\hat{P}^{-1} = -\hat{\vec{V}}$ **vector** $\qquad$ $\hat{P}\hat{\vec{V}}'\hat{P}^{-1} = +\hat{\vec{V}}'$ **pseudovector (axial vector)**

$\hat{P}\hat{S}\hat{P}^{-1} = +\hat{S}$ **scalar** $\qquad$ $\hat{P}\hat{S}'\hat{P}^{-1} = -\hat{S}'$ **pseudoscalar**

So for example, the angular momentum $\hat{\vec{J}}$ is not a true vector, but pseudovector, and a scalar product $\hat{\vec{p}}\cdot\hat{\vec{J}}$ is not a true scalar, but pseudoscalar.

▶ Invariance sensu stricto

N-particle Hamiltonian $\hat{H} = \hat{P}\hat{H}\hat{P}^{-1} = \sum_{k=1}^{N} \frac{1}{2M_k} \overbrace{\hat{P}\hat{\vec{p}}_k{}^2\hat{P}^{-1}}^{(-\hat{\vec{p}}_k)\cdot(-\hat{\vec{p}}_k)} + \overbrace{\hat{P}V(\{\hat{\vec{x}}_k\},\{\hat{\vec{S}}_k\})\hat{P}^{-1}}^{V(\{-\hat{\vec{x}}_k\},\{\hat{\vec{S}}_k\})}$

$\Rightarrow \boxed{V(\{\hat{\vec{x}}_k\},\{\hat{\vec{S}}_k\}) = V(\{-\hat{\vec{x}}_k\},\{\hat{\vec{S}}_k\})}$ potential must be even

▶ Parity

Operator $\hat{P}$ not only defines the space-inversion transformation, but also represents a physical observable called parity:

$\hat{P}^2 = \hat{I}$ $\quad\boxed{\hat{P} = \hat{P}^\dagger = \hat{P}^{-1}}\quad \Rightarrow$ eigenvalues $\quad\boxed{\pi = \pm 1}$

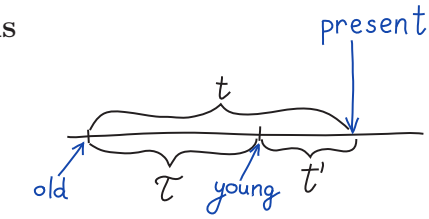
For single-particle wavefunctions we get:
$\hat{P}\Psi_{\text{even}}(\vec{x}) = +\Psi_{\text{even}}(\vec{x}) \quad \hat{P}\Psi_{\text{odd}}(\vec{x}) = -\Psi_{\text{odd}}(\vec{x})$
$\hat{P}[R(r)Y_{lm}(\vartheta,\varphi)] = R(r)\underbrace{Y_{lm}(\pi-\vartheta,\varphi+\pi)}_{P_{lm}(-\cos\vartheta)e^{im\varphi}e^{im\pi}} = \underbrace{(-)^{l-m}(-)^m}_{(-)^l}[R(r)Y_{lm}(\vartheta,\varphi)]$

■ Time translation

We come to transformations involving time. The most important specimen of this type represents a shift of the time-axis origin—time translation. The unitary operator expressing the transition between observers with different time settings is closely related to the evolution operator, which describes the dynamics. Motions of quantum systems generated by this operator will be in our main focus starting from Sec. 5a.

▶ **Observations with different time origins**

$$\left.\begin{array}{l}|\psi_{\rm young}(t')\rangle \\ |\psi_{\rm old}(\underbrace{t'+\tau}_{t})\rangle\end{array}\right\} \equiv \begin{array}{l}\text{states of the system seen by} \\ \text{“young” \& “old” observers}\end{array}$$



Uniqueness requirement: $|\psi_{\rm young}(t')\rangle \stackrel{!}{=} |\psi_{\rm old}(t)\rangle$

Transformation between both time frames: $|\psi_{\rm young}(t')\rangle = \hat{U}(t,t')|\psi_{\rm old}(t')\rangle$

$\Rightarrow$ Evolution transformation from time t' to $t=t'+\tau$: $\boxed{|\psi_{\rm old}(t)\rangle = \hat{U}(t,t')|\psi_{\rm old}(t')\rangle}$

▶ **Properties of $\hat{U}(t,t')$**

$$\left.\begin{array}{ll}\text{(a)} & \hat{U}(t,t') \equiv \hat{U}(\overbrace{t-t'}^{\tau}) \\ \text{(b)} & \hat{U}(\tau)^{-1} = \hat{U}(\tau)^{\dagger} \\ \text{(c)} & \hat{U}(0) = \hat{I} \\ \text{(d)} & \hat{U}(\tau_1+\tau_2) = \hat{U}(\tau_2)\hat{U}(\tau_1)\end{array}\right\} \Rightarrow \left\{\begin{array}{l}\hat{U}(\tau) = e^{i\hat{\chi}\tau} \text{ with any } \hat{\chi}=\hat{\chi}^{\dagger} \\ \text{Consistent choice:} \quad \hat{\chi} = -\frac{1}{\hbar}\hat{H} \\ \boxed{\hat{U}(\tau) = e^{-i\frac{\hat{H}\tau}{\hbar}}} \quad \textbf{evolution operator}\end{array}\right.$$

The above association of the generator $\hat{\chi}$ with the full **Hamiltonian** $\hat{H}$ of the system will be shown to be equivalent to the nonstationary Schrödinger equation (see Sec. 5a). The above derivation of $\hat{U}(\tau)$, in particular the requirement (a), in fact assumes that the symmetry of the system under the time translation is meant **sensu stricto**, which in this case implies that the Hamiltonian is independent of time: $\boxed{\hat{H}(t) \equiv \hat{H}}$ For instance, a system depending on external fields that vary in time does not possess this symmetry. However, it turns out (Sec. 5a) that even in such situations the time-dependent Hamiltonian $\hat{H}(t)$ fully determines the evolution operator $\hat{U}(t,t') \neq \hat{U}(t-t')$ of the system.

▶ **Evolution in the general case**

Postulate: Hamiltonian $\hat{H}(t)$ of the system at time t
$= \hbar\times$ generator of *infinitesimal* time translation $\equiv$ evolution from t to $t+dt$

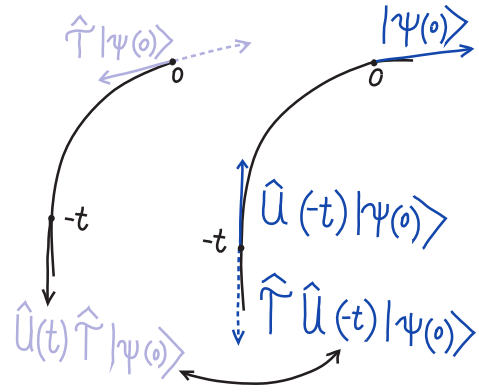
■ Time reversal

Time reversal means an inversion of the time arrow: going from future to past. One can imagine a movie played backwards. When watching such a movie, how to assign vectors to states and operators to observables to get a consistent QM description? Like the space inversion, the time reversal is just a discrete transformation, but a more difficult one. In quantum physics it cannot be represented by a unitary operator and there is no physical observable (analogous to spatial parity) associated with it. Similarly as in the case of the space inversion, the symmetry sensu stricto under the time reversal is slightly violated in nature (in weak interactions).

▶ Basic requirements

We seek for operator $\hat{\mathcal{T}}$ satisfying: $\boxed{\hat{U}(t)\hat{\mathcal{T}}|\psi(0)\rangle = \hat{\mathcal{T}}\hat{U}(-t)|\psi(0)\rangle}$ $\forall|\psi(0)\rangle$

This means: forward evolution of the time-reversed state = time reversal of the backward-evolved state, see the figure:



For infinitesimal time δt this implies:

$$\left(1 - i\tfrac{\hat{H}\delta t}{\hbar}\right)\hat{\mathcal{T}} = \hat{\mathcal{T}}\left(1 + i\tfrac{\hat{H}\delta t}{\hbar}\right)$$

$\Rightarrow$ We require: $\boxed{(-i\hat{H})\hat{\mathcal{T}} = \hat{\mathcal{T}}(i\hat{H})}$

For $\hat{\mathcal{T}}$ unitary this would mean:

$$\hat{H}\hat{\mathcal{T}} + \hat{\mathcal{T}}\hat{H} \equiv \underbrace{\{\hat{H}, \hat{\mathcal{T}}\}}_{\textbf{anticommutator}} = 0$$

$\Rightarrow$ $\hat{H}|E\rangle = E|E\rangle$ $\Rightarrow$ $\hat{H}(\hat{\mathcal{T}}|E\rangle) = -E(\hat{\mathcal{T}}|E\rangle)$

This would imply that energy has no lower bound, which would lead to catastrophic evolution accompanied by infinite release of energy. This is not physical.

$\Rightarrow$ $\hat{\mathcal{T}}$ is *not* a unitary operator!

▶ Operator $\hat{\mathcal{T}}$ is antiunitary

This means that it satisfies $\hat{\mathcal{T}}(\alpha\hat{A}) = \alpha^*\hat{\mathcal{T}}\hat{A}$ $\forall\,\alpha \in \mathbb{C}$

$\boxed{\hat{\mathcal{T}} \equiv \hat{U}\hat{K}}$ where $\begin{cases} \hat{U} \equiv \text{a unitary operator} \\ \hat{K} \equiv \text{complex conjugation operator: } \hat{K}\sum_i \alpha_i|i\rangle = \sum_i \alpha_i^*|i\rangle \\ \qquad \text{with respect to a selected basis } \{|i\rangle\}_{i=1,2,\ldots} \end{cases}$

$\Rightarrow$ Instead of $\{\hat{H}, \hat{\mathcal{T}}\} = 0$ the above requirement implies: $\boxed{[\hat{H}, \hat{\mathcal{T}}] = 0}$

The form of $\hat{\mathcal{T}}$ (the choice of $\hat{U}$ and the basis for $\hat{K}$) is not uniquely fixed but depends on the specific physical application.

▶ Properties of scalar products

$\langle\psi_1|\psi_2\rangle = \langle\hat{U}\psi_1|\hat{U}\psi_2\rangle = \sum_i \alpha'^*_{1i}\alpha'_{2i} = (\sum_i \alpha'_{1i}\alpha'^*_{2i})^* = \langle\hat{\mathcal{T}}\psi_1|\hat{\mathcal{T}}\psi_2\rangle^* = \langle\hat{\mathcal{T}}\psi_2|\hat{\mathcal{T}}\psi_1\rangle$

$\langle\psi_1|\hat{O}|\psi_2\rangle = \langle\hat{\mathcal{T}}\psi_2|\hat{\mathcal{T}}\hat{O}^\dagger\hat{\mathcal{T}}^{-1}|\hat{\mathcal{T}}\psi_1\rangle$ (e.g., transition matrix elements)

▶ Classification of observables with respect to time reversal

(1) $\hat{\mathcal{T}}\hat{A}\hat{\mathcal{T}}^{-1} = +\hat{A}$ **even observables** (e.g. $\hat{H}, \hat{\vec{x}}, \ldots$) $\hat{\mathcal{T}}$ keeps eigenvalues

(2) $\hat{\mathcal{T}}\hat{A}\hat{\mathcal{T}}^{-1} = -\hat{A}$ **odd observables** (e.g. $\hat{\vec{p}}, \hat{\vec{L}}, \hat{\vec{S}}, \ldots$) $\hat{\mathcal{T}}$ inverts eigenvalues

▶ Invariance sensu stricto

N-particle Hamiltonian $\hat{H} = \hat{\mathcal{T}}\hat{H}\hat{\mathcal{T}}^{-1} = \sum_k \frac{1}{2M_k}\overbrace{\hat{\mathcal{T}}\hat{\vec{p}}_k{}^2\hat{\mathcal{T}}^{-1}}^{(-\hat{\vec{p}}_k)\cdot(-\hat{\vec{p}}_k)} + \overbrace{\hat{\mathcal{T}}V(\{\hat{\vec{x}}_k\}, \{\hat{\vec{S}}_k\})\hat{\mathcal{T}}^{-1}}^{V^*(\{\hat{\vec{x}}_k\}, \{-\hat{\vec{S}}_k\})}$

$\Rightarrow$ $\boxed{V(\{\hat{\vec{x}}_k\}, \{\hat{\vec{S}}_k\}) = V^*(\{\hat{\vec{x}}_k\}, \{-\hat{\vec{S}}_k\})}$ real potential function (no losses) invariant under spin inversion (no external mag. field)

◂ Historical remark
1924: O. Laporte introduces spatial parity of electron wavefunctions in atoms
1931: E. Wigner shows that time reversal is represented by an antiunitary operator
1956: C.-S. Wu experimentally verifies that parity is violated in nuclear β decay
2012: experimental evidence of the time-reversal violation in weak decays

■ Galilean transformations

Nonrelativistic quantum mechanics must be invariant under transformations between inertial frames with relative speed $\vec{v}$. These transformations involve space, momentum and time variables.

▸ Quantum Galilean transformation

Classical Galilean transformation: $\begin{pmatrix}\vec{x}\\ \vec{p}\\ t\end{pmatrix} \mapsto \begin{pmatrix}\vec{x}'\\ \vec{p}'\\ t'\end{pmatrix} \equiv \mathbf{G}_{\vec{v}} \begin{pmatrix}\vec{x}\\ \vec{p}\\ t\end{pmatrix} = \begin{pmatrix}\vec{x}-\vec{v}\,t\\ \vec{p}-M\vec{v}\\ t\end{pmatrix}$

Unitary operators $\hat{G}_{\vec{v}}$ must satisfy $\boxed{\hat{G}_{\vec{v}}\,\hat{\vec{x}}\,\hat{G}_{\vec{v}}^{-1} = \hat{\vec{x}}-\vec{v}t\hat{I},\quad \hat{G}_{\vec{v}}\,\hat{\vec{p}}\,\hat{G}_{\vec{v}}^{-1} = \hat{\vec{p}}-M\vec{v}\hat{I}}$

$\boxed{\hat{G}_{\vec{v}} = e^{\frac{i}{\hbar}(M\hat{\vec{x}}-t\hat{\vec{p}})\cdot\vec{v}}} = \prod_{i=1}^{3} e^{\frac{i}{\hbar}Mv_i\hat{x}_i}\; e^{-\frac{i}{\hbar}tv_i\hat{p}_i}\; e^{\frac{i}{\hbar}\frac{1}{2}Mv_i^2t}$ (using the BCH formula)

Systems with $N>1$ particles: $\hat{G}_{\vec{v}} = \prod_{k=1}^{N} \hat{G}_{\vec{v}}^{(i)}$

Trasformation of single-particle wavefunction:
Coordinate representation: $\hat{G}_{\vec{v}}\,\psi(\vec{x},t) = e^{\frac{i}{\hbar}(M\vec{v}\cdot\vec{x}-\frac{1}{2}Mv^2t)}\,\psi(\vec{x}-\vec{v}t,t)$
Momentum representation: $\hat{G}_{\vec{v}}\,\tilde{\psi}(\vec{p},t) = e^{\frac{i}{\hbar}(-t\vec{v}\cdot\vec{p}+\frac{1}{2}Mv^2t)}\,\tilde{\psi}(\vec{p}-M\vec{v},t)$

▸ Relativistic quantum theory

To implement the relativistic Lorenz transformation into the quantum theory turned out to be a much more difficult task. It was not possible — at least not in a consistent way — before an essential reinterpretation of the wavefunction. In the relativistic theory, it does not describe a single particle, but a quantized field of particles whose number is not fixed. We do not follow this story here.

◂ Historical remark
1925: Erwin Schrödinger attempts to create a Lorenz-invariant wave equation, but because of problems he remains with the non-relativistic formulation
1926: Oskar Klein and Walter Gordon (simultaneously V. Fock and others) develop a relativistic wave equation for spinless particles
1927: Paul Dirac initiates quantum field theory (the correct unification of relativity with QM), in 1928 he creates a relativistic wave equation for spin-$\frac{1}{2}$ particle

■ Symmetry and degeneracy

Degeneracy of energy levels is an important signature of the system's symmetry sensu stricto. It occurs because for transformations $\hat{U}_g \equiv e^{i\hat{\vec{G}}\cdot\vec{s}}$ belonging to the symmetry group $\mathcal{G}$ the vector $\hat{U}_g|E\rangle$, where $|E\rangle$ is any eigenstate of the system's

Hamiltonian $\hat{H}$, remains an eigenstate of $\hat{H}$ with the same energy E. However, some symmetries cause no degeneracy, and some degeneracies are not caused by usual geometric symmetries.

► **Abelian symmetry group**: Eigenstates of $\hat{H}$ are simultaneous eigenstates of all generators $\hat{G}_i$ $\Rightarrow$ $e^{i\hat{\vec{G}}\cdot\vec{s}}|E\rangle = e^{i\varphi}|E\rangle$ (with $\varphi \equiv$ just a phase) $\Rightarrow$ The symmetry does not necessarily imply degeneracy. If degeneracy of eigenstates with different eigenvalues of $\hat{\vec{G}}$ occurs, it has some other ("dynamical") origins.

► **Non-Abelian symmetry group**: Some generators $\hat{G}_i$ act nontrivially on the eigenstates of $\hat{H}$ $\Rightarrow$ $e^{i\hat{\vec{G}}\cdot\vec{s}}|E\rangle = |E'\rangle$ with $\hat{H}|E'\rangle = E|E'\rangle$ and $\langle E|E'\rangle \neq 0$ $\Rightarrow$ Degeneracy in general occurs. Example: rotationally invariant $\hat{H}$ shows degeneracy of eigenstates $\{|ajm\rangle\}_{m=-j}^{+j}$, where $j, m \equiv$ total angular momentum quantum numbers and $a \equiv$ additional q. numbers.

► **Dynamical symmetry**

This term refers to situations when the Hamiltonian $\hat{H}$ has a higher symmetry than the commonly required space-time symmetries (like those under translations, rotations etc.). The sensu-stricto symmetry group $\mathcal{G}$ of such a system usually contains these space-time groups as subgroups. This leads to so-called **accidental degeneracies** of energy levels beyond those dictated by the common symmetries.

Example (a): **3D isotropic harmonic oscillator**
Dimensionless coordinate and momentum operators $\begin{cases} \hat{\vec{\mathrm{x}}} = \frac{1}{\sqrt{2\hbar/M\omega}}\hat{\vec{x}} \\ \hat{\vec{\mathrm{p}}} = \frac{1}{\sqrt{2\hbar M\omega}}\hat{\vec{p}} \end{cases}$

$$\hat{H} = \tfrac{1}{2M}\hat{\vec{p}}^{\,2} + \tfrac{M\omega^2}{2}\hat{\vec{x}}^{\,2} = \hbar\omega\big[\tfrac{3}{2} + \underbrace{(\hat{\vec{\mathrm{x}}} + i\,\hat{\vec{\mathrm{p}}})}_{\hat{\vec{b}}^\dagger}\cdot\underbrace{(\hat{\vec{\mathrm{x}}} - i\,\hat{\vec{\mathrm{p}}})}_{\hat{\vec{b}}}\big]$$

Beyond the rotational symmetry defined by transformations $\left\{ \begin{smallmatrix} \hat{R}\,\hat{\vec{x}}\,\hat{R}^{-1} = \mathbf{R}\,\hat{\vec{x}} \\ \hat{R}\,\hat{\vec{p}}\,\hat{R}^{-1} = \mathbf{R}\,\hat{\vec{p}} \end{smallmatrix} \right\}$ with orthogonal matrices $\mathbf{R} \in \mathrm{SO}(3)$, the Hamiltonian is also symmetric under a class of unitary transformations $\left\{ \begin{smallmatrix} \hat{U}\,\hat{\vec{b}}\,\hat{U}^{-1} = \mathbf{U}\,\hat{\vec{b}} \\ \hat{U}\,\hat{\vec{b}}^\dagger\,\hat{U}^{-1} = \mathbf{U}^\dagger\,\hat{\vec{b}}^\dagger \end{smallmatrix} \right\}$ with unitary matrices $\mathbf{U} \in \mathrm{U}(3)$. We have $\mathrm{U}(3) \supset \mathrm{SO}(3)$, so the system's actual symmetry is higher than rotational. This causes "accidental" degeneracies of oscillator eigenstates with different orbital quantum numbers l (see Sec. 2b).

Example (b): **Coulomb potential** (i.e., the hydrogen atom or Kepler problem)
Accidental degeneracy of the Hamiltonian eigenstates with different orbital quantum numbers l exists also in isotropic potential $V(r) = -\frac{K}{r}$ (see Sec. 2b). In this case the symmetry chain is $\mathrm{SO}(4) \supset \mathrm{SO}(3)$, where 6 generators of the SO(4) group coincide with components of the orbital angular momentum $\hat{\vec{L}}$ and those of the Runge-Lenz vector $\hat{\vec{R}} = \frac{1}{2}(\hat{\vec{p}} \times \hat{\vec{L}} - \hat{\vec{L}} \times \hat{\vec{p}}) - MK\hat{\vec{x}}$, all satisfying $[\hat{H}, \hat{L}_i] = [\hat{H}, \hat{R}_i] = 0$.

◀ Historical remark
1926: Wolfgang Pauli associates the accidental degeneracy in the hydrogen atom with the additional symmetry (using Lenz result from 1924)
1935-6: V. Fock & V. Bargmann analyze the dynamical symmetry of hydrogen
1960-70's: elaboration of techniques based on dynamical symmetries in particle and nuclear physics (A.O. Barut, Y. Ne'eman, A. Böhm, F. Iachello, D.J. Rowe *et al.*)

5a. UNITARY TIME EVOLUTION

After all, we are now coming to the dynamics of quantum systems, i.e., the evolution of state vectors in the Hilbert space with running time variable t. The standard treatment of quantum mechanics declares two types of quantum evolution: (i) the spontaneous one — motions signifying perpetual flow of time, and (ii) an induced one — changes provoked by quantum measurements. At first we will focus on type (i), the unitary evolution of systems which are not disturbed by any external interactions. Later, when we elaborate a more sophisticated statistical description of quantum states, we will argue that evolution of type (ii) may also be treated under type (i) if the external probes are included into the full quantum description.

■ Evolution operator and Schrödinger equation for systems with time-independent Hamiltonians

For quantum mechanics, the nonstationary Schrödinger equation means the same as what the Newton equation means for classical mechanics. We have already introduced the evolution operator from the time translation (Sec. 4b), so we do not need to make a special postulate on the spontaneous dynamics.

► Spontaneous evolution of a quantum system

$$\boxed{|\psi(t)\rangle = e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle} \quad \Leftrightarrow \quad i\hbar\tfrac{d}{dt}[e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle] = \hat{H}[e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle] \quad \boxed{i\hbar\tfrac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle}$$

evolution operator **nonstationary Schrödinger equation**

This description of the time evolution, with proper definitions of the system's state vectors and the Hamiltonian (operator of total energy), is quite general — valid in both non-relativistic and relativistic quantum theory. However, in the relativistic domain (i.e., within the quantum field theory) it becomes too complex and more viable approaches are applied instead. The non-relativistic QM follows from from considering the wavefunction of a fixed number of particles (in relativistic physics, particles can be created and annihilated) and from using the non-relativistic approximation of the Hamiltonian.

Example: Non-relativistic spinless particle with Hamiltonian $\hat{H}=\frac{\hat{\vec{p}}^2}{2M}+V(\hat{\vec{x}})$:

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t)=\left[-\frac{\hbar^2}{2M}\Delta+V(\vec{x})\right]\psi(\vec{x},t)$$

▸ Expression via stationary states

Assume a discrete energy spectrum of $\hat{H}$ that provides a complete basis $\{|E_i\rangle\}_{i=1}^{d}$

$\hat{H}|E_i\rangle=E_i|E_i\rangle \quad \Rightarrow \quad |\psi(0)\rangle\equiv|E_i\rangle \xrightarrow{t}|\psi(t)\rangle=e^{-i\frac{E_i t}{\hbar}}|\psi(0)\rangle$

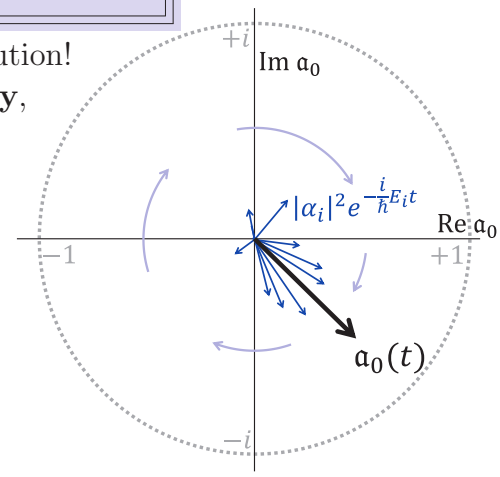
Eigenstates of $\hat{H}$ evolve just through their phase factors ⇒ they are "stationary"
⇒ Evolution of a general state is expressed by its expansion to eigenstates $|E_i\rangle$:

$$|\psi(0)\rangle\equiv\sum_i \underbrace{\alpha_i}_{\alpha_i(0)}|E_i\rangle \quad\xrightarrow{t}\quad \sum_i \underbrace{\alpha_i e^{-i\frac{E_i t}{\hbar}}}_{\alpha_i(t)}|E_i\rangle\equiv|\psi(t)\rangle$$

This yields a rather simple picture of evolution!

Example: **quantum survival probability**, i.e., the probability that the initial state $|\psi(0)\rangle$ is found in the evolved state $|\psi(t)\rangle$

$$\begin{aligned}\mathfrak{p}_0(t) &= \left|\mathfrak{a}_0(t)\right|^2=\left|\langle\psi(0)|\psi(t)\rangle\right|^2\\ &=\left|\langle\psi(0)|e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle\right|^2\\ &=\boxed{\left|\sum_i|\alpha_i|^2e^{-i\frac{E_i t}{\hbar}}\right|^2=\mathfrak{p}_0(t)}\end{aligned}$$



■ Single-particle probability current

If the dynamical Schrödinger equation is applied to the scalar wavefunction of a single particle in external fields, the resulting dependence $\psi(\vec{x},t)$ describes how the probability density $\rho(\vec{x},t)=|\psi(\vec{x},t)|^2$ flows in space. This process can be described in terms of ordinary fluid dynamics.

▸ Continuity equation

Particle in scalar and vector potentials $V(\vec{x},t)$ and $\vec{A}(\vec{x},t)$:

$$\frac{\partial}{\partial t}\underbrace{|\psi|^2}_{\rho}=\underbrace{\frac{\partial\psi}{\partial t}}_{\text{from Schrödinger eq.}}\psi^*+\psi\underbrace{\frac{\partial\psi^*}{\partial t}}=\frac{1}{i\hbar}\psi^*\left[\frac{1}{2M}(-i\hbar\vec{\nabla}-q\vec{A})^2+V\right]\psi+\left\{\begin{smallmatrix}\text{complex}\\ \text{conjugate}\end{smallmatrix}\right\}=$$

$$=\frac{1}{M\hbar}\,\mathrm{Im}\underbrace{\left[\psi^*(-\hbar^2\vec{\nabla}\cdot\vec{\nabla}+i\hbar q\vec{\nabla}\cdot\vec{A}+i\hbar q\vec{A}\cdot\vec{\nabla}+q^2\vec{A}^2)\psi\right]}_{\begin{smallmatrix}-\hbar^2\vec{\nabla}\cdot(\psi^*\vec{\nabla}\psi)+i\hbar q\vec{\nabla}\cdot(\psi^*\vec{A}\psi)\\ +\hbar^2(\vec{\nabla}\psi^*)\cdot(\vec{\nabla}\psi)-i\hbar q\left[(\vec{\nabla}\psi^*)\cdot\vec{A}\psi-\text{C.C.}\right]+q^2\vec{A}^2|\psi|^2\end{smallmatrix}}=-\vec{\nabla}\cdot\underbrace{\left[\frac{\hbar}{M}\mathrm{Im}(\psi^*\vec{\nabla}\psi)-\frac{q}{M}\psi^*\vec{A}\psi\right]}_{\vec{j}}$$

We obtain the familiar continuity equation:

$$\frac{\partial}{\partial t}\rho(\vec{x},t)+\vec{\nabla}\cdot\vec{j}(\vec{x},t)=0$$

The change of probability in an infinitesimal volume is in balance with the incoming/outgoing flux of probability. The probability density $\rho(\vec{x},t)$ behaves like the density of a fluid whose "substance" is locally conserved.

Conservation of total probability: Take a sphere of radius R (volume V_R, surface S_R). Then $\frac{d}{dt}\int\limits_{V_R} |\psi(\vec{x},t)|^2\, d\vec{x} = -\int\limits_{V_R} \vec{\nabla}\cdot\vec{j}(\vec{x},t) d\vec{x} = -\int\limits_{S_R} \vec{j}(\vec{x},t)\cdot d\vec{S}_R \xrightarrow[R\to\infty]{} 0$

(since for normalizable wavefunctions $\vec{j} \to 0$ faster than $1/S_R$)

$\Rightarrow$ The norm $\langle\psi|\psi\rangle = \int |\psi(\vec{x},t)|^2\, d\vec{x} = 1$ is conserved in time, as was already clear from unitarity of the evolution operator $\hat{U}(t)$.

▶ Probability current (flux)

$$\vec{j}(\vec{x},t) = \frac{\hbar}{M} \underbrace{\mathrm{Im}\left[\psi^*\vec{\nabla}\psi\right]}_{-\frac{i}{2}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*)} - \frac{q}{M}\psi^*\vec{A}\psi = \boxed{\frac{1}{2M}\left[\psi^*(\hat{\vec{\pi}}\psi) + \psi(\hat{\vec{\pi}}\psi)^*\right] = \vec{j}}$$

$\hat{\vec{\pi}} = (-i\hbar\vec{\nabla} - q\vec{A}) \equiv$ mechanical momentum

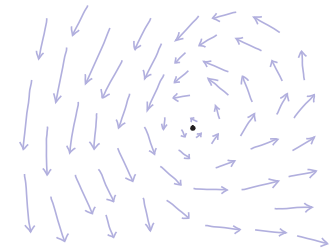
Parametrization: $\boxed{\psi(\vec{x},t) = R(\vec{x},t)e^{\frac{i}{\hbar}S(\vec{x},t)}}$ $\Rightarrow$ $\boxed{\vec{j} = \underbrace{R^2}_{\rho}\underbrace{\frac{1}{M}\left[\vec{\nabla}S - q\vec{A}\right]}_{\vec{v}}}$

This helps to understand the meaning of complex single-particle wavefunctions:

- The squared absolute value $|\psi(\vec{x},t)|^2 = R(\vec{x},t)^2$ is the probability density.
- The gradient of phase $\vec{\nabla}S(\vec{x},t)$ determines the velocity field $\Rightarrow$ flux.

This means that even a stationary wavefuction $\psi(\vec{x}) = R(\vec{x})e^{\frac{i}{\hbar}S(\vec{x})}$ can have a **dynamical content** if $\psi(\vec{x}) \in \mathbb{C}$ and the phase $S(\vec{x}) \neq$ const.

The wavefunction $\psi(\vec{x})$ can be visualized as a mesh of arrows whose lengths are proportional to $\vec{v}(\vec{x}) = \frac{1}{M}\vec{\nabla}S(\vec{x})$ (the velocity field) and whose density is proportional to $\rho(\vec{x}) = R(\vec{x})^2$ (the density field), see an artificial example here:

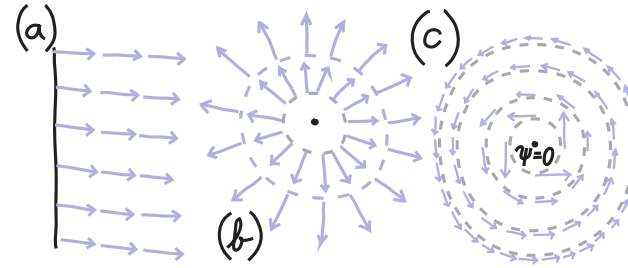


▶ Probability currents for simple wavefunctions

(a) Planar wave:	$\psi = \mathcal{N}e^{i\vec{k}\cdot\vec{x}}$	$\vec{j} = \lvert\mathcal{N}\rvert^2\frac{\hbar\vec{k}}{M}$
(b) Spherical wave:	$\psi = \mathcal{N}\frac{1}{r}e^{ik_r r}$	$\vec{j} = \lvert\mathcal{N}\rvert^2\frac{\hbar k_r}{Mr^2}\vec{n}_r$
(c) Eigenstate of orbital momentum:	$\psi = \underbrace{R(r)}_{\lvert R\rvert e^{i\phi_r(r)}}\underbrace{Y_{lm}(\vartheta,\varphi)}_{P_{lm}(\cos\vartheta)e^{im\varphi}}$	$\vec{j} \propto \frac{d\phi_r}{dr}\vec{n}_r + \frac{m\hbar}{r\sin\vartheta}\vec{n}_\varphi$

The corresponding probability currents are:

(a) translational
(b) divergent
(c) rotational



▶ Interference of probability currents

Let $\psi(\vec{x}) = \psi_1(\vec{x}) + \psi_2(\vec{x})$, with $\psi_1(\vec{x})$ and $\psi_2(\vec{x})$ being wavefunctions with currents $\vec{j}_1(\vec{x})$ and $\vec{j}_2(\vec{x})$. The probability current corresponding to $\psi(\vec{x})$ reads:

$$\boxed{\vec{j} = \vec{j}_1 + \vec{j}_2 + \underbrace{\tfrac{1}{M}\mathrm{Re}\left[\psi_1^*(-i\hbar\vec{\nabla})\psi_2 + \psi_2^*(-i\hbar\vec{\nabla})\psi_1 - 2q\vec{A}\psi_1^*\psi_2\right]}_{\text{interference term } \vec{j}_{\rm int}}}$$

Example:
plane waves

$$\left.\begin{aligned}\psi_1(\vec{x}) &= \mathcal{N}e^{i\vec{k}_1\cdot\vec{x}}\\ \psi_2(\vec{x}) &= \mathcal{N}e^{i\vec{k}_2\cdot\vec{x}}\end{aligned}\right\} \quad\Rightarrow\quad \vec{j}_{\rm int}(\vec{x}) = |\mathcal{N}|^2\left[\tfrac{\hbar}{M}(\vec{k}_1+\vec{k}_1) - 2q\vec{A}(\vec{x})\right]\cos\left[(\vec{k}_1-\vec{k}_2)\cdot\vec{x}\right]$$

In particular, we obtain no interference for $\vec{k}_1 = \pm\vec{k}_2$ and $\vec{A}=0$

▶ Stationary solutions of dynamical problems

The continuity equation enables us to solve some nonstationary single-particle problems, like **scattering on a potential** $V(\vec{x})$, via the stationary Schr. equation. These techniques will be elaborated in Secs. 12 & 13. Here just shortly.

Stationary state: $\frac{\partial}{\partial t}|\psi|^2 = 0 \quad\Rightarrow\quad$ continuity equation reads: $\boxed{\vec{\nabla}\cdot\vec{j} = 0}$

For systems inviariant under time reversal there exist degenerate Hamiltonian eigenstates $\left\{\begin{smallmatrix}\psi_E\\ \psi_E^*\end{smallmatrix}\right\}$ with flows $\left\{\begin{smallmatrix}\vec{j}\\ -\vec{j}\end{smallmatrix}\right\}$. We can combine these solutions to a real solution with $\vec{j}=0$. However, when solving the dynamical problems we proceed with complex solutions.

Example: Consider the **1D scattering** problem describing passage of a particle through a finite-range potential $V(x)$ with $V(x)\to 0$ for $x\to\pm\infty$.

We search for the solutions of

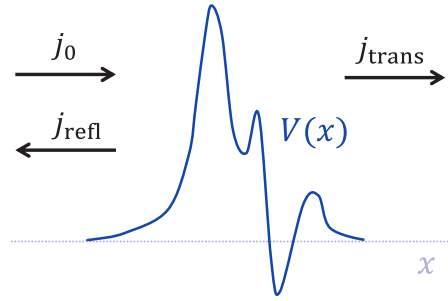
$$\left[-\tfrac{\hbar^2}{2M}\tfrac{d^2}{dx^2} + V(x)\right]\psi_E(x) = \overbrace{\tfrac{(\hbar k)^2}{2m}}^{E}\psi_E(x)$$

with $\psi_E(x)$ having the asymptotic forms:

$x\to-\infty$: $\psi_E(x) \sim \underbrace{e^{+ikx}}_{\text{incoming}} + \underbrace{a_{\rm refl}(E)e^{-ikx}}_{\text{reflected}}$

$a_{\rm refl}, a_{\rm trans} \equiv$ coefficients

$x\to+\infty$: $\psi_E(x) \sim \overbrace{a_{\rm trans}(E)e^{+ikx}}^{\text{transmitted waves}}$



1D continuity eq. $\frac{d}{dx}j(x)=0 \Rightarrow j(x)=\text{const} \Rightarrow \overbrace{\left(1-|a_{\rm refl}(E)|^2\right)\tfrac{\hbar k}{M}}^{j(-\infty)=j_0+j_{\rm refl}} = \overbrace{|a_{\rm trans}(E)|^2\tfrac{\hbar k}{M}}^{j_{\rm trans}=j(+\infty)}$

Hence the solution of $\psi_E(x)$ of the stationary Schrödinger equation with the above asymptotics directly yields the reflection probability $\mathfrak{p}_{\rm refl}(E) = |a_{\rm refl}(E)|^2$ $(= \frac{j_{\rm refl}}{j_0})$ and transmission propability $\mathfrak{p}_{\rm trans}(E) = |a_{\rm trans}(E)|^2$ $(= \frac{j_{\rm trans}}{j_0})$ satisfying $\mathfrak{p}_{\rm refl}+\mathfrak{p}_{\rm trans}=1$. It turns out that, in general, even a particle with $E<\mathrm{Max}_x V(x)$ has a chance $\mathfrak{p}_{\rm trans}(E) > 0$ to pass (**quantum tunneling** effect), and also a particle with $E>\mathrm{Max}_x V(x)$ has a chance $\mathfrak{p}_{\rm refl}(E)>0$ to get reflected.

► **Vorticity of the flow** $\boxed{\vec{\mathfrak{v}} \equiv \vec{\nabla} \times \vec{v}}$

This quantity quantifies the spinning motion of the 3D velocity flow.

(a) $\vec{A} = 0$: $\vec{\mathfrak{v}} = \vec{\nabla} \times \left(\frac{1}{M}\vec{\nabla}S\right) = 0$ except points satisfying $\psi = 0$, where the phase S is not determined ⇒ In absence of mag. field, the probability flow may produce vortices only at the points where $\psi = 0$, cf. the rotational flow (c) in the above example.

(b) $\vec{A} \neq 0$: $\vec{\mathfrak{v}} = -\frac{q}{M}\overbrace{(\vec{\nabla} \times \vec{A})}^{\vec{B}}$ ⇒ The flow is vortical in all points where $\vec{B} \neq 0$.

◄ **Historical remark**

1926: Erwin Schrödinger presents the nonrelativistic wave equation for single electron & Max Born finds its probabilistic interpretation using the probability flux

1928: George Gamow explains nuclear α-decays with the aid of quantum tunneling

■ Conservation laws and symmetries

We are ready now to appreciate the deepest dynamical consequence of symmetry. According to the famous theorem by Emmy Noether, the symmetry sensu stricto of a given system under an n-parameter Lie group generates n conserved quantities. This has rather fundamental connotations. One may imagine that the very recognition of all physical quantities relies on the particular symmetries that imply the conservation of these quantities in some systems. But what the conservation law means in the indeterministic environment of QM, where all physical quantities yield just statistical values?

► **Conservation laws in QM**

Time evolution of the probability distribution for measurement outcomes a of quantity A for a system in initial state $|\psi(0)\rangle$: $p_\psi(a,t) \equiv \langle\psi(t)|\hat{P}_a|\psi(t)\rangle$

Quantity A is conserved in a given quantum system *iff* its probability distribution $p_\psi(a,t)$ for any initial state does not change in time:

⇒ $\boxed{\frac{\partial}{\partial t}p_\psi(a,t) = 0}$ $\forall\,|\psi(0)\rangle$ & $\forall\, a$

⇒ statistical moments $\underbrace{\langle\psi(t)|\hat{A}^k|\psi(t)\rangle}_{\langle\psi(0)|e^{i\frac{\hat{H}t}{\hbar}}\hat{A}^k e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle} = \langle\psi(0)|\hat{A}^k|\psi(0)\rangle$ ⇒ $e^{i\frac{\hat{H}t}{\hbar}}\hat{A}e^{-i\frac{\hat{H}t}{\hbar}} = \hat{A}$

⇒ $\boxed{\boxed{[\hat{A},\hat{H}] = 0}}$

So, the conserved quantities are those that commute with the Hamiltonian.

► **Evolution of averages**

$$i\hbar\tfrac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle = \overbrace{-\langle\psi(0)|e^{i\frac{\hat{H}t}{\hbar}}\hat{H}\hat{A}e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle + \langle\psi(0)|e^{i\frac{\hat{H}t}{\hbar}}\hat{A}\hat{H}e^{-i\frac{\hat{H}t}{\hbar}}|\psi(0)\rangle}^{\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle}$$

Time-derivative "operator": $\boxed{\boxed{\hat{\dot{A}} \equiv \tfrac{1}{i\hbar}[\hat{A},\hat{H}]}}$ $\qquad \boxed{\tfrac{d}{dt}\langle A\rangle_\psi \equiv \langle\psi(t)|\hat{\dot{A}}|\psi(t)\rangle}$

Analogy with the Poisson bracket: $\dot{A} = \sum_i \left(\frac{\partial A}{\partial p_i} \underbrace{\dot{p}_i}_{-\frac{\partial H}{\partial q_i}} + \frac{\partial A}{\partial q_i} \underbrace{\dot{q}_i}_{+\frac{\partial H}{\partial p_i}} \right) = \{A, H\}$

$\Rightarrow$ correspondence $[\hat{A}, \hat{H}] \leftrightarrow i\hbar \{A, H\}$

Example: **particle speed** "operator" for $\hat{H} = \frac{1}{2M}(\hat{\vec{p}} - q\vec{A})^2 + V$

$\dot{\hat{\vec{x}}} = \frac{1}{i\hbar}[\hat{\vec{x}}, \hat{H}] = \frac{1}{2iM\hbar}[\hat{\vec{x}}, (\hat{\vec{p}} - q\vec{A})^2] = \frac{1}{M}(\hat{\vec{p}} - q\vec{A}) = \frac{1}{M}\hat{\vec{\pi}}$

► Conservation laws generated by symmetries

Let quantity $\hat{G}$ be a Hermitian generator of an $n=1$ Lie group $\mathcal{G} \equiv \{e^{i\hat{G}s}\}_{s\in\mathbb{R}}$

$$\left.\begin{array}{r} [\hat{G}, \hat{H}] = 0 \\ \hat{G} \text{ is conserved} \end{array}\right\} \Leftrightarrow \left\{\begin{array}{l} [e^{i\hat{G}s}, \hat{H}] = 0 \\ \mathcal{G} \text{ is the } \textbf{symmetry group} \text{ of } \hat{H} \text{ (sensu stricto)} \end{array}\right.$$

Generalizing to higher dimensional Lie groups, we obtain the QM version of the **Noether theorem**: invariance of $\hat{H}$ under a Lie group with n generators implies conservation of quantities associated with all generators

Standard spatio-temporal symmetries of $\hat{H}$ and related **conservation laws**:

translational invariance	$\Leftrightarrow$	**linear momentum** $\hat{\vec{p}}$
rotational invariance	$\Leftrightarrow$	**angular momentum** $\hat{\vec{J}}$
time translation invariance	$\Leftrightarrow$	**energy** $\hat{H}$
space reflection invariance	$\Leftrightarrow$	**parity** $\hat{P}$

Note: Space reflection is not a continuous transformation; parity conservation follows from an "accidental" Hermiticity of the reflection operator $\hat{P}$

◄ Historical remark

1915: E. Noether proves the theorem relating conservation laws with symmetries
1924: N. Bohr, H. Kramers & J. Slater propose that in QM the conservation laws hold only "statistically" (not in every event), but this is later disproved experimentally
1927: Eugene Wigner writes about symmetry & conservation laws in QM, he relates parity conservation in elmag. decays with reflection symmetry of interaction
1956-64: Discoveries of the violation of the spatial and combined parity $\hat{P}$ and $\hat{C}\hat{P}$

■ Energy × time uncertainty relation

Time does not appear as a standard physical observable. It is just "a parameter" whose only role is "to fly" — and we all have to fly with it! In particular, quantum theory offers no operator to be associated with time. It is possible to find various observables that can be used for time measurements in association with some specific initial states, but to find a universal time operator is not possible. Nevertheless, it is often stated that time and energy form a pair of conjugated quantities similar to coordinate and momentum. This can be valid only in a limited sense, which we explore in the following.

▶ Survival probability and energy distribution

We return to the above-outlined problem of survival probability. The amplitude $\mathfrak{a}_0(t) \equiv \langle\psi(0)|\psi(t)\rangle$ and probability $\mathfrak{p}_0(t) = |\mathfrak{a}_0(t)|^2$ to find the system in its $t = 0$ state $|\psi(0)\rangle$ at a positive or negative time t must satisfy conditions:

$$\mathfrak{a}_0(t)=\langle\psi(0)|e^{-i\frac{\hat{H}t}{\hbar}}\psi(0)\rangle=\langle e^{+i\frac{\hat{H}t}{\hbar}}\psi(0)|\psi(0)\rangle = \mathfrak{a}_0^*(-t) \quad \Rightarrow \quad \boxed{\mathfrak{p}_0(t) = \mathfrak{p}_0(-t)}$$

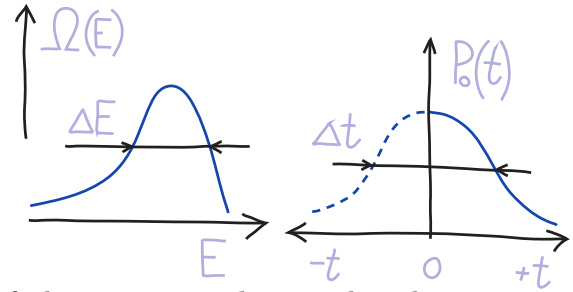
To evaluate $\mathfrak{a}_0(t)$, we use the completeness:
(for continuous E & discrete k; other possibilities analogous)

$$\begin{cases} \int\limits_{\mathcal{S}(\hat{H})} \sum\limits_{k\in\mathcal{D}_E} |Ek\rangle\langle Ek|\, dE = \hat{I} \\ \langle E'k'|Ek\rangle = \delta(E-E')\delta_{kk'} \end{cases}$$

$$\mathfrak{a}_0(t)=\langle\psi(0)|\underset{\hat{I}}{\uparrow} e^{-i\frac{\hat{H}t}{\hbar}} \underset{\hat{I}}{\uparrow}|\psi(0)\rangle=\iint \sum_{k,k'} \underbrace{\langle\psi(0)|E'k'\rangle}_{\omega^*(E',k')} \underbrace{\langle E'k'|e^{-i\frac{\hat{H}t}{\hbar}}|Ek\rangle}_{e^{-i\frac{Et}{\hbar}}\delta(E-E')\delta_{kk'}} \underbrace{\langle Ek|\psi(0)\rangle}_{\omega(E,k)} dE\, dE'$$

$$= \int \underbrace{\left[\sum_k |\omega(E,k)|^2\right]}_{\Omega(E)\ \textbf{energy distribution}} e^{-i\frac{Et}{\hbar}}dE = \boxed{\int\limits_{\mathcal{S}(\hat{H})} \Omega(E)e^{-i\frac{Et}{\hbar}}dE = \mathfrak{a}_0(t)}$$

So the survival amplitude $\mathfrak{a}_0(t)$ is the Fourier transform of the energy distribution $\Omega(E)$. The general rule is that $\left\{\begin{smallmatrix}\text{wide}\\ \text{narrow}\end{smallmatrix}\right\}$ energy distributions yeild the survival probabilities that decay $\left\{\begin{smallmatrix}\text{quickly}\\ \text{slowly}\end{smallmatrix}\right\}$.



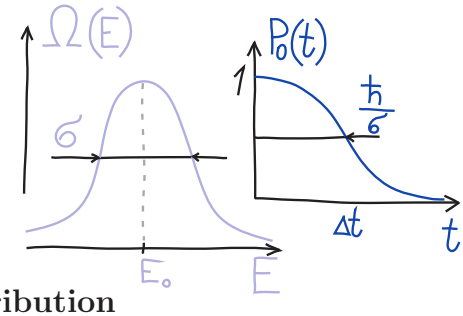
Defining some widths ΔE and Δt of the energy and time distributions, we expect an approximate relation $\Delta E \cdot \Delta t \sim \hbar$, where however Δt is not an uncertainty in the usual quantum sense. Below we illustrate this by two examples:

(1) **Gaussian energy distribution**

$$\boxed{\Omega(E) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(E-E_0)^2}{2\sigma^2}}}$$ the energy width is naturally defined as $\Delta E = \sigma$

$$\mathfrak{a}_0(t)=\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} \underbrace{e^{-\frac{(E-E_0)^2}{2\sigma^2}-i\frac{Et}{\hbar}}}_{e^{-\frac{1}{2\sigma^2}E^2+\left(\frac{E_0}{\sigma^2}-\frac{it}{\hbar}\right)E-\frac{E_0^2}{2\sigma^2}}} dE = e^{-\frac{\sigma^2}{2\hbar^2}t^2}e^{-i\frac{E_0 t}{\hbar}}$$

$$\boxed{\mathfrak{p}_0(t) = e^{-\left(\frac{\sigma}{\hbar}\right)^2 t^2}} = e^{-\left(\frac{t}{\Delta t}\right)^2} \Rightarrow \text{the time width can be defined as } \Delta t = \frac{\hbar}{\sigma} \quad \Rightarrow \boxed{\Delta E \cdot \Delta t = \hbar}$$



(2) **Breit-Wigner (Cauchy) energy distribution**

$$\boxed{\Omega(E) = \frac{1}{\pi}\frac{\frac{\Gamma}{2}}{(E-E_0)^2+\left(\frac{\Gamma}{2}\right)^2}}$$

Γ = finite halfwidth of $\Omega(E)$

$\langle\langle E^2\rangle\rangle = \infty$ energy disperion infinite as the decrease of $\Omega(E)$ for $E\to\pm\infty$ is too slow (algebraic)

We obtain $\boxed{\mathfrak{p}_0(t) = e^{-\frac{t}{\tau}}}$ **exponential decay** with average lifetime $\tau = \frac{\hbar}{\Gamma}$

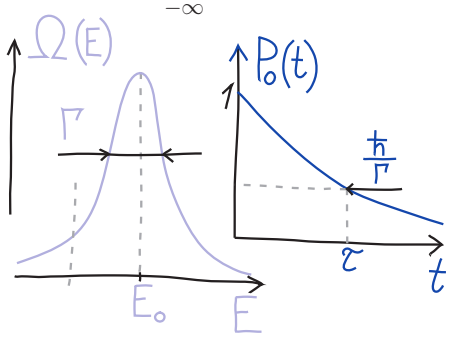
So the energy-time uncertainty satified: $\boxed{\overbrace{\Delta E}^{\Gamma} \cdot \overbrace{\Delta t}^{\tau} = \hbar}$

Inverse proof (from exponential decay to Breit-Wigner distribution):

Assume $\mathfrak{a}_0(t) = \left\{ \begin{array}{l} e^{-\Gamma t/(2\hbar)} e^{-iE_0 t/\hbar} \\ e^{+\Gamma t/(2\hbar)} e^{-iE_0 t/\hbar} \end{array} \right\}$ for $\left\{ \begin{array}{l} t \geq 0 \\ t < 0 \end{array} \right.$ Coherent assumption on the phase factors. The $t>0$ exponential decay is extended also to $t<0$

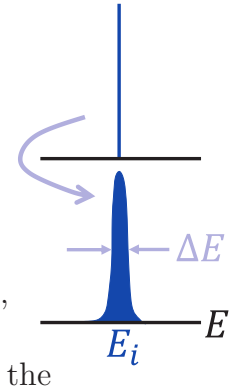
$$\Omega(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \mathfrak{a}_0(t) e^{+i\frac{Et}{\hbar}} dt = \frac{1}{2\pi\hbar} \Bigg(\underbrace{\int_{-\infty}^{0} e^{\left[\frac{\Gamma}{2\hbar} + i\frac{E-E_0}{\hbar}\right]t} dt}_{\frac{\hbar}{(\Gamma/2)+i(E-E_0)}} + \underbrace{\int_{0}^{+\infty} e^{\left[-\frac{\Gamma}{2\hbar} + i\frac{E-E_0}{\hbar}\right]t} dt}_{\frac{-\hbar}{-(\Gamma/2)+i(E-E_0)}} \Bigg) =$$

$$= \frac{1}{\pi} \frac{\Gamma/2}{(E-E_0)^2 + (\Gamma/2)^2}$$



So the exponential decay of unstable nuclei, particles and other objects is related to the continuous Breit-Wigner distribution of energy, which is called the **natural lineshape**. However, the Breit-Wigner distribution $\Omega(E)$ is not physical as it has the infinite energy dispersion. The real lineshape can be very close to the natural one but must deviate from it in both low- and high-energy tails. This leads to small deviations from the exponential law, in particular, to a smoothening of the $t = 0$ cusp of the extended function $\mathfrak{p}_0(t)$; see below.

▶ Mechanism of generating a smooth lineshape



The decay of an unstable quantum system Q is often due to its interaction with a certain quantized field F (e.g., the electromagnetic field). The Q + F system has Hamiltonian $\hat{H} = \hat{H}_{\rm Q} + \hat{H}_{\rm S} + \hat{H}_{\rm QF}$, where $\hat{H}_{\rm Q}$ (with a discrete spectrum) and $\hat{H}_{\rm F}$ (with a continuous spectrum) are self-Hamiltonians of Q and F, and $\hat{H}_{\rm QF}$ is a Q-F interaction. Assume an initial state $|\psi(0)\rangle = |E_i\rangle_{\rm Q}|0\rangle_{\rm F}$ in the full Hilbert space $\mathcal{H} = \mathcal{H}_{\rm Q} \otimes \mathcal{H}_{\rm F}$, where $|E_i\rangle_{\rm Q}$ is an excited state of Q (so $\hat{H}_{\rm Q}|E_i\rangle_{\rm Q} = E_i|E_i\rangle_{\rm Q}$) and $|0\rangle_{\rm F}$ is the lowest-energy eigenstate (vacuum) of F. Thus the state $|E_i\rangle_{\rm Q}|0\rangle_{\rm F}$ is an eigenstate of $\hat{H}_{\rm Q} + \hat{H}_{\rm S}$, but not of the full Hamiltonian $\hat{H}$. Hence this state evolves with time. The energy distribution $\Omega(E)$ in the continuous eigenbasis of $\hat{H}$ determines the survival probability function $P_0(t)$.

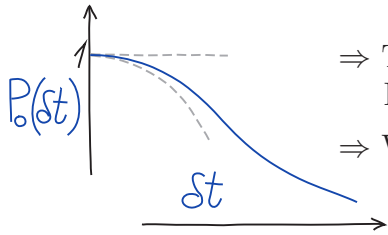
▶ Non-exponential decay

The decay of unstable nuclei, particles or excited states is described by the exponential decay law, but necessary low- & high-energy deviations from the

Breit-Wigner energy distribution imply that this law is only an approximation. This becomes particularly apparent at very small and very large times. Deviations at the small times: The exponential decay yields $\frac{d}{dt}\mathfrak{p}_0(t)\big|_{t=0} = -\frac{1}{\tau}$ while QM always yields $\boxed{\frac{d}{dt}\mathfrak{p}_0(t)\big|_{t=0} = 0}$

$|\mathfrak{a}_0(\delta t)|^2 = \langle\psi(0)|e^{-i\frac{\hat{H}\delta t}{\hbar}}|\psi(0)\rangle\langle\psi(0)|e^{+i\frac{\hat{H}\delta t}{\hbar}}|\psi(0)\rangle \approx$ expand up to 2nd order in δt

$\approx 1 + \langle\psi(0)|\hat{H}|\psi(0)\rangle^2\frac{(\delta t)^2}{\hbar^2} - \langle\psi(0)|\hat{H}^2|\psi(0)\rangle\frac{(\delta t)^2}{\hbar^2} = \boxed{1 - \underbrace{\frac{\langle\langle E^2\rangle\rangle}{\hbar^2}}_{\tau^{-2}}(\delta t)^2 \approx \mathfrak{p}_0(\delta t)}$



⇒ The QM decay for small times is always quadratic. However, this is usually very hard to measure!

⇒ We again get: $\underbrace{\Delta E}_{\sqrt{\langle\langle E^2\rangle\rangle}}\ \underbrace{\Delta t}_{\tau} = \hbar$

◀ Historical remark

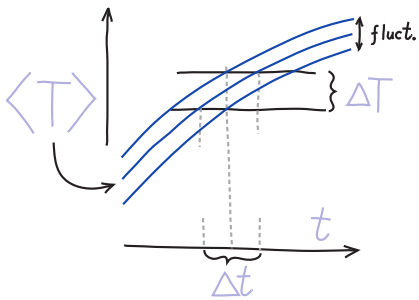
1950-60s: Theoretical study of deviations from the exponential decay law
1997: The first experimental detection of the short-time deviations

► Energy × time uncertainty in real measurements

Assume the situation in which an evolution of a certain quantity T (with quantum operator $\hat{T}$) for some particular initial states is used for the determination of time (for a given system). What is the precision of such a chronometer?

For $\hat{T}$ being an applicable **"clock" operator** there must be $\boxed{[\hat{T}, \hat{H}] \neq 0}$ (otherwise the distribution of quantity T for any initial state $|\psi(0)\rangle$ would be conserved in time) ⇒ standard $\hat{T} \times \hat{H}$ uncertainty relation can be applied in the evolving state $|\psi(t)\rangle$:

$$\sqrt{\langle\langle E^2\rangle\rangle_{\psi(t)}\langle\langle T^2\rangle\rangle_{\psi(t)}} \geq \frac{\hbar}{2}\left|\langle\psi(t)|\overbrace{\tfrac{1}{i\hbar}[\hat{T}, H]}^{\dot{\hat{T}}}|\psi(t)\rangle\right|$$



Quantity $\frac{\sqrt{\langle\langle T^2\rangle\rangle_{\psi(t)}}}{|\langle\psi(t)|\dot{\hat{T}}|\psi(t)\rangle|} = \frac{\Delta_{\psi(t)}T}{\frac{d}{dt}\langle T\rangle_{\psi(t)}} \equiv \Delta t$ can be identified with an uncertainty of time determination via the clock observable $\hat{T}$ for initial state $|\psi(0)\rangle$

⇒ real uncertainty relation $\boxed{\Delta E \cdot \Delta t \geq \frac{\hbar}{2}}$

Time operator in QM? For a certain *subset of initial states* of the given system, it is possible to find a suitable clock operator $\hat{T}$. However, there exists *no universal time operator* $\hat{T}$ satisfying the canonical commutation relation $[\hat{T}, \hat{H}] = -i\hbar\hat{I}$, applicable for all initial states $\in \mathcal{H}$. For instance, this would imply the absence of a lower bound of energy, which is unphysical.

◀ Historical remark
1926, 1933: W. Pauli shows the difficulty in building a quantum operator of time
1928: N. Bohr proposes the $E \times t$ uncertainty principle, 1930's debate with Einstein
1945: L. Mandelstam & I. Tamm derive $E \times t$ uncertainty for "clock observables"
1960's–present: Discussions on the ways to formulate QM with a time operator

■ Hamiltonians depending on time

Let us have a closer look on quantum dynamics generated by a Hamiltonian which itself changes in time: $\boxed{\hat{H} = \hat{H}(t)}$. This means that, for the system under study, the time-translation invariance is violated, as is actually the case if a variable external field is applied. However, as explained in the following paragraph, time-dependent Hamiltonians naturally appear also in time-translation invariant situations—in the so-called Dirac picture of quantum dynamics.

▶ Nonstationary Schrödinger equation for time-dependent Hamiltonians

The form of the evolution operator remains valid in the local sense (for infinitesimal time intervals δt): $\hat{U}(t_0+\delta t, t_0) = e^{-i\frac{\hat{H}(t)\delta t}{\hbar}}$

$\Rightarrow$ The nonstationary Schr. eq. remains the same: $\boxed{i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle}$

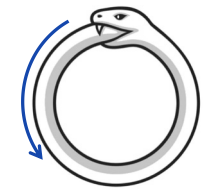
We distinguish 2 cases:
$$\begin{cases} \boxed{\text{(a)} \quad [\hat{H}(t), \hat{H}(t')] = 0 \quad \forall\, t, t'} & \text{...easy but rare} \\ \boxed{\text{(b)} \quad [\hat{H}(t), \hat{H}(t')] \neq 0 \quad t \neq t'} & \text{...normal \& difficult} \end{cases}$$

Schrödinger equation can be presented as an equation for the **general evolution operator** $\hat{U}(t, t_0)$:
$$i\hbar\frac{\partial}{\partial t}\overbrace{\hat{U}(t, t_0)|\psi(t_0)\rangle}^{|\psi(t)\rangle} = \hat{H}(t)\overbrace{\hat{U}(t, t_0)|\psi(t_0)\rangle}^{|\psi(t)\rangle} \quad \text{valid } \forall\ |\psi(t_0)\rangle$$

$\Rightarrow$ operator equation $\boxed{i\hbar\frac{\partial}{\partial t}\hat{U}(t, t_0) = \hat{H}(t)\,\hat{U}(t, t_0)}$ with $\boxed{\hat{U}(t_0, t_0) = \hat{I}}$

▶ Dyson series for general evolution operator

The formal solution of the above operator equation reads as follows:
$$\hat{U}(t, t_0) = \hat{I} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{H}(t_1)\underbrace{\hat{U}(t_1, t_0)}_{\hat{I} - \frac{i}{\hbar}\int_{t_0}^{t_1}\hat{H}(t_2)\underbrace{\hat{U}(t_2,t_0)}_{\cdots}\,dt_2}\,dt_1$$



By repeatedly inserting this equation into itself we obtain the solution in the form of an infinite Dyson series:

$$\hat{U}(t, t_0) = \hat{I} + \left(-\tfrac{i}{\hbar}\right)^1 \int_{t_0}^{t} \hat{H}(t_1)\,dt_1 + \left(-\tfrac{i}{\hbar}\right)^2 \int_{t_0}^{t}\int_{t_0}^{t_1} \hat{H}(t_1)\hat{H}(t_2)\,dt_2 dt_1 + \ldots$$
$$+ \left(-\tfrac{i}{\hbar}\right)^n \int_{t_0}^{t}\int_{t_0}^{t_1}\ldots\int_{t_0}^{t_{n-1}} \hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)\;dt_n \ldots dt_2 dt_1 + \ldots$$

In general, the Dyson series can be summed up to a compact form only in case (a) of the Hamiltonian time dependence. In case (b), which is much more generic, the evolution operator can only be expressed in the infinite-series form.

► **Case (a) commuting Hamiltonians**: $[\hat{H}(t), \hat{H}(t')] = 0$

$$\int_{t_0}^{t}\int_{t_0}^{t_1} \hat{H}(t_1)\hat{H}(t_2)\,dt_2dt_1 = \tfrac{1}{2}\int_{t_0}^{t}\int_{t_0}^{t} \hat{H}(t_1)\hat{H}(t_2)\,dt_2dt_1 = \tfrac{1}{2}\left[\int_{t_0}^{t} \hat{H}(t_1)\,dt_1\right]^2$$

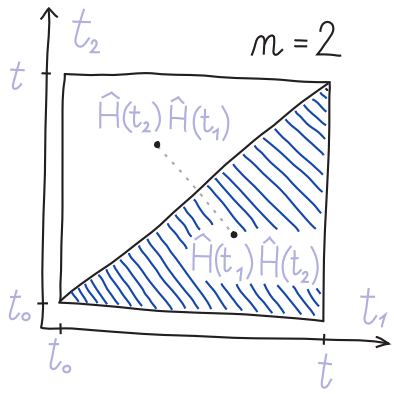
$$\int_{t_0}^{t}\int_{t_0}^{t_1}\cdots\int_{t_0}^{t_{n-1}} \hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)\;dt_n\ldots dt_2dt_1 = \tfrac{1}{n!}\left[\int_{t_0}^{t} \hat{H}(t_1)\,dt_1\right]^n$$

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t_1)\,dt_1}$$

... compact expression of the evolution operator

► **Case (b) non-commuting Hamiltonians**: $[\hat{H}(t), \hat{H}(t')] \neq 0$

Note that $\int_{t_0}^{t}\int_{t_0}^{t_1}\cdots\int_{t_0}^{t_{n-1}} \hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)\;dt_n\ldots dt_2dt_1 =$



$$\tfrac{1}{n!}\int_{t_0}^{t}\int_{t_0}^{t}\cdots\int_{t_0}^{t} \underbrace{\mathfrak{T}\left[\hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)\right]}_{\hat{H}(t_{i_1})\hat{H}(t_{i_2})\ldots\hat{H}(t_{i_n})} dt_n\ldots dt_2dt_1$$

time ordering
$(t_1, t_2 \ldots t_n) \mapsto (t_{i_1} \geq t_{i_2} \geq \cdots \geq t_{i_n})$

In each term of Dyson series do the following:
(1) change the subintegral operator function to the t-ordered product: $[\ldots] \mapsto \mathfrak{T}[\ldots]$
(2) extend integ. domain ⇒ all upper limits $= t$
(3) reduce the integral by factor $\frac{1}{n!}$

$$\hat{U}(t,t_0) = \mathfrak{T}e^{-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t_1)\,dt_1}$$

... symbolic compact expression in the form of the time ordered exponential−just an abbreviation of the full Dyson series

The Dyson series for a general time-dependent Hamiltonian is not a perturbation series, i.e., it is not guaranteed that the size of individual contributions decreases with increasing order. So it might be generally difficult to make it useful. However, below we will see that convergence properties of the Dyson series get much better in the so-called interaction picture of the time evolution.

■ Alternative descriptions of time evolution

So far we have followed an approach to quantum dynamics in which the vectors corresponding to physical states vary in time while the operators associated with fundamental observables (such as coordinates and momenta) stay constant. The varying Hamiltonians considered in the last paragraph were exceptions that

we related to externally varied fields. However, this most common description of the time evolution is not the only one. All equivalent descriptions can be sorted into 3 groups, according to whether the evolution is attributed to state vectors, operators of observables, or to both.

► **3 equivalent ways** to express action of any unitary transformation $\hat{U}$

	varying vectors		varying operators		varying both
(1)	$\|\psi\rangle \mapsto \hat{U}\|\psi\rangle$	**(2)**	$\|\psi\rangle \mapsto \|\psi\rangle$	**(3)**	$\|\psi\rangle \mapsto \hat{U}_1\|\psi\rangle$
	$\hat{A} \mapsto \hat{A}$		$\hat{A} \mapsto \hat{U}^{-1}\hat{A}\hat{U}$		$\hat{A} \mapsto \hat{U}_0^{-1}\hat{A}\hat{U}_0$

for any factorization $\hat{U} = \hat{U}_0\hat{U}_1$

In all cases, matrix elements $\langle\psi'|\hat{A}|\psi\rangle$ are the same ⇒ equivalent descriptions

These possibilities constitute 3 equivalent types of description of quantum dynamics with unitary evolution operator $\boxed{\hat{U}(t) = e^{-i\frac{\hat{H}t}{\hbar}}}$ which is invariant under the time translations.

► **(1) Schrödinger picture**

It assumes varying state vectors and constant operators:

$$\boxed{\begin{array}{l}|\psi(t)\rangle_{\mathrm{S}} = \hat{U}(t)|\psi(0)\rangle_{\mathrm{S}} \\ \hat{A}_{\mathrm{S}} \equiv \text{const.}\end{array}} \quad \Rightarrow \begin{cases} \text{usual time evolution of state vectors} \\ \qquad\qquad \boxed{i\hbar\frac{d}{dt}|\psi(t)\rangle_{\mathrm{S}} = \hat{H}_{\mathrm{S}}|\psi(t)\rangle_{\mathrm{S}}} \\ \text{time independent operators} \end{cases}$$

In nonrelativistic QM, this is the most common description of dynamics.

► **(2) Heisenberg picture**

It works with constant state vectors and varying operators. Assuming that vectors and operators in the Heisenberg picture coincide with those of the Schrödinger picture at time $t = 0$, we obtain:

$$\boxed{\begin{array}{l}|\psi(t)\rangle_{\mathrm{H}} = |\psi\rangle_{\mathrm{H}} \equiv \text{const.} \\ \hat{A}_{\mathrm{H}}(t) = \hat{U}^{\dagger}(t)\,\hat{A}_{\mathrm{S}}\,\hat{U}(t)\end{array}} \quad \Rightarrow \begin{cases} \text{time independent state vectors} \\ \qquad\qquad |\psi\rangle_{\mathrm{H}} = \hat{U}^{\dagger}(t)|\psi(t)\rangle_{\mathrm{S}} \\ \text{time dependent operators} \end{cases}$$

⇒ Hamiltonian $\hat{H}_{\mathrm{H}} = \hat{H}_{\mathrm{S}} \equiv \hat{H}$

⇒ General observable evolution equation: $\boxed{i\hbar\frac{d}{dt}\hat{A}_{\mathrm{H}}(t) = [\hat{A}_{\mathrm{H}}(t), \hat{H}]}$

► **(3) Dirac (interaction) picture**

It is intermediate between the Schrödinger and Heisenberg pictures.

The Hamiltonian is split to the "free" and "interaction" parts: $\boxed{\hat{H} = \hat{H}_0 + \hat{H}'}$

While the evolution operator with the "free" Hamiltonian $\hat{H}_0$ evolves the operators, the state vectors are evolved by the remaining part of the full evolution operator. Mind that in a generic situation we have to assume that $[\hat{H}_0, \hat{H}'] \neq 0$, so the factorization of the full evolution operator is not the trivial one:

$$\hat{U}(t) = \overbrace{\hat{U}_0(t)}^{=e^{-i\frac{\hat{H}_0 t}{\hbar}}}\ \overbrace{\hat{U}_1(t)}^{\neq e^{-i\frac{\hat{H}' t}{\hbar}}}$$

Operators evolve by $\hat{U}_0(t) = e^{-i\frac{\hat{H}_0 t}{\hbar}}$ $\Rightarrow$ $\boxed{\hat{A}_{\rm D}(t) = \hat{U}_0^\dagger(t)\,\hat{A}_{\rm S}\,\hat{U}_0(t)}$

$\Rightarrow$ $\hat{H}_{0\rm D} = \hat{H}_{0\rm S} \equiv \hat{H}_0$

$\Rightarrow$ operators satisfy differential equation $\boxed{\boxed{i\hbar\frac{d}{dt}\hat{A}_{\rm D}(t) = [\hat{A}_{\rm D}(t), \hat{H}_0]}}$

Vectors evolve by $\hat{U}_1(t) = \hat{U}_0^\dagger(t)\hat{U}(t)$ $\Rightarrow$ $\boxed{|\psi(t)\rangle_{\rm D} = \hat{U}_0^\dagger(t)|\psi(t)\rangle_{\rm S}}$

$$i\hbar\tfrac{d}{dt}|\psi(t)\rangle_{\rm D} = -\hat{H}_0|\psi(t)\rangle_{\rm D} + \hat{U}_0^\dagger(t)\underbrace{\big(i\hbar\tfrac{d}{dt}|\psi(t)\rangle_{\rm S}\big)}_{(\hat{H}_0+\hat{H}')\hat{U}_0(t)|\psi(t)\rangle_{\rm D}} = \underbrace{\hat{U}_0^\dagger(t)\hat{H}'\hat{U}_0(t)}_{\hat{H}'_{\rm D}(t)}|\psi(t)\rangle_{\rm D}$$

$$\boxed{\boxed{i\hbar\tfrac{d}{dt}|\psi(t)\rangle_{\rm D} = \hat{H}'_{\rm D}(t)|\psi(t)\rangle_{\rm D}}}$$

Schwinger-Tomonaga equation
just the Schrödinger eq. with $\hat{H} \mapsto \hat{H}'_{\rm D}(t)$

The evolution according to the Schwinger-Tomonaga equation can be represented by **state evolution operator** $\hat{U}(t, t_0)_{\rm D}$, which is expressed via the **Dyson series** with $\hat{H}(t) \equiv \hat{H}'_{\rm D}(t)$. In this case, due to the assumed "smallness" of $\hat{H}'_{\rm D}$ with respect to $\hat{H}_0$, the series can be used in a **perturbative way**, i.e., neglecting higher-order terms (see Sec. 11). The Dirac interaction picture is a common framework in the relativistic quantum field theory.

◂ Historical remark
1925-6: W. Heisenberg & E. Schrödinger use the two descriptions of QM dynamics
1930: Paul Dirac connects these descriptions in a unified picture
1934: Julian Schwinger (S.-I. Tomonaga in 1940's) introduce the interaction picture
1949: Freeman Dyson uses the expansion of the evolution operator in QED

■ Green operator

We now briefly outline an approach to evolution which becomes very useful later, in the context of relativistic quantum theory. Based on the old idea of Green's function, known from the general theory of differential equations, this approach leads to a rather new, revealing view of quantum dynamics.

▸ General Green's function

Assume a general differential equation $\boxed{\hat{D}_x f(x) = R(x)}$ for an unknown function $f(x)$, where $\hat{D}_x$ is a differential operator in variable x and $R(x)$ is a fixed function. The Green's function $G_0(x)$ associated with this equation satisfies

$\boxed{\hat{D}_x G_0(x) = \delta(x)}$ $\Rightarrow$ general solution $\boxed{f(x) = f_0(x) + \int dx' G_0(x-x')R(x') \quad \text{with } \hat{D}_x f_0(x)=0}$

▸ Quantum Green operator

We define the **retarded Green operator** $\hat{G}_0^+(t, t_0)$ for nonstationary Schrödinger equation with Hamiltonian $\hat{H}_0(t)$ as the evolution operator $\hat{U}_0(t, t_0)$ restricted to $t \geq t_0$. It satisfies the following Green-like operator equation:

$$\boxed{\hat{G}_0^+(t,t_0) = \underbrace{\Theta(t-t_0)}_{=\begin{cases}1 \text{ for } t\geq t_0\\ 0 \text{ for } t<t_0\end{cases}} \hat{U}_0(t,t_0)} \qquad \boxed{\left[i\hbar\tfrac{\partial}{\partial t} - \hat{H}_0(t)\right]\hat{G}_0^+(t,t_0) = i\hbar\delta(t-t_0)}$$

Proof:
$$i\hbar\tfrac{\partial}{\partial t}\overbrace{\Theta(t-t_0)\hat{U}_0(t,t_0)}^{\hat{G}_0^+(t,t_0)} = i\hbar\overbrace{\delta(t-t_0)\hat{U}_0(t,t_0)}^{i\hbar\delta(t-t_0)\hat{U}_0(t_0,t_0)=i\hbar\delta(t-t_0)\hat{I}} + \overbrace{\Theta(t-t_0)\hat{H}_0(t)\hat{U}_0(t,t_0)}^{\hat{H}_0(t)\hat{G}_0^+(t,t_0)}$$

Note: The meaning of word "retarded" should be understood here in the sense that $\hat{G}_0^+(t,t_0)$ evolves the system from a past time t_0 to a future time t. Similarly, **advanced Green operator** (evolving from future t_0 to past t) is defined by $\boxed{\hat{G}_0^-(t,t_0) = -\Theta(t_0-t)\hat{U}_0(t,t_0)}$ and satisfies the same Green-like equation. Below we continue our discussion with the retarded operator only.

▶ Transition from free to full Green operator

We assume that the above Green operators with $\hat{H}_0(t)$ describes free evolution and the full Hamiltonian contains also an interaction $\hat{H}'(t)$. The retarded Green operator of the full Hamiltonian $\boxed{\hat{H}(t) = \hat{H}_0(t) + \hat{H}'(t)}$ is defined by

$$\boxed{\hat{G}^+(t,t_0) = \Theta(t-t_0)\hat{U}(t,t_0)} \qquad \boxed{\left[i\hbar\tfrac{\partial}{\partial t} - \hat{H}(t)\right]\hat{G}^+(t,t_0) = i\hbar\delta(t-t_0)}$$

and satisfies the following integral equation:

$$\boxed{\hat{G}^+(t,t_0) = \hat{G}_0^+(t,t_0) - \tfrac{i}{\hbar}\int_{-\infty}^{+\infty}\hat{G}_0^+(t,t_1)\hat{H}'(t_1)\hat{G}^+(t_1,t_0)\,dt_1}$$

... this is an analog of the above general form of solution of $\hat{D}_x f(x)=R(x)$

Proof: application of $\left[i\hbar\frac{\partial}{\partial t}-\hat{H}_0\right]$ to the first term and inside the integral yields the defining eq. of $\hat{G}^+$:
$$\left[i\hbar\tfrac{\partial}{\partial t} - \hat{H}_0(t)\right]\hat{G}^+(t,t_0) = i\hbar\delta(t-t_0) + \overbrace{\int_{-\infty}^{+\infty}\delta(t-t_1)\hat{H}'(t_1)\hat{G}^+(t_1,t_0)\,dt_1}^{\hat{H}'(t)\hat{G}^+(t,t_0)}$$

▶ Iterative solution of the full Green operator

The above integral expression of the full Green operator $\hat{G}^+(t,t_0)$ through the free Green operator $\hat{G}_0^+(t,t_0)$ enables us to reuse the above-introduced "insert-to-itself" (*time-reversed uroboros*) technique. We obtain an infinite series:

$$\hat{G}^+(t,t_0) = \hat{G}_0^+(t,t_0) - \tfrac{i}{\hbar}\int_{-\infty}^{+\infty}\hat{G}_0^+(t,t_1)\hat{H}'(t_1)\hat{G}_0^+(t_1,t_0)\,dt_1 \;+\; \cdots$$
$$+\left(-\tfrac{i}{\hbar}\right)^n\underbrace{\int_{-\infty}^{+\infty}\!\!\cdots\!\int_{-\infty}^{+\infty}}_{n\times}\hat{G}_0^+(t,t_n)\hat{H}'(t_n)\hat{G}_0^+(t_n,t_{n-1})\,....\,\hat{G}_0^+(t_2,t_1)\hat{H}'(t_1)\hat{G}_0^+(t_1,t_0)\,dt_n\,...\,dt_1$$
$$+\;\cdots\cdots$$

This series is analogous to the Dyson series, except (a) the zeroth term $\hat{G}_0^+ \neq \hat{I}$, (b) all integrals have the same limits, and (c) the alternating operators $\hat{G}_0^+$ and $\hat{H}'$ inside integrals. If $\hat{H}'$ is small compared to $\hat{H}_0$, the series can again be used in the **perturbative way**, i.e., neglecting the terms of higher order. The meaning of this expansion will become clear in the following.

▶ Propagator

Forward evolution of a single-particle state can be written as:

$$\langle\vec{x}|\psi(t)\rangle = \langle\vec{x}|\hat{G}^+(t,t_0)|\psi(t_0)\rangle = \int\langle\vec{x}|\hat{G}^+(t,t_0)|\vec{x}_0\rangle\langle\vec{x}_0|\psi(t_0)\rangle\, d\vec{x}_0$$

$$\Rightarrow \boxed{\psi(\vec{x},t) = \int \underbrace{G^+(\vec{x}t|\vec{x}_0t_0)}_{\langle\vec{x}|\hat{G}^+(t,t_0)|\vec{x}_0\rangle}\psi(\vec{x}_0,t_0)\, d\vec{x}_0}$$

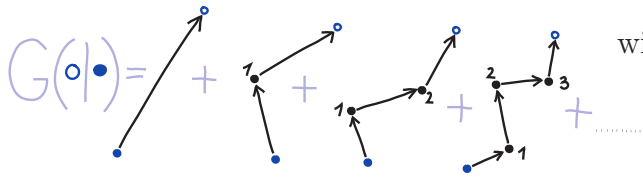
with $G^+(\vec{x}t|\vec{x}_0t_0)$ (coordinate representation of the single-particle Green operator) being called "propagator"

The propagator $G^+(\vec{x}t|\vec{x}_0t_0)$ can be interpreted as the wavefunction $\psi(\vec{x},t)$ evolved from ideally localized initial state $\psi(\vec{x},t_0) = \delta(\vec{x}-\vec{x}_0) \equiv |\vec{x}_0\rangle$. It satisfies the equation: $\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2M}\Delta - V(\vec{x},t)\right] G^+(\vec{x}t|\vec{x}_0t_0) = i\hbar\delta(t-t_0)\delta(\vec{x}-\vec{x}_0)$

Let $\boxed{V(\vec{x},t) = V_0(\vec{x},t) + V'(\vec{x},t)}$ and let $G_0^+(\vec{x}t|\vec{x}_0t_0)$ be the solution for $V_0(\vec{x},t)$. The iterative solution for the full potential $V(\vec{x},t)$ reads as:

$$\begin{aligned} G^+(\vec{x}t|\vec{x}_0t_0) \;&= G_0^+(\vec{x}t|\vec{x}_0t_0) + \cdots + \left(-\tfrac{i}{\hbar}\right)^n \underbrace{\int\!\!\ldots\!\!\int}_{2n\times} G_0^+(\vec{x}t|\vec{x}_nt_n)V'(\vec{x}_n,t_n)\ldots \\ &\ldots G_0^+(\vec{x}_2t_2|\vec{x}_1t_1)V'(\vec{x}_1,t_1)G_0^+(\vec{x}_1t_1|\vec{x}_0t_0)\; d\vec{x}_n dt_n \ldots d\vec{x}_1 dt_1 + \cdots \end{aligned}$$

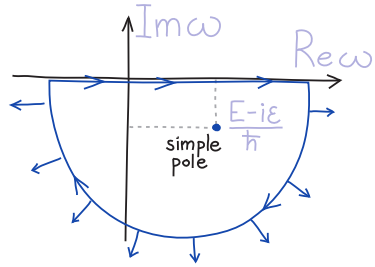
This series has a visual interpretation:



with each intermediate interaction bringing the factor $\frac{1}{i\hbar}V'(\vec{x}_k,t_k)$ and the integration over all space-time points $(\vec{x}_k,t_k)$

▶ Green operator for time-independent Hamiltonian $\hat{H}(t) \equiv \hat{H}$

Expansion in stationary states: $\hat{G}^+(t,t_0) = \Theta(t-t_0)\sum_{i,k} e^{-i\frac{E_i(t-t_0)}{\hbar}}|E_ik\rangle\langle E_ik| =$



$$= \lim_{\varepsilon\to 0_+}\sum_{i,k}\left(\tfrac{i\hbar}{2\pi}\int_{-\infty}^{\infty}\tfrac{e^{-i\omega(t-t_0)}}{\hbar\omega-E_i+i\varepsilon}d\omega\right)|E_ik\rangle\langle E_ik|$$

using the result from complex analysis (see the sketch of integration path used in its derivation):

$$\tfrac{i\hbar}{2\pi}\int_{-\infty}^{\infty}\tfrac{e^{-i\omega t}}{\hbar\omega-E+i\varepsilon}d\omega = \Theta(t)e^{-i\frac{(E-i\varepsilon)t}{\hbar}} \text{ for } \varepsilon>0$$

$$\Rightarrow\ \hat{G}^+(t,t_0)=\boxed{\hat{G}^+(\overbrace{t-t_0}^{\tau})=\lim_{\varepsilon\to 0_+}\frac{i}{2\pi}\int_{-\infty}^{\infty}\overbrace{\frac{1}{E-\hat{H}+i\varepsilon}}^{\hat{G}^+(E)}e^{-\frac{i}{\hbar}E\tau}dE}$$

Similarly:
$\hat{G}^-(\tau)=\lim_{\varepsilon\to 0_+}$
$\frac{i}{2\pi}\int_{-\infty}^{\infty}\underbrace{\frac{1}{E-\hat{H}-i\varepsilon}}_{\hat{G}^-(E)}e^{-\frac{i}{\hbar}E\tau}\,dE$

Operators $\hat{G}^{\pm}(\tau)$ & $\hat{G}^{\pm}(E)$, mutually related by Fourier transformations, represent **time & energy images** of the retarded and advanced Green operators.

◄ Historical remark
1828: George Green applies math. analysis in electromagnetism ⇒ Green function
1949: Richard Feynman applies Green funcs. in QM+QED (later "propagator")

5b. EXAMPLES OF UNITARY EVOLUTION

Having digested all the general approaches to the description of quantum evolution, we need to see some concrete applications. A few examples discussed below represent just a personal selection—a multitude of other cases could serve the purpose as well.

■ Two-level (& few-level) systems

Two-level systems yield periodic evolution. A lot of examples of such behavior exists in nature: from oscillation phenomena in particle physics to excitation-deexcitation cycles in quantum optics. Note that any system with Hilbert space of a finite dimension $n \geq 2$ exhibits in general a *quasiperiodic* evolution: it can be expressed via a finite number of periodic motions, like the function $f(t) = g(e^{i\omega_1 t}, e^{i\omega_2 t}, \dots)$ where $\omega_1, \omega_2, \dots$ represent partial frequencies.

► General two-level Hamiltonian

The most general Hamiltonian $\hat{H}$ in $d = 2$ is determined (including the overall scale) by 4 real parameters, which can be associated with coefficients $\hbar(\omega_0, \vec{\omega})$ at the unit and Pauli matrices that comprise $\hat{H}$.

$$\boxed{\hat{H}=\begin{pmatrix}\hbar\omega_0+\hbar\omega_3 & \hbar\omega_1-i\hbar\omega_2\\ \hbar\omega_1+i\hbar\omega_2 & \hbar\omega_0-\hbar\omega_3\end{pmatrix}=\hbar\big[\omega_0\hat{I}+\underbrace{\omega_1\hat{\sigma}_1+\omega_2\hat{\sigma}_2+\omega_3\hat{\sigma}_3}_{\vec{\omega}\cdot\hat{\vec{\sigma}}}\big]}$$

$\sqrt{\omega_1^2+\omega_2^2+\omega_3^2}\equiv\omega$

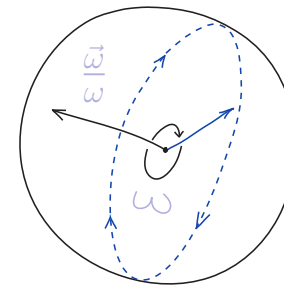
► Two-level evolution operator

is calculated as the spinor transformation (see Sec. 4b):

$$e^{-i\frac{\hat{H}t}{\hbar}}=e^{-i(\omega_0 t)\hat{I}}\,\underbrace{e^{-i(\vec{\omega}\cdot\hat{\vec{\sigma}})t}}$$

$$\boxed{\hat{U}(t)=e^{-i\omega_0 t}\left[(\cos\omega t)\,\hat{I}-i(\sin\omega t)\,\left(\frac{\vec{\omega}}{\omega}\cdot\hat{\vec{\sigma}}\right)\right]}$$

$$=e^{-i\omega_0 t}\begin{pmatrix}\cos\omega t-i\frac{\omega_3}{\omega}\sin\omega t & -\frac{\omega_2+i\omega_1}{\omega}\sin\omega t\\ \frac{\omega_2-i\omega_1}{\omega}\sin\omega t & \cos\omega t+i\frac{\omega_3}{\omega}\sin\omega t\end{pmatrix}$$

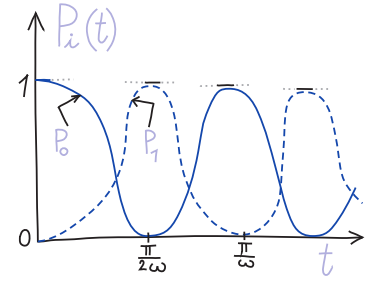


This yields quasiperiodic evolution with partial frequencies ω_0 and ω, but the global phase $\omega_0 t$ is not relevant. For a spin-$\frac{1}{2}$ particle, the motion represents a steady rotation around the spatial direction $\vec{n} = \vec{\omega}/\omega$ with frequency ω.

▶ **Special case**: $\hat{H} = \begin{pmatrix} \hbar\omega_0 & \hbar\omega \\ \hbar\omega & \hbar\omega_0 \end{pmatrix} \quad \Rightarrow \quad \hat{U}(t) = e^{-i\omega_0 t} \begin{pmatrix} \cos\omega t & -i\sin\omega t \\ -i\sin\omega t & \cos\omega t \end{pmatrix}$

$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow{t} |\psi(t)\rangle = e^{-i\omega_0 t} \begin{pmatrix} \cos\omega t \\ -i\sin\omega t \end{pmatrix}$

$$\Rightarrow \begin{cases} \mathfrak{p}_0(t) = |\langle\psi(0)|\psi(t)\rangle|^2 = \cos^2\omega t \\ \mathfrak{p}_1(t) = |\langle\psi(0)_\perp|\psi(t)\rangle|^2 = \sin^2\omega t \end{cases} \quad \begin{matrix} \textbf{oscillations} \\ \text{period } T = \frac{\pi}{\omega} \end{matrix}$$



▶ **Generalization to $d > 0$**

A general d-dimensional Hamiltonian $\hat{H}$ is determined (including the overall scale) by d^2 real parameters. The quasiperiodic evolution generated by this Hamiltonian has d independent frequencies $\omega_i = \frac{1}{\hbar}E_i$, where E_i with $i = 1, ..., d$ are eigevalues of $\hat{H}$. One of these frequencies (any of them) can be chosen to determine just the global phase.

◀ **Historical remark**

1954: M. Gell-Mann and A. Pais describe oscillations of neutral particles
1960's-present: Particle-antiparticle ($d = 2$) and neutrino ($d = 3$) oscillations studied in numerous experiments

■ Free particle

Although a scalar particle moving in empty space (no fields) represents the most trivial example of evolution, expressed in terms of an ordinary wavefunction, the related calculations are a bit unpleasant. Nevertheless, they yield two benefits of general importance: the discovery of the wavepacket spreading phenomenon and quantification of the limits of validity of nonrelativistic QM.

▶ **Free-particle propagator**

Hamiltonian: $\hat{H} = \frac{1}{2M}\hat{\vec{p}}^2 \quad \Rightarrow \quad$ Green operator: $\hat{G}^+(t, t_0) = \Theta(t-t_0)\, e^{-i\frac{t-t_0}{2M\hbar}\hat{\vec{p}}^2}$

Propagator: $G^+(\vec{x}t|\vec{x}_0 t_0) \equiv \langle\vec{x}|\hat{G}^+(t, t_0)|\vec{x}_0\rangle \quad \begin{matrix} \vec{x}-\vec{x}_0 \equiv \Delta\vec{x} \\ t-t_0 \equiv \Delta t \end{matrix}$

$$= \Theta(\Delta t) \iint \underbrace{\langle\vec{x}|\vec{p}\rangle}_{\frac{1}{\sqrt{2\pi\hbar}^3} e^{+i\vec{p}\cdot\vec{x}/\hbar}} \underbrace{\langle\vec{p}|e^{-i\frac{\Delta t}{2M\hbar}\hat{\vec{p}}^2}|\vec{p}_0\rangle}_{e^{-i\frac{\Delta t}{2M\hbar}\vec{p}^2}\delta(\vec{p}-\vec{p}_0)} \underbrace{\langle\vec{p}_0|\vec{x}_0\rangle}_{\frac{1}{\sqrt{2\pi\hbar}^3} e^{-i\vec{p}_0\cdot\vec{x}_0/\hbar}} d\vec{p}\, d\vec{p}_0 = \frac{\Theta(\Delta t)}{(2\pi\hbar)^3} \int e^{\frac{i}{\hbar}\left[\vec{p}\cdot\Delta\vec{x} - \frac{\vec{p}^2}{2M}\Delta t\right]} d\vec{p}$$

$$= \frac{\Theta(\Delta t)}{(2\pi\hbar)^3} \underbrace{\int e^{a(\vec{p}-\vec{q})^2 + b} d\vec{p}}_{\left(-\frac{\pi}{a}\right)^{3/2} e^b \text{ for } \mathrm{Re}\, a<0} \quad \text{with} \quad a = -i\frac{\Delta t}{2\hbar M} \quad b = i\frac{M(\Delta\vec{x})^2}{2\hbar\Delta t} \quad \vec{q} = \frac{M\Delta\vec{x}}{\Delta t}$$

To get $\mathrm{Re}\, a < 0$ assume: $\Delta t \longrightarrow \Delta t - i\varepsilon$ with $\varepsilon \to 0+$

$$\cdots = \lim_{\varepsilon\to 0+} \frac{\Theta(\Delta t)}{(2\pi\hbar)^3} \left(\frac{2\pi\hbar M}{\varepsilon + i\Delta t}\right)^{\frac{3}{2}} e^{i\frac{M(\Delta\vec{x})^2}{2\hbar\Delta t}} = \boxed{\Theta(\Delta t) \left(\frac{M}{2i\pi\hbar\Delta t}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\frac{M}{2}\left(\frac{\Delta\vec{x}}{\Delta t}\right)^2 \Delta t} = G^+(\Delta\vec{x}, \Delta t)}$$

$|G^+(\Delta\vec{x},\Delta t)|^2 = \left(\frac{M}{2\pi\hbar\Delta t}\right)^3$ for $\Delta t > 0$ $\quad\Rightarrow$ immediate spread of the particle in the whole space ($\Leftarrow$ nonrelativistic theory)

▶ Evolution of Gaussian wavepackets

If the particle localization is imperfect, the spreading rate of its wavefunction should become finite.

$$\psi(\vec{x},t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \underbrace{\tilde{\psi}(\vec{p})}_{\frac{e^{-(\vec{p}-\vec{p}_0)^2/4\sigma_p^2}}{(2\pi\sigma_p^2)^{3/4}}} e^{\frac{i}{\hbar}\left[\vec{p}\cdot\vec{x}-\frac{\vec{p}^2}{2M}t\right]} d\vec{p} = \frac{1}{(8\pi^3\hbar^2\sigma_p^2)^{3/4}} \int \underbrace{e^{\left(-\frac{1}{4\sigma_p^2}-\frac{it}{2\hbar M}\right)\vec{p}^2+\left(\frac{\vec{p}_0}{2\sigma_p^2}+\frac{i\vec{x}}{\hbar}\right)\cdot\vec{p}-\frac{\vec{p}_0^2}{4\sigma_p^2}}}_{e^{a(\vec{p}-\vec{q})^2+b}\quad \mathrm{Re}\,a<0} =$$

$$= \frac{1}{(8\pi^3\hbar^2\sigma_p^2)^{3/4}} \left(-\frac{\pi}{a}\right)^{\frac{3}{2}} e^b \qquad a=-\frac{1}{4\sigma_p^2}\left(1+i\frac{2\sigma_p^2 t}{\hbar M}\right) \quad \vec{q}=-\frac{1}{2a}\left(\frac{\vec{p}_0}{2\sigma_p^2}+i\frac{\vec{x}}{\hbar}\right) \quad b=-a\vec{q}^2-\frac{\vec{p}_0^2}{4\sigma_p^2}$$

Probability density: $|\psi(\vec{x},t)|^2 = \left(\frac{1}{8\pi\hbar^2\sigma_p^2|a|^2}\right)^{\frac{3}{2}} e^{2\mathrm{Re}\,b}$

Define $\sigma_x^2(t) \equiv 4\hbar^2\sigma_p^2|a|^2 = \frac{\hbar^2}{4\sigma_p^2}\left[1+\frac{4\sigma_p^4}{\hbar^2M^2}t^2\right]$ and evaluate the exponent:

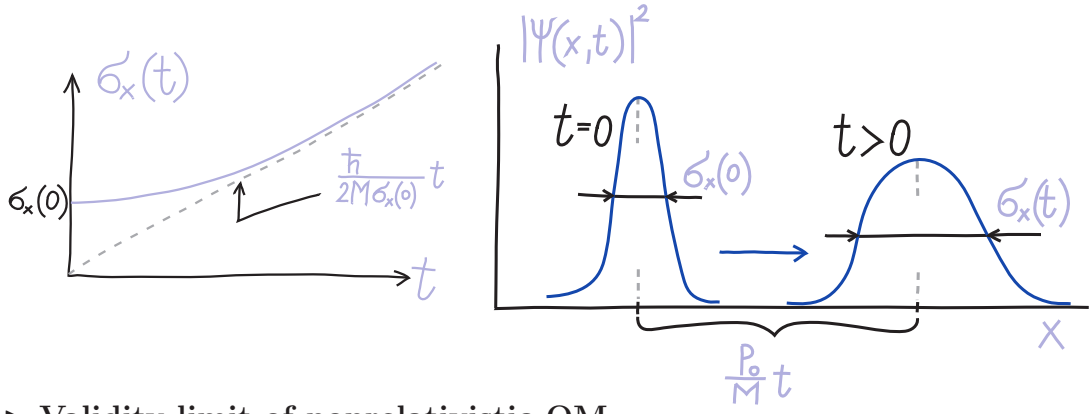
$$2\mathrm{Re}\,b = -\frac{1}{2\sigma_x(t)^2}\left[16\hbar^2\sigma_p^2|a|^2\mathrm{Re}(a\vec{q}^2)+4\hbar^2|a|^2\vec{p}_0^{\,2}\right] = -\frac{\left(\vec{x}-\frac{\vec{p}_0}{M}t\right)^2}{2\sigma_x(t)^2}$$

$$|\psi(\vec{x},t)|^2 = \frac{1}{[2\pi\sigma_x(t)^2]^{3/2}} e^{-\frac{[\vec{x}-\vec{x}_0(t)]^2}{2\sigma_x(t)^2}}$$

$$\vec{x}_0(t) = \frac{\vec{p}_0}{M}\,t \qquad \textbf{translation}$$

$$\sigma_x(t) = \sigma_x(0)\sqrt{1+\left[\frac{\hbar}{2M\sigma_x(0)^2}\right]^2 t^2} \qquad \textbf{spreading}$$

For short times, the wavepacket moves like a classical particle with average momentum $\vec{p}_0$, but for longer times the wavepackets spreads out in space. The smaller is the spread $\sigma_x(0)$ at $t=0$, the faster it grows at $t \gg 0$.



▶ Validity limit of nonrelativistic QM

Spreading speed of the wavepacket: $s \equiv \frac{1}{2}\frac{d}{dt}\sigma_x(t) = \frac{\frac{\sigma_x(0)}{2}\left[\frac{\hbar}{2M\sigma_x(0)^2}\right]^2 t}{\sqrt{1+\left[\frac{\hbar}{2M\sigma_x(0)^2}\right]^2 t^2}} \xrightarrow{\text{large } t} \frac{\hbar}{4M\sigma_x(0)}$

Nonrelativistic QM becomes *invalid* for $s \gtrsim c$. This will be so for the initial particle localization $\boxed{\sigma_x(0) \lesssim \frac{\hbar}{4Mc} = \frac{1}{4}\lambda\!\!\!^{-}_{\mathrm{C}}}$ where $\lambda\!\!\!^{-}_{\mathrm{C}}$ (for electron $\doteq 386\,\mathrm{fm}$) is

the reduced **Compton wavelength** of the given particle (see Sec. 2b). So the nonrelativistic Schrödiger equation of a free particle is applicable *iff* $\sigma_x(0) \gg \lambda\!\!\!^{-}_{\rm C}$

► **Phase & group velocities**

(a) A monochromatic planar wave $\psi(\vec{x},t) = e^{i\overbrace{[\vec{k}\cdot\vec{x}-\omega(\vec{k})t]}^{\phi(\vec{k},\vec{x},t)}}$

Phase velocity $\vec{v}_{\rm ph}$ given by the condition of a constant phase:

$$\phi(\vec{k},\,\vec{x},\,t)=\text{const.} \quad\Rightarrow\quad \vec{k}\cdot\vec{x}=\text{const.}+\omega(\vec{k})t \quad\Rightarrow\quad \vec{v}_{\rm ph}=\tfrac{\omega(\vec{k})}{k^2}\vec{k}$$
$$\vec{k}=\tfrac{\vec{p}}{\hbar},\;\; \hbar\omega(\vec{k})=\tfrac{(\hbar\vec{k})^2}{2M} \quad\Rightarrow\quad \text{QM:}\quad \boxed{\vec{v}_{\rm ph}=\tfrac{\vec{p}}{2M}=\tfrac{1}{2}\vec{v}_{\rm clas}}$$

(b) A wave packet $\psi(\vec{x},t)=\int a(\vec{k})\,e^{i[\vec{k}\cdot\vec{x}-\omega(\vec{k})t]}\,d\vec{k}$ with the amplitude function $a(\vec{k})=(\frac{\hbar}{2\pi})^{\frac{3}{2}}\tilde{\psi}(\hbar\vec{k})$ having a sharp maximum at $\vec{k}=\vec{k}_0$

Group velocity $\vec{v}_{\rm gr}$ represents the motion of the maximum of $\psi(\vec{x},t)$:

$$\psi(\vec{x},t)\approx a(\vec{k}_0)\,e^{i\phi(\vec{k}_0,\vec{x},t)}\int e^{i\vec{q}\cdot\vec{\nabla}_{\vec{k}}\phi(\vec{k},\vec{x},t)|_{\vec{k}=\vec{k}_0}}\,d\vec{q}$$

$\Rightarrow$ the integral ≈ 0 except when the phase has a stationary point:

$$\vec{\nabla}_{\vec{k}}\,\phi(\vec{k},\vec{x},\,t)|_{\vec{k}=\vec{k}_0}=0 \quad\Rightarrow\quad \vec{x}=\vec{\nabla}_{\vec{k}}\,\omega(\vec{k})|_{\vec{k}=\vec{k}_0}\,t \quad\Rightarrow\quad \vec{v}_{\rm gr}=\vec{\nabla}_{\vec{k}}\,\omega(\vec{k})|_{\vec{k}=\vec{k}_0}$$
$$\Rightarrow\quad \text{QM:}\quad \boxed{\boxed{\vec{v}_{\rm gr}=\tfrac{\vec{p}_0}{M}=\vec{v}_{0\rm clas}}}$$

■ Coherent states in harmonic oscillator

The harmonic oscillator potential has the magic power to prevent Gaussian wavepackets from spreading. It provides the simplest specimen from the large family of coherent states. These states generalized to more complex situations represent an important tool to construct the classical limit of a quantum system (cf. Sec. 8). For the sake of simplicity we will stay now in 1D space.

► **Coherent states as eigenstates of the lowering operator**

We know that the 1D oscillator Hamiltonian $\hat{H}=\frac{1}{2M}\hat{p}^2+\frac{M\omega^2}{2}\hat{x}^2=\hbar\omega\big(\hat{b}^\dagger\hat{b}+\frac{1}{2}\big)$ is naturally expressed through ladder (lowering & raising) operators

$$\left\{\begin{array}{l}\hat{b}^\dagger=\sqrt{\frac{M\omega}{2\hbar}}\big(\hat{x}-i\frac{1}{M\omega}\hat{p}\big)\\ \hat{b}=\sqrt{\frac{M\omega}{2\hbar}}\big(\hat{x}+i\frac{1}{M\omega}\hat{p}\big)\end{array}\right\}\Leftrightarrow\left\{\begin{array}{l}\hat{x}=\sqrt{\frac{\hbar}{2M\omega}}\big(\hat{b}^\dagger+\hat{b}\big)\\ \hat{p}=i\sqrt{\frac{M\hbar\omega}{2}}\big(\hat{b}^\dagger-\hat{b}\big)\end{array}\right\}\Rightarrow\left\{\begin{array}{l}\hat{b}^\dagger|E_n\rangle=\sqrt{n+1}\,|E_{n+1}\rangle\\ \hat{b}|E_n\rangle\;\;=\sqrt{n}\,|E_{n-1}\rangle\end{array}\right\}$$

satisfying the commutation relation $[\hat{b},\hat{b}^\dagger]=\hat{I}$. Operators $\hat{b}^\dagger$ and $\hat{b}$ are thought to create and annihilate quanta of vibrations — effective particles called phonons.

The coherent state is an eigenstate of the lowering operator:

$\boxed{\boxed{\hat{b}|\psi_z\rangle=z|\psi_z\rangle}}$ with an eigenvalue $z\in\mathbb{C}$

► **Coherent states in the energy eigenbasis** $\quad\boxed{\boxed{|\psi_z\rangle=e^{-\frac{|z|^2}{2}}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,|E_n\rangle}}$

Proof: $\hat{b}|\psi_z\rangle=e^{-\frac{|z|^2}{2}}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\;\overbrace{\hat{b}|E_n\rangle}^{\sqrt{n}|E_{n-1}\rangle}=ze^{-\frac{|z|^2}{2}}\sum_{n=1}^{\infty}\frac{z^{n-1}}{\sqrt{(n-1)!}}|E_{n-1}\rangle=z|\psi_z\rangle$

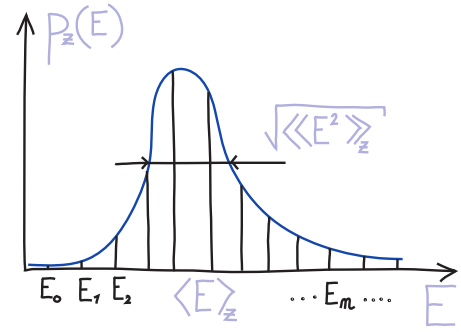
The coherent state $|\psi_z\rangle$ shows
Poisson energy distribution

$$\mathfrak{p}_z(E_n) = e^{-\lambda}\,\frac{\lambda^n}{n!}$$

with $\lambda \equiv |z|^2 = \langle n\rangle_z = \langle\langle n^2\rangle\rangle_z$.

The energy average & dispersion read as:

$$\boxed{\langle E\rangle_z = \hbar\omega\left(|z|^2+\tfrac{1}{2}\right) \quad \langle\langle E^2\rangle\rangle_z = (\hbar\omega)^2|z|^2}$$



Note: There exists **no** eigenstate of the raising operator $\hat b^\dagger$. Indeed, assume a general state $|\psi\rangle = \sum_{n=0}^\infty \alpha_n |E_n\rangle$, where coefficients α_n vanish $\forall\, n$ below a certain n_0 (possibly $n_0=0$). We have $\hat b^\dagger|\psi\rangle = \sum_{n=0}^\infty \sqrt{n+1}\alpha_n|E_{n+1}\rangle = \sum_{n=1}^\infty \alpha'_n|E_n\rangle$, where coefficients α'_n vanish $\forall\, n$ below n_0+1. So $\hat b^\dagger|\psi\rangle \not\propto |\psi\rangle$.

▸ Normalization & scalar products of coherent states

$$\underbrace{\langle\psi_z|\psi_{z'}\rangle}_{\substack{z=|z|e^{i\phi}\\ z'=|z'|e^{i\phi'}}} = e^{-\frac{|z|^2+|z'|^2}{2}} \sum_n\sum_{n'} \frac{(z^*)^n (z')^{n'}}{\sqrt{n!\,n'!}} \underbrace{\langle E_n|E_{n'}\rangle}_{\delta_{nn'}} = e^{-\frac{|z|^2+|z'|^2}{2}} \sum_n \frac{(z^*z')^n}{n!} =$$

$$\cdots = e^{-\frac{|z|^2+|z'|^2}{2}+|z||z'|[\cos(\phi'-\phi)+i\sin(\phi'-\phi)]} = \boxed{e^{-\frac{|z'-z|^2}{2}+i|z||z'|\sin(\phi'-\phi)} = \langle\psi_z|\psi_{z'}\rangle}$$

Coherent states $\{|\psi_z\rangle\}_{z\in\mathbb{C}}$ form an **overcomplete set** in $\mathcal{H}$: $\begin{cases}\langle\psi_z|\psi_z\rangle = 1\\ \langle\psi_z|\psi_{z'}\rangle \neq 0 \text{ for } z\neq z'\end{cases}$

▸ Coordinate & momentum averages

$$\langle\psi_z|\hat x|\psi_z\rangle = \sqrt{\tfrac{\hbar}{2M\omega}}\overbrace{\langle\psi_z|(\hat b^\dagger+\hat b)|\psi_z\rangle}^{z^*+z} =$$

$$\langle\psi_z|\hat p|\psi_z\rangle = i\sqrt{\tfrac{M\hbar\omega}{2}}\underbrace{\langle\psi_z|(\hat b^\dagger-\hat b)|\psi_z\rangle}_{z^*-z} =$$

$$\boxed{\begin{array}{l}\sqrt{\frac{2\hbar}{M\omega}}\,\mathrm{Re}\, z = \langle x\rangle_z\\ \sqrt{2M\hbar\omega}\,\mathrm{Im}\, z = \langle p\rangle_z\end{array}}$$

▸ Coordinate representation

$$\psi_z(x) = \langle x|\psi_z\rangle = e^{-\frac{|z|^2}{2}} \sum_{n=0}^\infty \frac{z^n}{\sqrt{n!}} \underbrace{\langle x|E_n\rangle}_{\left(\frac{M\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}} e^{-\frac{M\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{M\omega}{\hbar}}x\right)} = \left(\tfrac{M\omega}{\pi\hbar}\right)^{\frac14} e^{-\frac{|z|^2}{2}-\frac{M\omega}{2\hbar}x^2} \underbrace{\sum_{n=0}^\infty \frac{\left(\frac{z}{\sqrt2}\right)^n}{n!} H_n\left(\sqrt{\tfrac{M\omega}{\hbar}}x\right)}_{e^{\frac{M\omega}{\hbar}x^2-\left(\sqrt{\frac{M\omega}{\hbar}}x-\frac{z}{\sqrt2}\right)^2}}$$

Applying the generating function of Hermite polynomials

$$H_n(\xi) \equiv \tfrac{d^n}{d\eta^n} e^{\xi^2-(\xi-\eta)^2}\big|_{\eta=0} \quad\Rightarrow\quad e^{\xi^2-(\xi-\eta)^2} = \sum_n H_n(\xi)\tfrac{\eta^n}{n!}$$

we arrive to:

$$\cdots = \left(\tfrac{M\omega}{\pi\hbar}\right)^{\frac14} e^{-\frac{|z|^2}{2}+\frac{M\omega}{2\hbar}x^2} e^{-\left(\sqrt{\frac{M\omega}{\hbar}}x-\frac{z}{\sqrt2}\right)^2} = \left(\tfrac{M\omega}{\pi\hbar}\right)^{\frac14} e^{-\frac{M\omega}{2\hbar}x^2+2z\sqrt{\frac{M\omega}{2\hbar}}x-z\mathrm{Re}\, z}$$

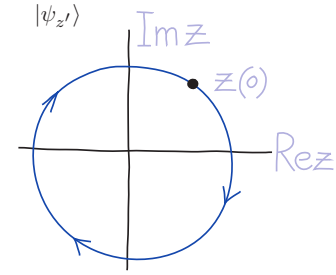
$$\boxed{|\psi_z(x)|^2 = \left(\tfrac{M\omega}{\pi\hbar}\right)^{\frac12} e^{-\frac{M\omega}{\hbar}\left(x-\langle x\rangle_z\right)^2}} \quad \textbf{Gaussian distribution} \text{ with } \sigma_x^2 = \tfrac{\hbar}{2M\omega}$$

So coherent states of the harmonic oscillator are Gaussian wavepackets with the z-dependent cooordinate & momentum averages and constant dispersions.

▶ Time evolution of coherent states

$$e^{-i\frac{\hat{H}t}{\hbar}}|\psi_z\rangle = e^{-\frac{|z|^2}{2}}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}e^{-i\left(n+\frac{1}{2}\right)\omega t}|E_n\rangle = e^{-i\frac{\omega t}{2}}\underbrace{e^{-\frac{|z|^2}{2}}\sum_{n=0}^{\infty}\frac{\overbrace{(ze^{-i\omega t})^n}^{(z')^n}}{\sqrt{n!}}|E_n\rangle}_{|\psi_{z'}\rangle}$$

$$\boxed{\hat{U}(t)|\psi_{z(0)}\rangle = e^{-i\frac{\omega t}{2}}|\psi_{z(t)}\rangle \qquad z(t) = z(0)e^{-i\omega t}}$$



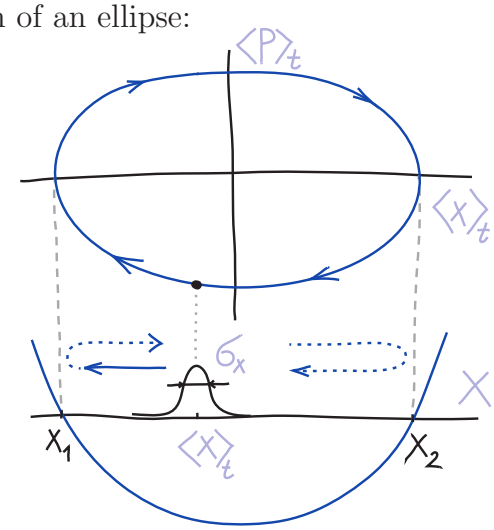
Evolution of coordinate & momentum averages

$$\langle x\rangle_t = \underbrace{\sqrt{\tfrac{2\hbar}{M\omega}}\left[\mathrm{Re}z(0)}_{\langle x\rangle_0}\cos(\omega t) + \mathrm{Im}z(0)\sin(\omega t)\right]$$

$$\langle p\rangle_t = \underbrace{-\sqrt{2M\hbar\omega}\left[\mathrm{Im}z(0)}_{\langle p\rangle_0}\cos(\omega t) - \mathrm{Re}z(0)\sin(\omega t)\right]$$

The averages satisfy the following equation of an ellipse:

$$\boxed{\tfrac{1}{2M}\langle p\rangle_t^2 + \tfrac{M\omega^2}{2}\langle x\rangle_t^2 = \underbrace{\hbar\omega|z(0)|^2}_{\langle E\rangle_{z(0)}-\frac{\hbar\omega}{2}}}$$



Coherent state approximately imitates the **classical oscillator trajectory** in the phase space, which satisfies:

$$\tfrac{1}{2M}p^2 + \tfrac{M\omega 2}{2}x^2 = E$$

Since $\langle E\rangle_z \gg \frac{\hbar\omega}{2}$ for $|z|^2 \gg 1$, the approximation is getting improved with increasing $|z| \leftrightarrow \langle E\rangle_z$

Constant widths $\boxed{\sigma_x = \sqrt{\frac{\hbar}{2M\omega}} \quad \sigma_p = \frac{\hbar}{2\sigma_x}}$ minimize the Heisenberg relation.

◀ Historical remark

1925: Erwin Schrödinger discovers oscillator coherent states (he wrongly anticipates that such states will make the notion of pointlike particles irrelevant)
1950-60's: J. Schwinger and J.Klauder use coherent states in the field-theory context
1963: Roy Glauber shows the key importance of coherent states in quantum optics

■ Heisenberg picture of particle in general potential

The above-derived results concerning the free particle and particle in the harmonic-oscillator potential indicate that coordinate and momentum averages may evolve in agreement with the laws of classical dynamics. Indeed, this correspondence can be generalized to the case of a particle moving in an arbitrary potential $V(\vec{x})$. To practice non-Schrödinger views of evolution, we switch for a moment to the Heisenberg picture.

▶ Ehrenfest theorem

We assume a single spinless particle with Hamiltonian: $\hat{H} = \frac{1}{2M}\hat{\vec{p}}^2 + V(\hat{\vec{x}})$

Evolving operators in the Heisenberg picture satisfy the following equations:

$$\left.\begin{array}{l} \frac{d}{dt}\hat{p}_i = \frac{1}{i\hbar}[\hat{p}_i, \hat{H}] = \frac{1}{i\hbar}[\hat{p}_i, V(\hat{\vec{x}})] = -\frac{\partial V}{\partial x_i}(\hat{\vec{x}}) \\ \frac{d}{dt}\hat{x}_i = \frac{1}{i\hbar}[\hat{x}_i, \hat{H}] = \frac{1}{i\hbar}[\hat{x}_i, \frac{1}{2M}\hat{p}_i^2] = \frac{1}{M}\hat{p}_i \end{array}\right\} \Rightarrow \left\{ \boxed{\begin{array}{l} \frac{d}{dt}\hat{\vec{p}} = -\vec{\nabla}V(\hat{\vec{x}}) \\ \frac{d}{dt}\hat{\vec{x}} = \frac{1}{M}\hat{\vec{p}} \end{array}} \right.$$

$$\frac{d^2}{dt^2}\hat{x}_i = \frac{d}{dt}\left(\frac{1}{M}\hat{p}_i\right) = -\frac{1}{M}\frac{\partial V}{\partial x_i}(\hat{\vec{x}}) \Rightarrow \boxed{M\frac{d^2}{dt^2}\hat{\vec{x}} = -\vec{\nabla}V(\hat{\vec{x}})}$$ **"quantum Newton law"**

▶ Semiclassical behavior

Consider an arbitrary state $|\psi_{\rm H}\rangle = |\psi_{\rm S}(t=0)\rangle$.

Coordinate averages $\langle x_i(t)\rangle_\psi = \langle\psi_{\rm S}(t)|\hat{x}_{i\rm S}|\psi_{\rm S}(t)\rangle = \langle\psi_{\rm H}|\hat{x}_i(t)_{\rm H}|\psi_{\rm H}\rangle$ evolve in accord with an averaged Newton law; in particular: $\boxed{M\frac{d^2}{dt^2}\langle\vec{x}(t)\rangle_\psi = -\langle\vec{\nabla}V(\hat{\vec{x}})\rangle_\psi}$

$\Rightarrow$ Semiclassical evolution of average coordinates is obtained for convenient initial states, like narrow wavepackets. However, as we saw, the **dispersions** $\langle\langle x_i^2(t)\rangle\rangle_\psi$ are not fixed and may behave in a crazy way (like in the case of a free particle, and in contrast to the exceptional case of the harmonic oscillator).

◀ Historical remark

1927: P. Ehrenfest formulates the relation between quantum and classical dynamics

■ Spin in rotating magnetic field

In the following example we describe the evolution of quantum spin in a time dependent external field. Although the time dependence of the Hamiltonian is of the nontrivial type [case (b) of Sec. 5a], the solution can be found analytically — not as the Dyson series. The example touches on the physics of nuclear magnetic resonance, which has a number of very important applications.

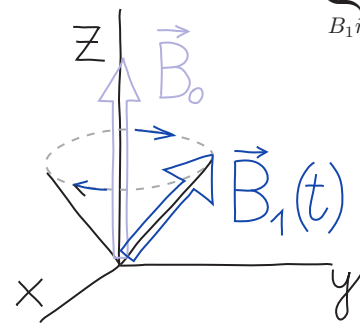
▶ **Magnetic resonance setup**: a particle (e.g. the proton) with magnetic moment (operator $\hat{\mu}$) is placed in a combined stationary (homogeneous) + variable (rotating) magnetic field. Hamiltonian reads as:

$$\hat{H}(t) = \overbrace{-\hat{\mu}_z B_0}^{\text{stationary field}} \overbrace{-\hat{\vec{\mu}}\cdot\underbrace{\vec{B}_1(t)}_{B_1\vec{n}(t)}}^{\text{varying field}}$$

Magnetic dipole operator: $\hat{\vec{\mu}} = g\mu_{\rm N}\frac{1}{\hbar}\hat{\vec{S}}$

$$\boxed{\hat{H}(t) = -\underbrace{g\mu_{\rm N}B_0}_{\hbar\omega_0}\frac{1}{\hbar}\hat{S}_3 - \underbrace{g\mu_{\rm N}B_1}_{\hbar\omega_1}\left(\vec{n}(t)\cdot\frac{1}{\hbar}\hat{\vec{S}}\right)}$$

$$\boxed{\vec{n}(t) = \begin{pmatrix} \sin\vartheta\cos\omega t \\ -\sin\vartheta\sin\omega t \\ \cos\vartheta \end{pmatrix}}$$ **rotating field**



Without loss of generality one may set $\vec{B}_1(t) \perp \vec{B}_0$

In the resonance case, the frequency ω of rotating field B_1 ($\ll B_0$) is tuned to the **Larmor frequency** ω_0 of the spin precession in the stationary filed B_0, and is applied in the form of pulses of certain duration. These pulses are used to prepare the spin in a desired state.

▶ Hamiltonians at various time instants *do not commute*:

$$[\hat{H}(t),\hat{H}(t')] = \omega_1^2\Big[\big(\vec{n}(t)\cdot\hat{\vec{S}}\big),\big(\vec{n}(t')\cdot\hat{\vec{S}}\big)\Big]+\omega_0\omega_1\Big[\hat{S}_3,\big(\vec{n}(t')\cdot\hat{\vec{S}}\big)\Big]+\omega_1\omega_0\Big[\big(\vec{n}(t)\cdot\hat{\vec{S}}\big),\hat{S}_3\Big] =$$
$$= i\hbar\omega_1\Big(\omega_1[\vec{n}(t)\times\vec{n}(t')]\cdot\hat{\vec{S}}+\omega_0[\vec{n}(t')\times\hat{\vec{S}}]_3-\omega_0[\vec{n}(t)\times\hat{\vec{S}}]_3\Big)\neq 0$$

▶ **Separation of the time dependence**

$$\hat{H}(t) = -(\omega_0+\omega_1\cos\vartheta)\hat{S}_3-\omega_1\sin\vartheta\underbrace{\big[(\cos\omega t)\hat{S}_1-(\sin\omega t)\hat{S}_2\big]}_{e^{+\frac{i}{\hbar}\omega t\hat{S}_3}\hat{S}_1e^{-\frac{i}{\hbar}\omega t\hat{S}_3}}$$

BCH formula: $e^{+\hat{A}}\hat{B}e^{-\hat{A}}=\sum\limits_k\frac{1}{k!}[\hat{A},[\hat{A},\dots[\hat{A},\hat{B}]\dots]_k$

$$e^{\frac{i\varphi}{\hbar}\hat{S}_3}\hat{S}_1e^{-\frac{i\varphi}{\hbar}\hat{S}_3} = \hat{S}_1+\tfrac{1}{1!}\left(\tfrac{i\varphi}{\hbar}\right)^1\underbrace{[\hat{S}_3,\hat{S}_1]}_{i\hbar\hat{S}_2}+\tfrac{1}{2!}\left(\tfrac{i\varphi}{\hbar}\right)^2\underbrace{[\hat{S}_3,i\hbar\hat{S}_2]}_{\hbar^2\hat{S}_1}+\tfrac{1}{3!}\left(\tfrac{i\varphi}{\hbar}\right)^3\underbrace{[\hat{S}_3,\hbar^2\hat{S}_1]}_{i\hbar^3\hat{S}_2}+\dots =$$
$$= \overbrace{\big(1-\tfrac{\phi^2}{2!}+\dots\big)}^{\cos\varphi}\hat{S}_1-\overbrace{\big(\tfrac{\phi}{1!}-\tfrac{\phi^3}{3!}+\dots\big)}^{\sin\varphi}\hat{S}_2$$

$$\hat{H}(t) = e^{+\frac{i}{\hbar}\omega t\hat{S}_3}\underbrace{\Big[-(\omega_0+\omega_1\cos\vartheta)\hat{S}_3-(\omega_1\sin\vartheta)\hat{S}_1\Big]}_{\hat{H}(0)}e^{-\frac{i}{\hbar}\omega t\hat{S}_3}$$

"rotating" Hamiltonian

So the Hamiltonian time dependence has been separated to the overall rotation. This enables us to solve the dynamics explicitly, using the rotating frame.

▶ **Transformation to the rotating frame**

$|\psi(t)\rangle\mapsto|\psi'(t)\rangle\equiv e^{-\frac{i}{\hbar}\omega t\hat{S}_3}|\psi(t)\rangle$ the evolving state in the frame that rotates with $\vec{B}_1(t)$

$$i\hbar\tfrac{d}{dt}|\psi'(t)\rangle = \omega\hat{S}_3\underbrace{e^{-\frac{i}{\hbar}\omega t\hat{S}_3}|\psi(t)\rangle}_{|\psi'(t)\rangle}+\underbrace{e^{-\frac{i}{\hbar}\omega t\hat{S}_3}\hat{H}(t)e^{+\frac{i}{\hbar}\omega t\hat{S}_3}}_{\hat{H}(0)}\underbrace{e^{-\frac{i}{\hbar}\omega t\hat{S}_3}|\psi(t)\rangle}_{|\psi'(t)\rangle}$$

Schrödinger equation in rotating frame:

$$\boxed{i\hbar\tfrac{d}{dt}|\psi'(t)\rangle = \underbrace{\Big[\hat{H}(0)+\omega\hat{S}_3\Big]}_{\hat{H}_{\rm eff}}|\psi'(t)\rangle}$$

$$\boxed{\hat{H}_{\rm eff} = (\omega-\omega_0-\omega_1\cos\vartheta)\hat{S}_3-(\omega_1\sin\vartheta)\hat{S}_1}$$

So, in the rotating frame we obtain a stationary **effective Hamiltonian** $\hat{H}_{\rm eff}$, for which the evolution $|\psi'(t)\rangle$ can be easily found analytically as it is just a certain rotation. To obtain $|\psi(t)\rangle$, we have to finally apply an inverse transformation from the rotation frame back to the laboratory frame.

▶ **Solution**

For $|\psi(0)\rangle\equiv|\psi'(0)\rangle$ we obtain: $|\psi(t)\rangle = e^{+\frac{i}{\hbar}\omega t\hat{S}_3}e^{-\frac{i}{\hbar}\hat{H}_{\rm eff}t}|\psi(0)\rangle$

The leftmost operator is a rotation around the $\vec{n}_z$ axis by angle $-\omega t$, the rightmost operator represents a rotation around a direction $\vec{n}_\Omega$ by an angle Ωt.

We assume $\vec{B}_1(t)\perp\vec{B}_0$ ($\vartheta=\frac{\pi}{2}$), as the parallel component can be included in $\vec{B}_0$:

$\hat{U}(t) = e^{+\frac{i}{\hbar}\omega t \hat{S}_3} e^{-\frac{i}{\hbar}\Omega t(\vec{n}_\Omega \cdot \hat{\vec{S}})}$ $\quad \Omega = \sqrt{(\omega-\omega_0)^2+\omega_1^2} \quad \vec{n}_\Omega = \frac{1}{\Omega}\begin{pmatrix} -\omega_1 \\ 0 \\ \omega-\omega_0 \end{pmatrix}$

resonant case $\omega = \omega_0$: $\Omega = \omega_1, \ \vec{n}_\Omega = -\vec{n}_x$

◄ Historical remark

1938: I. Rabi proposes the magnetic resonance method to measure mag. moments
1946: F. Bloch & E.M. Purcell develop a spectroscopic method based on the magnetic resonance and provide its theoretical description
1971: dawn of the magnetic resonance imaging (tomography) applications

6a. QUANTUM STATISTICAL ENSEMBLES

Physics would not be nearly as powerful if it did not have the branch of statistical physics. It deals with situations — rather generic for all complex systems — when the system's initial state cannot be precisely determined. Instead, one has some knowledge on the probability distribution characterizing a multitude of possible states in which the system may occur. In classical statistical physics, a single realization of the given system at a point $(\vec{p}_0, \vec{q}_0)$ of a multidimensional phase space is replaced by a *statistical ensemble* of replicas of the system at different points. This means that $\delta(\vec{p}-\vec{p}_0, \vec{q}-\vec{q}_0)$ changes into a delocalized probability distribution $\rho(\vec{p}, \vec{q})$. We are ready now to apply this kind of statistical description to quantum physics.

■ Generalization of quantum states in terms of the density operator

Statistical description implies **statistical uncertainty** resulting from the imperfect knowledge of the system's state. However, quantum physics, as we have learned it so far, already contains **quantum uncertainty**, which exists even if the system's state is known exactly. It is useful to unify both these types of uncertainty in a generalized notion of quantum state. It is expressed by a positive-definite Hermitian operator in $\mathcal{H}$, called the density operator.

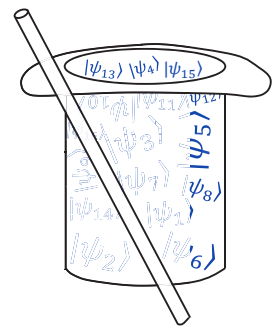
► Unified description of quantum & statistical uncertainties

In analogy to classical statistical ensemble, we want to introduce a quantum statistical ensemble. We assume that the state vector describing a given system is randomly selected from a certain predefined set:

$$\left\{ \begin{array}{ll} |\psi_1\rangle & \ldots \text{drawn with probability } \mathfrak{p}_1 \\ |\psi_2\rangle & \ldots \text{drawn with probability } \mathfrak{p}_2 \\ \vdots & \vdots \end{array} \right\}$$

where $\langle\psi_k|\psi_k\rangle = 1 \ \forall\, k$ and $\sum_k \mathfrak{p}_k = 1$.

We stress that the orthogonality of states is *not* required, so in general $\langle\psi_k|\psi_l\rangle \neq 0$ for $k \neq l$.



We note that probabilities $\mathfrak{p}_k$ express only the statistical uncertainty of drawing a state from the ensemble. An additional quantum uncertainty expresses the fact that the actually drawn state $|\psi_k\rangle$ can be mixed up with other states $|\psi_l\rangle$ in the process of measurement.

Example: electrons from an accelerator are delivered to the target in the spin states:

$$\left\{\begin{array}{ll} |\uparrow\rangle & \text{...probability } \mathfrak{p}_\uparrow \\ |\rightarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{i}{\sqrt{2}}|\downarrow\rangle & \text{...probability } \mathfrak{p}_\rightarrow \\ |\leftarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{i}{\sqrt{2}}|\downarrow\rangle & \text{...probability } \mathfrak{p}_\leftarrow \end{array}\right\}$$

The probability of measuring the spin z-projection $\uparrow$ in an unknown state that has been delivered is $\mathfrak{p}_\uparrow + \frac{\mathfrak{p}_\rightarrow}{2} + \frac{\mathfrak{p}_\leftarrow}{2} = \sum_k \mathfrak{p}_k |\langle\uparrow|\psi_k\rangle|^2$, which takes into account both statistical and quantum uncertainties.

This statistical ensemble of quantum states is described by the

density operator $\Leftrightarrow$ **density matrix**

$$\boxed{\hat{\rho} \equiv \sum_k \mathfrak{p}_k |\psi_k\rangle\langle\psi_k|} \qquad \rho_{ij} = \langle i|\hat{\rho}|j\rangle = \sum_k \mathfrak{p}_k \langle i|\psi_k\rangle\langle\psi_k|j\rangle$$

Taking into account both satatistical and quantum uncertainties, we see that the density operator $\hat{\rho}$ generates **probabability distribution** in the **entire Hilbert space** $\mathcal{H}$: The probability to find an arbitrary $|\psi\rangle \in \mathcal{H}$ in a state randomly drawn from the ensemble is given by $\sum_k \mathfrak{p}_k \underbrace{|\langle\psi|\psi_k\rangle|^2}_{\mathfrak{p}_{\psi_k}(\psi)} = \boxed{\langle\psi|\hat{\rho}|\psi\rangle = \mathfrak{p}_{\hat{\rho}}(\psi)}$

▶ Pure and mixed states

Since statistical and quantum uncertainties involved in quantum statistical ensembles cannot be resolved, it is convenient to incorporate both of them into a **generalized definition of quantum state**. So the general state of a quantum system with Hilbert space $\mathcal{H}$ is described by the density operator $\hat{\rho}$ acting in $\mathcal{H}$. This formalism naturally includes the previous definition of states as vectors in $\mathcal{H}$, i.e., the description in absence of statistical uncertainty.

pure state	$\hat{\rho} = \|\psi\rangle\langle\psi\|$	$\Leftrightarrow$	$\|\psi\rangle$	$\exists$ state vector
mixed state	$\hat{\rho} = \sum_k \mathfrak{p}_k \|\psi_k\rangle\langle\psi_k\|$	$\Leftrightarrow$	$\times$	$\nexists$ state vector

no stat. uncertainty

stat. uncertainty exists

▶ Properties of the density operator

(a) Hermiticity $\boxed{\hat{\rho} = \hat{\rho}^\dagger}$

(b) $\mathrm{Tr}\big[\sum_k \mathfrak{p}_k |\psi_k\rangle\langle\psi_k|\big] = \sum_i \sum_k \mathfrak{p}_k \langle i|\psi_k\rangle\langle\psi_k|i\rangle = \sum_k \mathfrak{p}_k \overbrace{\sum_i \langle\psi_k|i\rangle\langle i|\psi_k\rangle}^{\langle\psi_k|\psi_k\rangle=1} = \boxed{1 = \mathrm{Tr}\hat{\rho}}$

(c) $\langle\psi|\hat{\rho}|\psi\rangle \equiv \mathfrak{p}_\psi(\rho) \in [0,1] \quad \forall\,|\psi\rangle \quad \Rightarrow$ eigenvalues $\boxed{\rho_i \in [0,1]}$

(d) **Diagonalized density matrix**:

$$\boxed{\hat\rho=\sum_i \rho_i|\phi_i\rangle\langle\phi_i|} \equiv \begin{pmatrix} \rho_1 & 0 & 0 & \cdots \\ 0 & \rho_2 & 0 & \\ 0 & 0 & \rho_3 & \\ \vdots & & & \ddots \end{pmatrix} \quad \begin{array}{l} \sum_i \rho_i = 1 \quad \rho_i \ldots \text{probability to find } |\phi_i\rangle \\ \sum_i \rho_i^2 \le 1 \end{array}$$

For a pure state $|\psi\rangle$, the diagonalization yields $\hat\rho = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \\ 0 & 0 & 0 & \\ \vdots & & & \ddots \end{pmatrix}$ with $|\phi_1\rangle = |\psi\rangle$.

The quantity $\boxed{\gamma_\rho = \mathrm{Tr}\,\hat\rho^2 \in [0,1]}$ is called **purity** of the state $\hat\rho$. It allows one to distinguish pure & mixed states, and for mixed states to quantify the degree of impurity $1-\gamma_\rho$.

$$\gamma_\rho \begin{cases} = 1 & \text{for pure state} \\ < 1 & \text{for mixed state} \end{cases}$$

► Ambiguity in the expansion of $\hat\rho$

The **diagonalized form** $\hat\rho = \sum_i \rho_i|\phi_i\rangle\langle\phi_i|$ (with $\{|\phi_i\rangle\}$ orthonormal) can be considered to be a **"canonical expression"** of a general density operator. This form represents an ideal statistical ensemble, in which the states $|\phi_i\rangle$ are mutually distinguishable. However, the same diagonalized form is assigned to different non-diagonal expressions $\hat\rho = \sum_k \mathfrak{p}_k|\psi_k\rangle\langle\psi_k|$ $\left(\begin{smallmatrix}\text{with } \{|\psi_k\rangle\} \text{ normalized} \\ \text{but otherwise arbitrary}\end{smallmatrix}\right)$. This indicates equivalence of various statistical ensembles (those with the same diagonal form), which is due to some kind of arbitrariness in dividing the total uncertainty between the statistical and quantum components.

► Statistical properties of observables

If the density operator $\hat\rho$ defines the state of the system, we have to learn how to use it for the determination of statistical properties of measurement outcomes.

$\langle A\rangle_\rho \equiv$ **average** of quantity $\hat A$ in state $\hat\rho \equiv \sum_k \mathfrak{p}_k|\psi_k\rangle\langle\psi_k|$

$$\langle A\rangle_\rho = \int a \overbrace{\sum_k \mathfrak{p}_k \underbrace{\langle\psi_k|\hat P_a|\psi_k\rangle}_{\mathfrak{p}_{\psi_k}(a)}}^{\mathfrak{p}_\rho(a)} da = \sum_k \mathfrak{p}_k\langle\psi_k|\hat A|\psi_k\rangle = \sum_{ij}\sum_k \mathfrak{p}_k\langle\psi_k|i\rangle\langle i|\hat A|j\rangle\langle j|\psi_k\rangle =$$

$$= \sum_{ij} \underbrace{\sum_k \mathfrak{p}_k\langle j|\psi_k\rangle\langle\psi_k|i\rangle}_{\langle j|\hat\rho|i\rangle}\langle i|\hat A|j\rangle = \boxed{\mathrm{Tr}(\hat\rho\,\hat A) = \mathrm{Tr}(\hat A\,\hat\rho) = \langle A\rangle_\rho}$$

For a pure state: $\langle A\rangle_\psi = \sum_i \langle i|\psi\rangle\langle\psi|\hat A|i\rangle = \langle\psi|\hat A|\psi\rangle$

Dispersion: $\langle\!\langle A^2\rangle\!\rangle_\rho = \langle A^2\rangle_\rho - \langle A\rangle_\rho^2 = \boxed{\mathrm{Tr}(\hat A^2\hat\rho) - \mathrm{Tr}^2(\hat A\,\hat\rho) = \langle\!\langle A^2\rangle\!\rangle_\rho}$

Probability distribution $\mathfrak{p}_\rho(a) = \sum_k \mathfrak{p}_k\langle\psi_k|\hat P_a|\psi_k\rangle = \mathrm{Tr}(\hat P_a\,\hat\rho)$

◄ Historical remark

1927: John von Neumann introduces the density operator (matrix) to build quantum statistical mechanics; simultaneously, Lev Landau uses the density operator to describe quantum states of subsystems of a larger composite system

■ Entropy and canonical ensemble

The concept of entropy plays an important role in thermodynamics as well as in mathematical information theory. Statistical physics is a bridge between both these seemingly distant coasts. States with null entropy are the pure states of ordinary QM. In contrast, states whose entropy is maximal—within given constraints upon some physical averages—represent equilibrated systems in contact with a thermal bath.

▸ Shannon information entropy

General probability distribution for a finite set of events:

$$\text{event } i \in \{1, 2, \dots n\} \;\leftrightarrow\; \text{probability } \{\mathfrak{p}_i\} \equiv \{\mathfrak{p}_1, \mathfrak{p}_2, \dots, \mathfrak{p}_n\}$$

Information entropy is a functional on the space of probability distributions:

$$\boxed{S[\{\mathfrak{p}_i\}] = -\sum_{i=1}^{n} \mathfrak{p}_i \ln \mathfrak{p}_i}$$

Properties

Maximum	$S = \ln n$ for $\mathfrak{p}_i = \text{const} = \frac{1}{n} \quad \forall\, i$	maximal uncertainty
Minimum	$S = 0$ for $\mathfrak{p}_i = \delta_{ij}$ (with any j)	minimal uncertainty

Additivity: 2 sets of **independent events** $\left\{ \begin{smallmatrix} i \leftrightarrow \mathfrak{p}_i \\ j \leftrightarrow \mathfrak{p}_j \end{smallmatrix} \right\} \Rightarrow$ entropy $\left\{ \begin{smallmatrix} S_1 \\ S_2 \end{smallmatrix} \right\}$

Joint distribution: event $(i \wedge j)$ with prob. $\mathfrak{p}_{ij} = \mathfrak{p}_i \mathfrak{p}_j \Rightarrow$ entropy $\boxed{S_{12} = S_1 + S_2}$

However, for correlated events $(\mathfrak{p}_{ij} \neq \mathfrak{p}_i \mathfrak{p}_j)$: $S_{12} = S_1 + S_2 + \Delta S$ with $\Delta S \gtrless 0$

▸ Von Neumann entropy

$$\boxed{\boxed{S_\rho = -k \sum_{i=1}^{d} \rho_i \ln \rho_i = -k \operatorname{Tr}\big[\hat{\rho} \ln \hat{\rho}\big]}}$$

To make contact with the **thermodynamic entropy** we use the Boltzmann const. $k = 8.6 \cdot 10^{-5}$eV/K

$S_\rho = 0$ for pure state

$S_\rho > 0$ for mixed state ($S_\rho = S_{\max} = \ln d$ for "maximally mixed" state)

▸ **Equilibrium state** of a quantum system which exchanges energy with the surrounding environment (**thermal bath**):

$\hat{\rho}$ diagonal in the system's energy eigenbasis: $\hat{\rho} = \sum_i \rho_i |E_i\rangle\langle E_i| \Rightarrow$ stationary state with respect to system's Hamiltonian: $\hat{\rho}(t) = \sum_i \rho_i e^{-i\frac{E_i t}{\hbar}} |E_i\rangle\langle E_i| e^{+i\frac{E_i t}{\hbar}} = \hat{\rho}(0)$

Probabilities ρ_i determined from **constrained maximal entropy prinicple**: Search for max. S_ρ with fixed **energy average** $\langle E \rangle_\rho = \sum_i \rho_i E_i$ and $\sum_i \rho_i = 1$ $\Rightarrow$ method of Lagrange multipliers: we look for an extreme of function

$$f = -\sum_i \rho_i \ln \rho_i + (\alpha + 1) \sum_i \rho_i - \beta \sum_i \rho_i E_i$$

$$\frac{\partial f}{\partial \rho_i} = -\ln \rho_i - \rho_i \tfrac{1}{\rho_i} + (\alpha + 1) - \beta E_i = 0 \quad \Rightarrow \quad \boxed{\rho_i = e^{\alpha - \beta E_i}} = \overbrace{e^{\alpha}}^{\text{normalization}}\, e^{-\beta E_i}$$

Constants α, β determined from the $\operatorname{Tr} \hat{\rho} = 1$ & fixed average $\langle E \rangle_\rho$ conditions

▶ Canonical density operator

From the above-derived result $\hat{\rho}_\beta = e^\alpha \sum_i e^{-\beta E_i} |E_i\rangle\langle E_i|$ we obtain:

$$\boxed{\hat{\rho}_\beta = \tfrac{1}{Z(\beta)}\, e^{-\beta \hat{H}}} \quad \text{with} \quad \boxed{\beta = \tfrac{1}{kT}} \quad \textbf{inverse temperature}$$
the only parameter of the canonical state

$$\boxed{Z(\beta) = \sum_i e^{-\beta E_i} = \mathrm{Tr}\, e^{-\beta \hat{H}}} \quad \textbf{canonical partition function}$$
normalization factor $e^\alpha \equiv \frac{1}{Z(\beta)}$

▶ $Z(\beta)$ contains complete information on thermal properties

$$\tfrac{d}{d\beta} Z(\beta) = \tfrac{d}{d\beta} \mathrm{Tr}\, e^{-\beta \hat{H}} = -\mathrm{Tr}\big[\hat{H} \underbrace{e^{-\beta \hat{H}}}_{Z(\beta)\hat{\rho}_\beta}\big] = -Z(\beta) \underbrace{\mathrm{Tr}[\hat{H}\hat{\rho}_\beta]}_{\langle E\rangle_\beta}$$

$$\boxed{\langle E\rangle_\beta = -\tfrac{1}{Z(\beta)} \tfrac{d}{d\beta} Z(\beta) = -\tfrac{d}{d\beta} \ln Z(\beta)} \quad \textbf{energy average}$$

$$-\tfrac{d}{d\beta}\langle E\rangle_\beta = kT^2 \underbrace{\tfrac{d}{dT}\langle E\rangle_T}_{c_V(T)} \quad \text{specific heat at temperature } T$$

$$-\tfrac{d}{d\beta}\langle E\rangle_\beta = \tfrac{d^2}{d\beta^2} \ln Z(\beta) = \overbrace{\tfrac{1}{Z(\beta)} \tfrac{d^2 Z(\beta)}{d\beta^2}}^{\frac{1}{Z(\beta)}\mathrm{Tr}\left[\hat{H}^2 e^{-\beta\hat{H}}\right]} - \overbrace{\tfrac{1}{Z(\beta)^2}\left[\tfrac{dZ(\beta)}{d\beta}\right]^2}^{\langle E\rangle_\beta^2} = \langle E^2\rangle_\beta - \langle E\rangle_\beta^2 = \langle\langle E^2\rangle\rangle_\beta$$

$$\boxed{\langle\langle E^2\rangle\rangle_\beta = \tfrac{1}{k\beta^2} c_V(\beta) = \tfrac{d^2}{d\beta^2} \ln Z(\beta)} \quad \textbf{energy dispersion \& specific heat}$$

▶ $Z(\beta)$ contains complete information on energy spectrum

energy levels $\{E_i\}$ $\Rightarrow$ **level density**

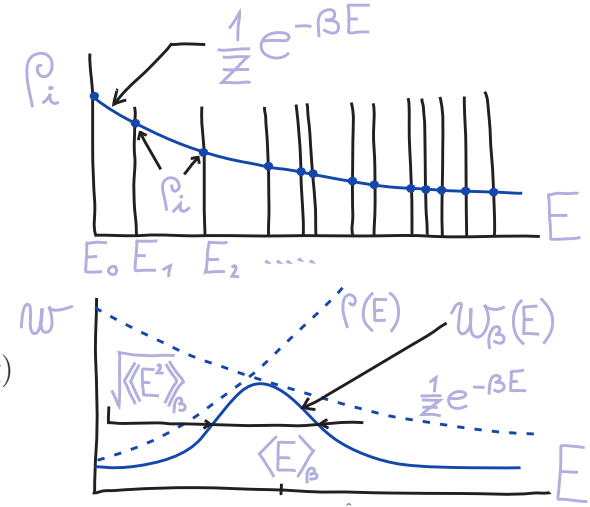
$$\boxed{\varrho(E) = \sum_i \delta(E - E_i)}$$

$\varrho(E)$ can be obtained as the inverse Laplace transform of $Z(\beta) = \int \varrho(E) e^{-\beta E} dE$

Thermal distribution of energy $w_\beta(E)$ (probabability density for finding the system at energy E if temperature is T) is expressed via the level density $\varrho(E)$:

$$\boxed{w_\beta(E) \propto \varrho(E)\, \tfrac{e^{-\beta E}}{Z(\beta)}}$$

Usually the (increasing $\times$ decreasing) function product yields a peak at a certain value $[E]_\beta$ close to $\langle E\rangle_\beta$



▶ Imaginary time $t = -i\hbar\beta$ evolution operator $\hat{U}(t) = e^{-i\frac{\hat{H}t}{\hbar}}$ is equivalent to the unnormalized canonical density operator $\boxed{e^{-\beta\hat{H}} = Z(\beta)\,\hat{\rho}_\beta = \hat{U}(-i\hbar\beta)}$

This is used in some advanced calculations of thermal & dynamical properties.

► Similar procedure (using maximal entropy principle) is applicable also for systems with variable numbers N_i of particles (types $i = 1, 2, \ldots n$) but fixed averages $\langle N_i \rangle$ (particles exchanged with the bath) ⇒ grand-canonical ensemble characterized by inverse temperature β and chemical potentials μ_i (see Sec. 15).

◄ Historical remark
1878: J.W. Gibbs presents the concept of canonical ensemble & entropy formula
1927: J. von Neumann introduces the density operator & entropy in QM
1948: C. Shannon applies entropy in the information theory

■ Wigner quasiprobability distribution

As the density-operator formalism merges statistical and quantal fluctuations into a unified picture, it may raise hopes of formulating quantum mechanics in a purely statistical language—via some appropriate statistical distributions in the classical phase space. Although it turns out that such a formulation is not possible, the product of this effort is useful by itself.

► **Motivation**: Assume a system with f degrees of freedom with coordinate & momentum eigenvectors $|\vec{x}\rangle$ & $|\vec{p}\rangle$. The $\left\{ \begin{smallmatrix} \text{coordinate} \\ \text{momentum} \end{smallmatrix} \right\}$ representations of an arbitrary density operator $\hat{\rho}$ are given by functions $\left\{ \begin{smallmatrix} \langle \vec{x}\,' | \hat{\rho} | \vec{x} \rangle \equiv \rho(\vec{x}\,', \vec{x}) \\ \langle \vec{p}\,' | \hat{\rho} | \vec{p} \rangle \equiv \rho(\vec{p}\,', \vec{p}) \end{smallmatrix} \right\}$. Could we also construct $\rho(\vec{x}, \vec{p})$, i.e., an analog of the classical phase-space distribution?

► Characteristic function of a probability distribution

Any continuous probability distribution $\rho(x)$ is equivalently expressed through its so-called characteristic function $\chi_\rho(\eta)$, which is the Fourier transform of $\rho(x)$. For a distribution $\rho(\vec{x}, \vec{p})$ in the classical phase space we can write:

$$\chi_\rho(\vec{\xi}, \vec{\eta}) = \int \rho(\vec{x}, \vec{p}) e^{\frac{i}{\mathfrak{h}}(\vec{\eta}\cdot\vec{x} + \vec{\xi}\cdot\vec{p})} d\vec{x}\, d\vec{p} \;\leftrightarrow\; \rho(\vec{x}, \vec{p}) = \frac{1}{(2\pi\mathfrak{h})^{2f}} \int \chi_\rho(\vec{\xi}, \vec{\eta}) e^{-\frac{i}{\mathfrak{h}}(\vec{\eta}\cdot\vec{x} + \vec{\xi}\cdot\vec{p})} d\vec{\xi}\, d\vec{\eta}$$

where $\left\{ \begin{smallmatrix} \vec{\xi} \\ \vec{\eta} \end{smallmatrix} \right\}$ are f-dimensional variables having the same units as $\left\{ \begin{smallmatrix} \vec{x} \\ \vec{p} \end{smallmatrix} \right\}$, and $\mathfrak{h}$ is an arbitrary constant in units of the product xp

⇒ characteristic function expressed as the average: $\boxed{\chi_\rho(\vec{\xi}, \vec{\eta}) = \left\langle e^{\frac{i}{\mathfrak{h}}(\vec{\eta}\cdot\vec{x} + \vec{\xi}\cdot\vec{p})} \right\rangle_\rho}$

► Quantum characteristic function and its inverse

The last expression enables us to find a quantum analog of characteristic function. In QM we naturally set $\mathfrak{h} = \hbar$ and obtain:

$$\boxed{\chi_\rho(\vec{\xi}, \vec{\eta}) \equiv \mathrm{Tr}\left[e^{\frac{i}{\hbar}(\vec{\eta}\cdot\hat{\vec{x}} + \vec{\xi}\cdot\hat{\vec{p}})} \hat{\rho} \right]}$$

Fourier inverse:

$$\boxed{W_\rho(\vec{x}, \vec{p}) \equiv \frac{1}{(2\pi\hbar)^{2f}} \int \chi_\rho(\vec{\xi}, \vec{\eta})\, e^{-\frac{i}{\hbar}(\vec{\eta}\cdot\vec{x} + \vec{\xi}\cdot\vec{p})}\, d\vec{\xi}\, d\vec{\eta}}$$

Wigner distribution

This represents a distribution in the phase space. Some of its properties are consistent with the interpretation in terms of a probability distribution, but there is one essential drawback: The distribution can take negative values!

► Wigner distribution for $f = 1$

The characteristic function:

$$\chi_\rho(\xi,\eta) = \int \langle x|\hat\rho\, e^{\frac{i}{\hbar}(\eta\hat x+\xi\hat p)}|x\rangle\, dx \overset{\text{BCH}}{=} e^{i\frac{\eta\xi}{2\hbar}} \int \langle x|\hat\rho\, e^{\frac{i}{\hbar}\eta\hat x} e^{\frac{i}{\hbar}\xi\hat p}|x\rangle\, dx$$

special BCH formula for $[\hat A,\hat B]=\hat C$, $[\hat A,\hat C]=[\hat B,\hat C]=0$: $e^{\hat A+\hat B} = e^{\hat A}e^{\hat B}e^{-\frac{1}{2}\hat C}$

$$= e^{i\frac{\eta\xi}{2\hbar}} \iint \underbrace{\langle x|\hat\rho e^{\frac{i}{\hbar}\eta\hat x}|x'\rangle}_{e^{\frac{i}{\hbar}\eta x'}\langle x|\hat\rho|x'\rangle} \underbrace{\langle x'|e^{\frac{i}{\hbar}\xi\hat p}|x\rangle}_{\langle x'|x-\xi\rangle=\delta(x'-x+\xi)} dx\, dx' = e^{-i\frac{\eta\xi}{2\hbar}} \int \underbrace{\langle x|\hat\rho|x-\xi\rangle}_{\rho(x,x-\xi)} e^{\frac{i}{\hbar}\eta x}\, dx \qquad \text{subst. } x'=x-\tfrac{\xi}{2}$$

$$\Rightarrow \quad \boxed{\chi_\rho(\xi,\eta) = \int \rho(x'+\tfrac{\xi}{2}, x'-\tfrac{\xi}{2})\, e^{\frac{i}{\hbar}\eta x'}\, dx'}$$

The Wigner distribution:

$$W_\rho(x,p) = \tfrac{1}{(2\pi\hbar)^2} \iint \Big[\int \rho(x'+\tfrac{\xi}{2}, x'-\tfrac{\xi}{2})\, e^{\frac{i}{\hbar}\eta x'}\, dx'\Big] e^{-\frac{i}{\hbar}(\eta x+\xi p)}\, d\eta\, d\xi =$$

$$= \tfrac{1}{(2\pi\hbar)^2} \iint \rho(x'+\tfrac{\xi}{2}, x'-\tfrac{\xi}{2}) \underbrace{\Big[\int e^{\frac{i}{\hbar}\eta(x'-x)}\, d\eta\Big]}_{2\pi\hbar\delta(x'-x)} e^{-\frac{i}{\hbar}\xi p}\, dx'\, d\xi$$

$$\boxed{W_\rho(x,p) = \tfrac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \rho\big(x+\tfrac{\xi}{2}, x-\tfrac{\xi}{2}\big)\, e^{-\frac{i}{\hbar}\xi p}\, d\xi}$$

where
$\rho(x'+\frac{\xi}{2}, x'-\frac{\xi}{2}) = \langle x'+\frac{\xi}{2}|\hat\rho|x'-\frac{\xi}{2}\rangle$

Reality: $W_\rho(x,p)^* = \frac{1}{2\pi\hbar}\int \rho\big(x-\frac{\xi}{2}, x+\frac{\xi}{2}\big)\, e^{+\frac{i}{\hbar}\xi p}\, d\xi = W_\rho(x,p)$

Normalization: $\iint W_\rho(x,p)dx\, dp = \frac{1}{(2\pi\hbar)^2} \iint \underbrace{\big[\int e^{-\frac{i}{\hbar}\xi p}\, dp\big]}_{2\pi\hbar\delta(\xi)} \rho\big(x+\frac{\xi}{2}, x-\frac{\xi}{2}\big) dx\, d\xi =$

$$= \int \rho(x,x)dx = \mathrm{Tr}\hat\rho = 1$$

These are properties of a probability distribution.

However, $W_\rho(x,p) = \frac{1}{2\pi\hbar}\int \big[\mathrm{Re}\rho(x+\frac{\xi}{2}, x-\frac{\xi}{2})\cos(\frac{\xi p}{\hbar}) + \mathrm{Im}\rho(x+\frac{\xi}{2}, x-\frac{\xi}{2})\sin(\frac{\xi p}{\hbar})\big] \not\geq 0$

Taking **negative values** in some phase-space domains, the distribution function $W_\rho(x,p)$ does *not* have the meaning of an ordinary probability density. It is sometimes called the *quasiprobability* distribution.

Moral: quantum oddity is unremovable!

◄ Historical remark

1927: H. Weyl derives a mapping of Hermitian operators to phase-space functions
1932: E. Wigner introduces quasiprobability distribution related to density operators
1940's-present: developments in the phase-space formulation of QM

■ Density operator for open systems

The way we introduced the density operator invokes a picture of somebody drawing numbered balls from a wheel of fortune. The balls are prepared there, one just does not know which number will be drawn. However, there

is another—and probably more important—use of the density-matrix formalism. It deals with open quantum systems, i.e., systems interacting with some other quantum systems, such as the surrounding environment or some intrinsic degrees of freedom, which are not explicitly considered on a given level of description. Such composite objects generically occur in entangled quantum states and the density operator is the only tool that allows one to extract states of individual subsystems.

▶ Two coupled systems $\begin{cases} 1 \equiv \text{the quantum system of interest} \\ 2 \equiv \text{environment (external system or internal degrees of freedom)} \end{cases}$

The total Hilbert space $\boxed{\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2}$ with $\{|\phi_{kl}\rangle\}_l \equiv$ basis of $\mathcal{H}_k$ $(k=1,2)$

A general pure state of the whole system 1+2 is given by: $\boxed{|\Psi\rangle = \sum_{ij} \alpha_{ij} |\phi_{1i}\rangle |\phi_{2j}\rangle}$

This is in general an entangled state

$\Rightarrow$ state vectors of subsystems 1 or 2 do not exist!

▶ Reduced density operator

The information on the **state of any subsystem** of a larger system is available only in the form of a density operator. This means that any such state represents in general a statistical ensemble. The density operator of a given subsystem is obtained as a **partial trace** of the density operator of the whole system over the Hilbert spaces of all the other subsystems. In our present case, the density operator $\hat{\rho}_1$ of system 1 is given as a partial trace of the full density operator $\hat{\rho}_{12}$ over the basis of system 2:

$$\text{pure state } |\Psi\rangle \quad \longmapsto \quad |\Psi\rangle\langle\Psi| \equiv \hat{\rho}_{12} \quad \longmapsto \quad \boxed{\hat{\rho}_1 \equiv \mathrm{Tr}_2\, \hat{\rho}_{12} \equiv \sum_l \langle \phi_{2l} | \hat{\rho}_{12} | \phi_{2l} \rangle}$$

$$|\Psi\rangle = \sum_{ij} \alpha_{ij} |\phi_{1i}\rangle |\phi_{2j}\rangle \quad \Rightarrow \quad \hat{\rho}_1 = \sum_l \sum_{ij} \sum_{i'j'} \alpha_{ij} \alpha^*_{i'j'} \underbrace{\langle \phi_{2l} | \phi_{2j} \rangle}_{\delta_{jl}} |\phi_{1i}\rangle\langle\phi_{1i'}| \underbrace{\langle \phi_{2j'} | \phi_{2l} \rangle}_{\delta_{j'l}}$$

$$\Rightarrow \boxed{\hat{\rho}_1 = \sum_{ii'} \underbrace{\left(\sum_j \alpha_{ij} \alpha^*_{i'j} \right)}_{\rho_{1ii'} = \rho^*_{1i'i}} |\phi_{1i}\rangle\langle\phi_{1i'}|}$$

This is an operator in $\mathcal{H}_1$ which has (as shown below) all the properties of a density operator, and therefore it **is** a density operator of system 1

▶ Properties of $\hat{\rho}_1 = \mathrm{Tr}_2\, \hat{\rho}_{12}$:

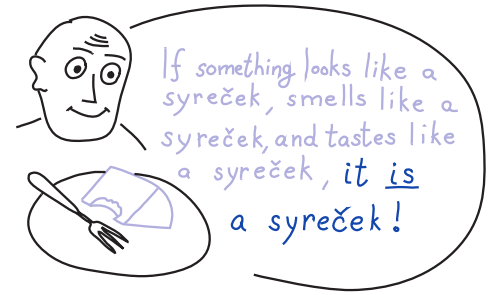
(a) $\hat{\rho}_1^\dagger = \sum_{ii'} \rho^*_{1ii'} |\phi_{1i'}\rangle\langle\phi_{1i}| = \hat{\rho}_1$

(b) $\mathrm{Tr}_1 \hat{\rho}_1 = \sum_{ij} |\alpha_{ij}|^2 = 1$

(c) $\langle \psi_1 | \hat{\rho}_1 | \psi_1 \rangle \geq 0 \quad \forall\, |\psi_1\rangle \equiv \sum_l \beta_l |\phi_{1l}\rangle$

$\Rightarrow$ eigenvalues ≥ 0

Proof: $\langle \psi_1 | \hat{\rho}_1 | \psi_1 \rangle = \sum_{ll'} \beta^*_{l'} \beta_l \sum_{ii'} \left(\sum_j \alpha_{ij} \alpha^*_{i'j} \right) \underbrace{\langle \phi_{1l'} | \phi_{1i} \rangle}_{\delta_{l'i}} \underbrace{\langle \phi_{1i'} | \phi_{1l} \rangle}_{\delta_{i'l}} = \sum_j \left| \sum_i \beta^*_i \alpha_{ij} \right|^2 \geq 0$



(d) $\mathrm{Tr}_1\hat{\rho}_1^2 \leq 1 \quad \Leftarrow$ (b),(c)

(e) Average value of a local observable $\hat{A} \equiv \hat{A}_1 \otimes \hat{I}_2$

$$\langle\Psi|\hat{A}|\Psi\rangle = \sum_{ij}\sum_{i'j'} \alpha_{ij}\alpha^*_{i'j'}\langle\phi_{1i'}|\hat{A}_1|\phi_{1i}\rangle \underbrace{\langle\phi_{2j'}|\phi_{2j}\rangle}_{\delta_{jj'}} = \overbrace{\sum_{ii'}\underbrace{\sum_{j}\alpha_{ij}\alpha^*_{i'j}}_{\rho_{1ii'}}\langle\phi_{1i'}|\hat{A}_1|\phi_{1i}\rangle}^{\mathrm{Tr}(\hat{A}_1\hat{\rho}_1)}$$

$$\Rightarrow \quad \boxed{\langle A\rangle_\Psi = \mathrm{Tr}(\hat{A}_1\hat{\rho}_1)}$$

▶ Pure states of the subsystem

The reduced density operator allows us to capture situations in which all predefined subsystems of the composite system are in pure states, which happens *iff* the state of the composite system is factorized with respect to the given decomposition: $\hat{\rho}_1 = \mathrm{Tr}_2\,\hat{\rho}_{12}$ is a pure state $|\psi_1\rangle \equiv \sum_i \beta_i|\phi_{1i}\rangle \;\Leftrightarrow\; |\Psi\rangle = \sum_{ij}\underbrace{\beta_i\gamma_j}_{\alpha_{ij}}|\phi_{1i}\rangle|\phi_{2j}\rangle = |\psi_1\rangle\big(\sum_j \gamma_j|\phi_{2j}\rangle\big) = |\psi_1\rangle|\psi_2\rangle$ is factorized.

$$\left.\begin{array}{lll} \hat{\rho}_1 = |\psi_1\rangle\langle\psi_1| & \Rightarrow & \rho_{1ii'} = \langle\phi_{1i}|\hat{\rho}_1|\phi_{1i'}\rangle = \beta_i\beta^*_{i'} \overbrace{\sum_j |\gamma_j|^2}^{1} \\ |\Psi\rangle = |\psi_1\rangle|\psi_2\rangle & \Rightarrow & \rho_{1ii'} = \sum_j \underbrace{\alpha_{ij}}_{\beta_i\gamma_j}\underbrace{\alpha^*_{i'j}}_{\beta^*_{i'}\gamma^*_j} = \beta_i\beta^*_{i'}\overbrace{\sum_j |\gamma_j|^2}^{1} \end{array}\right\} \text{same expressions}$$

▶ Schmidt decomposition of an entangled state

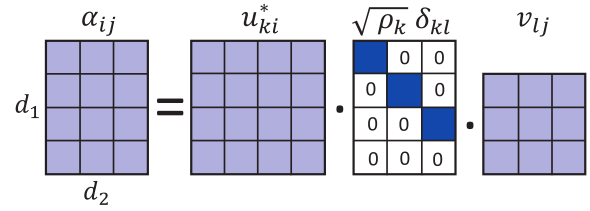
Any entangled state of a general coupled system composed of two subsystems 1 and 2 (with Hilbert space dimensions d_1 and d_2, respectively) can be expressed in a "canonical form" which makes use of the eigenvectors of both reduced density matrices $\hat{\rho}_1$ and $\hat{\rho}_2$. Consider the general state $|\Psi\rangle = \sum_{ij}\alpha_{ij}|\phi_{1i}\rangle|\phi_{2j}\rangle$:

State of subsystem 1:
$\hat{\rho}_1 = \mathrm{Tr}_2\,\hat{\rho}_{12} = \sum_{ii'}\big(\sum_j \alpha_{ij}\alpha^*_{i'j}\big)|\phi_{1i}\rangle\langle\phi_{1i'}|$

State of subsystem 2:
$\hat{\rho}_2 = \mathrm{Tr}_1\,\hat{\rho}_{12} = \sum_{jj'}\big(\sum_i \alpha_{ij}\alpha^*_{ij'}\big)|\phi_{2j}\rangle\langle\phi_{2j'}|$

Suppose $\boxed{\alpha_{ij} = \sqrt{\rho_i}\,\delta_{ij}} \Rightarrow \left\{\begin{array}{l} \rho_{1ii'} = \sum_j \alpha_{ij}\alpha^*_{i'j} = \sum_j \sqrt{\rho_i}\,\delta_{ij}\sqrt{\rho_{i'}}\,\delta_{i'j} = \rho_i\delta_{ii'} \\ \rho_{2jj'} = \sum_i \alpha_{ij}\alpha^*_{ij'} = \sum_i \sqrt{\rho_i}\,\delta_{ij}\sqrt{\rho_i}\,\delta_{ij'} = \rho_j\delta_{jj'} \end{array}\right\}$ diagonal $\left\{\begin{array}{l}\hat{\rho}_1 \\ \hat{\rho}_2\end{array}\right.$

This form of $|\Psi\rangle$ corresponds to the **singular value decomposition** of the generally non-square $d_1 \times d_2$ matrix $\boldsymbol{\alpha}$ of coefficients α_{ij} through the formula $\boxed{\boldsymbol{\alpha} = \boldsymbol{u}^\dagger\boldsymbol{\alpha}'\boldsymbol{v}}$, where $\boldsymbol{\alpha}'$ is semidiagonal and $\boldsymbol{u}$, $\boldsymbol{v}$ unitary. In particular, we get $\alpha_{ij} = \sum_{k=1}^{d_1}\sum_{l=1}^{d_2} u^*_{ki}(\sqrt{\rho_k}\delta_{kl})v_{lj}$ with $\sum_k \rho_k = \sum_{ij}|\alpha_{ij}|^2 = 1$ and $\left\{\begin{array}{l}\boldsymbol{u}\equiv u_{ik} \\ \boldsymbol{v}\equiv v_{lj}\end{array}\right\} \equiv$ some $\left\{\begin{array}{l}d_1\times d_1 \\ d_2\times d_2\end{array}\right\}$ unitary matrices.



$$\Rightarrow \quad |\Psi\rangle = \sum_{i=1}^{d_1}\sum_{j=1}^{d_2}\alpha_{ij}|\phi_{1i}\rangle|\phi_{2j}\rangle = \sum_{k=1}^{d_1}\sum_{l=1}^{d_2}\sqrt{\rho_k}\delta_{kl}\overbrace{\sum_{i=1}^{d_1}u^*_{ki}|\phi_{1i}\rangle}^{|\chi_{1k}\rangle}\overbrace{\sum_{j=1}^{d_2}v_{lj}|\phi_{2j}\rangle}^{|\chi_{2l}\rangle} \qquad \overbrace{\begin{array}{c}\text{from unitarity} \\ \text{of } \boldsymbol{u} \text{ and } \boldsymbol{v}\end{array}}^{\begin{array}{l}\langle\chi_{1k}|\chi_{1k'}\rangle = \delta_{kk'} \\ \langle\chi_{2l}|\chi_{2l'}\rangle = \delta_{ll'}\end{array}}$$

$$\Rightarrow \quad \boxed{|\Psi\rangle = \sum_{k=1}^{\mathrm{Min}\{d_1,d_2\}} \sqrt{\rho_k}\,|\chi_{1k}\rangle|\chi_{2k}\rangle} \quad \text{where} \quad \left\{ \begin{matrix} \{|\chi_{1k}\rangle\}_{k=1}^{d_1} \\ \{|\chi_{2k}\rangle\}_{k=1}^{d_2} \end{matrix} \right\} \text{ are } \textbf{eigenvectors} \text{ of } \left\{ \begin{matrix} \hat{\rho}_1 \\ \hat{\rho}_2 \end{matrix} \right\}$$

with the same sets of **eigenvalues** $\rho_k \left\{ \begin{matrix} > 0 & \text{for } k{=}1,\ldots,\mathrm{Min}\{d_1,d_2\} \\ = 0 & \text{for } k{=}\mathrm{Min}\{d_1,d_2\}{+}1,\ldots,\mathrm{Max}\{d_1,d_2\} \end{matrix} \right.$

Remark: Note the potentially large difference in the size of both expressions $|\Psi\rangle = \sum_{i=1}^{d_1}\sum_{j=1}^{d_2}\alpha_{ij}|\phi_{1i}\rangle|\phi_{2j}\rangle = \sum_{k=1}^{\mathrm{Min}\{d_1,d_2\}}\sqrt{\rho_k}\,|\chi_{1k}\rangle|\chi_{2k}\rangle$. The respective numbers of terms $d_1 d_2$ and $\mathrm{Min}\{d_1, d_2\}$ in these two formulas are for an example with $d_1 = 2$ (qubit) and $d_2 = 10^6$ (large environment) equal to $2 \cdot 10^6$ and 2. The use of the Schmidt decomposition can imply a huge simplification!

From the Schmidt decomposition we also see that:

$$\boxed{S_1 = S_2 \equiv S_{\mathrm{ent}} = -\sum_{k=1}^{\mathrm{Min}\{d_1,d_2\}} \rho_k \,\ln \rho_k}$$

Von Neumann entropies corresponding to both subsystems 1 & 2 are equal, expressing information on the mutual entanglement of both subsystems in the full state $|\Psi\rangle$, which was lost in the transition from $|\Psi\rangle$ to $\hat{\rho}_1$ & $\hat{\rho}_2$. The entropy S_{ent} (Boltzmann const. $= 1$ here) is called the **entanglement entropy** and quantifies the amount of entanglement involved in the given **pure state** $|\Psi\rangle$.

Example: $\mathcal{H}_1$ basis $\equiv \{|\uparrow\rangle, |\downarrow\rangle\}$ $\mathcal{H}_2$ basis $\equiv \{|1\rangle, |2\rangle, |3\rangle\}$

$$|\Psi\rangle = \tfrac{1}{\sqrt{6}}\left[|\uparrow\rangle_1|1\rangle_2 + |\uparrow\rangle_1|2\rangle_2 + |\uparrow\rangle_1|3\rangle_2 + \sqrt{2}|\downarrow\rangle_1|1\rangle_2 - \tfrac{1}{\sqrt{2}}|\downarrow\rangle_1|2\rangle_2 - \tfrac{1}{\sqrt{2}}|\downarrow\rangle_1|3\rangle_2\right]$$

$$= \underbrace{\sqrt{\tfrac{1}{2}}}_{\sqrt{\rho_1}}\,\underbrace{|\uparrow\rangle_1}_{|\chi_{11}\rangle}\,\underbrace{\tfrac{1}{\sqrt{3}}\left[|1\rangle_2 + |2\rangle_2 + |3\rangle_2\right]}_{|\chi_{21}\rangle} + \underbrace{\sqrt{\tfrac{1}{2}}}_{\sqrt{\rho_2}}\,\underbrace{|\downarrow\rangle_1}_{|\chi_{12}\rangle}\,\underbrace{\tfrac{1}{\sqrt{3}}\left[\sqrt{2}|1\rangle_2 - \tfrac{1}{\sqrt{2}}|2\rangle_2 - \tfrac{1}{\sqrt{2}}|3\rangle_2\right]}_{|\chi_{22}\rangle}$$

$$\hat{\rho}_1 = \tfrac{1}{2}|\chi_{11}\rangle\langle\chi_{11}| + \tfrac{1}{2}|\chi_{12}\rangle\langle\chi_{12}|, \quad \hat{\rho}_2 = \tfrac{1}{2}|\chi_{21}\rangle\langle\chi_{21}| + \tfrac{1}{2}|\chi_{22}\rangle\langle\chi_{22}| + 0|\chi_\perp\rangle\langle\chi_\perp|$$

◀ Historical remark
1907: E. Schmidt formulates the decomposition theorem (in theory of integral eqs.)

■ Evolution of density operator

The density operator in general depends on time. The form of this dynamics can be easily deduced from the evolution of individual states in $\mathcal{H}$. However, we come to an essential point here: There is a fundamental difference between the evolutions of density operators for closed and open systems! The density operator of a *closed system* undergoes just a continuous unitary transformation by ordinary evolution operator. This implies a fully reversible picture of dynamics. In contrast, the evolution of a reduced density operator associated with an *open system* is more complicated. Since the environment in general

interacts with the system, one cannot write its dynamical equation in an autonomous way (i.e., just in terms of the system's degrees of freedom). This is the place where irreversibility enters the physical description!

► **Evolution of a closed system**

Consider density operator in the form given by an initial set of state vectors. Evolution of the density operator determined by evolution of individual vectors:

$$\begin{array}{ccc} \text{initial state} & & \text{evolved state} \\ \hat\rho(0)=\sum_k \mathfrak{p}_k|\psi_k\rangle\langle\psi_k| & \xrightarrow{\ t\ } & \hat\rho(t)=\sum_k \mathfrak{p}_k\hat U(t)|\psi_k\rangle\langle\psi_k|\hat U(t)^{-1} \end{array}$$

General evolution:

$$\boxed{\hat\rho(t)=\hat U(t)\hat\rho(0)\hat U(t)^{-1}} \quad \begin{array}{c}\leftarrow \text{operator} \\ \text{forms}\end{array} \quad \begin{array}{c}\text{differential} \\ \rightarrow\end{array} \quad \boxed{i\hbar\tfrac{d}{dt}\hat\rho(t)=[\hat H,\hat\rho(t)]}$$

quantum Liouville equation

► Analogy with the **classical** Liouville equation for a statistical ensemble with the probability distribution $\rho(\vec q,\vec p,t)$ in phase space:

$$\tfrac{d}{dt}\rho(\vec q,\vec p,t)=\sum_i\Big[\tfrac{\partial\rho}{\partial q_i}\underbrace{\tfrac{dq_i}{dt}}_{+\frac{\partial H}{\partial p_i}}+\tfrac{\partial\rho}{\partial p_i}\underbrace{\tfrac{dp_i}{dt}}_{-\frac{\partial H}{\partial q_i}}\Big]+\tfrac{\partial\rho}{\partial t}=0 \quad\Rightarrow\quad \boxed{\tfrac{\partial\rho}{\partial t}=\{H,\rho\}}$$

► Evolution of a closed system does not change traces and entropy:

Unitary transformation $\hat\rho(t)=\hat U(t)\hat\rho(0)\hat U(t)^{-1}=\sum_k \rho_i\underbrace{\hat U(t)|\phi_i\rangle}_{|\phi_i(t)\rangle}\underbrace{\langle\phi_i|\hat U(t)^{-1}}_{\langle\phi_i(t)|}$

$\mathrm{Tr}\,\hat\rho(t)=\mathrm{Tr}\,\hat\rho(0)$ $\quad\Rightarrow\quad$ normalization conserved

$\mathrm{Tr}\,\hat\rho(t)^2=\mathrm{Tr}\,\hat\rho(0)^2$ $\quad\Rightarrow\quad$ any $\{\begin{smallmatrix}\text{pure}\\ \text{mixed}\end{smallmatrix}\}$ state remains a $\{\begin{smallmatrix}\text{pure}\\ \text{mixed}\end{smallmatrix}\}$ state

Eigenvalues ρ_i conserved $\Rightarrow$ **entropy** $\boxed{S_\rho(t)=-k\sum\rho_i\ln\rho_i=S_\rho(0)}=$**const**

► **Evolution of open systems: non-interacting case**

Consider first the case when the system under study and its environment do *not* interact with each other. Below we verify that this effectively coincides with the isolated case, as may be immediately anticipated.

The total Hamiltonian $\boxed{\hat H=\hat H_1\otimes\hat I_2+\hat I_1\otimes\hat H_2}\ \equiv\ \hat H_1+\hat H_2$ consists of two commuting components acting separately on the sybsystem 1 and subsystem 2

$\Rightarrow$ separable evolution $\boxed{\hat U(t)=e^{-i\frac{\hat Ht}{\hbar}}=\hat U_1(t)\otimes\hat U_2(t)}$

$$\left.\begin{array}{l}\hat U_1(t)=e^{-i\frac{\hat H_1t}{\hbar}}\\ \hat U_2(t)=e^{-i\frac{\hat H_2t}{\hbar}}\end{array}\right\}\Rightarrow\left\{\begin{array}{ll}\hat\rho_1(t)=\hat U_1(t)\hat\rho_1(0)\hat U_1(t)^{-1} & i\hbar\frac{d}{dt}\hat\rho_1(t)=[\hat H_1,\hat\rho_1(t)]\\ \hat\rho_2(t)=\hat U_2(t)\hat\rho_2(0)\hat U_2(t)^{-1} & i\hbar\frac{d}{dt}\hat\rho_2(t)=[\hat H_2,\hat\rho_2(t)]\end{array}\right.$$

For an initial pure state $|\Psi(0)\rangle=\sum_i\sqrt{\rho_i}\,|\chi_{1i}\rangle|\chi_{2i}\rangle$

of the whole system 1+2 we get: $|\Psi(t)\rangle=\sum_i\sqrt{\rho_i}\,\overbrace{\hat U_1(t)|\chi_{1i}\rangle}^{|\chi_{1i}(t)\rangle}\overbrace{\hat U_2(t)|\chi_{2i}\rangle}^{|\chi_{2i}(t)\rangle}$

⇒ The entropies of both partial density matrices remain equal and conserved: $\boxed{S_1(t)=S_2(t)=-k\sum_i \rho_i \ln \rho_i = \text{const}}$

⇒ Factorized initial states $|\Psi(0)\rangle = |\psi_1(0)\rangle|\psi_2(0)\rangle$ remain factorized: $|\Psi(t)\rangle = |\psi_1(t)\rangle|\psi_2(t)\rangle$

▶ Evolution of open systems: interacting case

If the system-environment interaction is turned on, the system's evolution becomes qualitatively different. We assume the total Hamiltonian in the form $\boxed{\hat{H} = \hat{H}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{H}_2 + \hat{V}_{12}}$ where $\hat{V}_{12}$ acts irreducibly on $\mathcal{H} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2$. Hence the evolution of the whole system is non-separable: $\boxed{\hat{U}(t) \neq \hat{U}_1(t) \otimes \hat{U}_2(t)}$

A general pure state of 1+2 evolves as $|\Psi(t)\rangle = \sum_{ij} \alpha_{ij}(t)|\phi_{1i}\rangle|\phi_{2j}\rangle$, which in the Schmidt decomposition yields $|\Psi(t)\rangle = \sum_i \sqrt{\rho_i(t)}\,|\chi_{1i}(t)\rangle|\chi_{2i}(t)\rangle$, where the common eigenvalues $\rho_i(t)$ of both partial density matrices vary in time.

⇒ The entropies of both subsystems are the same but vary: $\boxed{S_1(t)=S_2(t)=-k\sum_i \rho_i(t) \ln \rho_i(t) \neq \text{ const}}$

⇒ **non-unitary evolution of partial density matrices** $\hat{\rho}_1(t)$ and $\hat{\rho}_2(t)$, $i\hbar\frac{d}{dt}\hat{\rho}_1(t) - [\hat{H}_1, \hat{\rho}_1(t)] \neq 0 \neq i\hbar\frac{d}{dt}\hat{\rho}_2(t) - [\hat{H}_2, \hat{\rho}_2(t)]$

▶ Decoherence

Assume that the [system ⊗ environment] composite evolves from a *separable* [pure ⊗ general] initial state at t=0: $\underbrace{|\psi\rangle\langle\psi|_1}_{\hat{\rho}_1(0)} \otimes \underbrace{\hat{\rho}_2(0)}_{\text{may be a pure state } |\tilde{\psi}\rangle\langle\tilde{\psi}|_2} = \hat{\rho}_{12}(0) \quad \stackrel{t}{\longrightarrow} \quad \hat{\rho}_{12}(t)$

For $\hat{V}_{12} \neq 0$, the evolved total density operator at $t > 0$ is most probably unfactorizable, $\hat{\rho}_{12}(t) \neq \hat{\rho}_1(t) \otimes \hat{\rho}_2(t)$, and moreover yields the partial density operator $\hat{\rho}_1(t) \equiv \mathrm{Tr}_2\, \hat{\rho}_{12}(t)$ equivalent to a mixed state ⇒ Loss of the system's initial coherence (purity): $\boxed{\text{pure state } \hat{\rho}_1(0) \quad \stackrel{t}{\longrightarrow} \quad \hat{\rho}_1(t) \text{ mixed state}}$

Entropy relations:

$$\underbrace{\overbrace{S_1(0)}^{=0} + \overbrace{S_2(0)}^{\geq 0} + \overbrace{\Delta S(0)}^{=0}}_{S_{12}(0)} = \underbrace{\overbrace{S_1(t)}^{>0} + \overbrace{S_2(t)}^{>0} + \overbrace{\Delta S(t)}^{\neq 0}}_{S_{12}(t)}$$

where the correlation-induced term $\Delta S(t)$ compensates the change of $S_1(t)+S_2(t)$

The decoherence process results from the system's entanglement with environment, which takes place due to their mutual interaction. An increase of the system's entropy can be interpreted as *spreading of information* (quantum correlations) from the system alone to the composite system + environment. Since mixed states often carry semiclassical properties, decoherence usually induces loss of quantum features and emergence of classical behavior (cf. Sec. 8).

Note: The canonical (micro-canonical, grand-canonical) density operators represent equilibrium states resulting from a "generic" and "long-enough" interaction of the system with a "large-enough" environment. The reason why nature prefers these states is their maximal (under given constraints) entropy.

◄ Historical remark
1970: H.Dieter Zeh introduces the concept of environmentally-induced decoherence
1980's-present: intense research of various aspects of decoherence (W. Zurek *et al.*)

6b. EXAMPLES OF STATISTICAL ENSEMBLES

We will briefly present a few applications of the above-outlined theory of quantum statistical ensembles. It is worth emphasizing here that the density operator is not just a superfluous appendix of the quantum formalism, suitable only in some more or less exotic situations. Strictly speaking, hardly any quantum system is perfectly isolated. Almost all systems are embedded in some external environments and hide some effectively "irrelevant" internal degrees of freedom. Therefore, the density operator represents the most fundamental language of quantum theory, while the previously established description based on pure states appears as a mere approximation which holds only in some favorable situations.

■ Harmonic oscillator at nonzero temperature

Let us start with the most familiar system, the ordinary harmonic oscillator. It will be immersed now into a heat bath with temperature $T > 0$. This example has a great historical importance as it indicates the correct quantum solution of a so-called **specific-heat paradox**—the fact that the specific heat of solids gradually vanishes with the temperature going down to absolute zero (despite the equipartition theorem of classical thermodynamics, which predicts that the specific heat should be constant). The same calculation, just in slightly different clothes, applies also to the well-known problem of thermal blackbody radiation, which was historically the first hint of the coming quantum theory.

► Partition function of a 3D oscillator

Energies: $E_{n_1 n_2 n_3} = \sum_{i=1}^{3} \hbar\omega_i \left(n_i + \frac{1}{2}\right) \quad n_i = 0, 1, 2, \ldots$

Partition function: $Z(\beta) = \sum_{\left\{\begin{smallmatrix} n_1 \\ n_2 \\ n_3 \end{smallmatrix}\right\}=0}^{\infty} e^{-\beta E_{n_1 n_2 n_3}} = \prod_{i=1}^{3} \left[e^{-\beta\frac{\hbar\omega_i}{2}} \underbrace{\sum_{n_i=0}^{\infty} e^{-\beta\hbar\omega_i n_i}}_{\frac{1}{1-e^{-\beta\hbar\omega_i}}} \right] = \prod_{i=1}^{3} \frac{e^{-\beta\frac{\hbar\omega_i}{2}}}{1-e^{-\beta\hbar\omega_i}} =$

$$= \prod_{i=1}^{3} \underbrace{\left(e^{+\beta\frac{\hbar\omega_i}{2}} - e^{-\beta\frac{\hbar\omega_i}{2}}\right)^{-1}}_{\left[2\sinh\left(\beta\frac{\hbar\omega_i}{2}\right)\right]^{-1}}$$

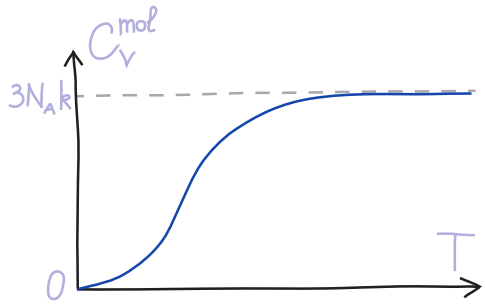
$$\boxed{\ln Z(\beta) = -\sum_{i=1}^{3} \ln\left(e^{+\beta\frac{\hbar\omega_i}{2}} - e^{-\beta\frac{\hbar\omega_i}{2}}\right)}$$

▶ **Specific heat**

We utilize the above-derived formulas:

Energy average: $\langle E\rangle_\beta = -\frac{d}{d\beta}\ln Z(\beta) = \sum_{i=1}^{3}\frac{\hbar\omega_i}{2}\overbrace{\frac{e^{+\beta\frac{\hbar\omega_i}{2}}+e^{-\beta\frac{\hbar\omega_i}{2}}}{e^{+\beta\frac{\hbar\omega_i}{2}}-e^{-\beta\frac{\hbar\omega_i}{2}}}}^{\coth\frac{\beta\hbar\omega_i}{2}}$

Molar specific heat: $c_V^{\rm mol}(\beta) = N_A k\beta^2\frac{d^2}{d\beta^2}\ln Z(\beta) = N_A k\sum_{i=1}^{3}\left(\frac{\beta\hbar\omega_i}{e^{+\beta\frac{\hbar\omega_i}{2}}-e^{-\beta\frac{\hbar\omega_i}{2}}}\right)^2$



High-$T \Rightarrow \beta \ll (\hbar\omega_i)^{-1}$

$$\boxed{c_V^{\rm mol}(T) \approx 3N_A k = \text{const}}$$

classical behavior

Low-$T \Rightarrow \beta \gg (\hbar\omega_i)^{-1}$

$$\boxed{c_V^{\rm mol}(T) \approx N_A k\sum_{i=1}^{3}\left(\frac{\hbar\omega_i}{kT}\right)^2 e^{-\frac{\hbar\omega_i}{kT}} \xrightarrow[T\to 0]{} 0}$$

quantum behavior

◀ **Historical remark**

1907: A. Einstein derives the specific heat formula for a quantized oscillator

■ Coherent superposition vs. statistical mixture

The following example attempts to clarify the difference between a coherent superposition, which is a pure state composed of several components weighted by complex/real *amplitudes*, and a statistical mixture, which is a mixed state involving the same components but just with the respective *probabilities*. We consider states of a single structureless particle.

▶ **Coherent superposition** of states $|\psi_{\rm I}\rangle$ & $|\psi_{\rm II}\rangle$

For a pure state $|\psi\rangle$ with wavefunction $\psi(\vec{x}) \equiv \langle\vec{x}|\psi\rangle$ the density operator $\hat\rho = |\psi\rangle\langle\psi|$ in the coordinate representation is: $\boxed{\langle\vec{x}|\hat\rho|\vec{x}\,'\rangle = \rho(\vec{x},\vec{x}\,') = \psi(\vec{x})\psi^*(\vec{x}\,')}$

For a superposition $\boxed{|\psi\rangle = \alpha|\psi_{\rm I}\rangle + \beta|\psi_{\rm II}\rangle} \equiv \alpha\psi_{\rm I}(\vec{x}) + \beta\psi_{\rm II}(\vec{x})$ we obtain

$$\rho(\vec{x},\vec{x}\,') = [\alpha\psi_{\rm I}(\vec{x}) + \beta\psi_{\rm II}(\vec{x})]\,[\alpha^*\psi_{\rm I}^*(\vec{x}\,') + \beta^*\psi_{\rm II}^*(\vec{x}\,')]$$

Probability distribution: $\rho(\vec{x},\vec{x}) = |\alpha\psi_{\rm I}(\vec{x})|^2 + |\beta\psi_{\rm II}(\vec{x})|^2 + \underbrace{2{\rm Re}\,[\alpha\beta^*\psi_{\rm I}(\vec{x})\psi_{\rm II}^*(\vec{x})]}_{\textbf{interference}}$

▶ **Statistical mixture** $\boxed{\hat\rho = |\alpha|^2|\psi_{\rm I}\rangle\langle\psi_{\rm I}| + |\beta|^2|\psi_{\rm II}\rangle\langle\psi_{\rm II}|}$

$$\rho(\vec{x},\vec{x}\,') = |\alpha|^2\psi_{\rm I}(\vec{x})\psi_{\rm I}^*(\vec{x}\,') + |\beta|^2\psi_{\rm II}(\vec{x})\psi_{\rm II}^*(\vec{x}\,')$$

Probability distribution: $\rho(\vec{x},\vec{x}) = |\alpha\psi_{\rm I}(\vec{x})|^2 + |\beta\psi_{\rm II}(\vec{x})|^2$ **no interference**

▶ **1D example**

(a) Coherent superposition $\boxed{\psi(x) \approx \frac{1}{\sqrt{2}}\delta_\epsilon(x+a) + \frac{1}{\sqrt{2}}\delta_\epsilon(x-a)}$

with $\delta_\epsilon(x\pm a)=\frac{1}{(2\pi\epsilon^2)^{\frac14}}e^{-\frac{(x\pm a)^2}{4\epsilon^2}}$, so that $|\delta_\epsilon(x\pm a)|^2=\frac{1}{\sqrt{2\pi\epsilon^2}}e^{-\frac{(x\pm a)^2}{2\epsilon^2}}$ are Gaussians with averages $\langle x\rangle=\mp a$ and small widths $\epsilon\ll a$ (normalization exact for $\epsilon\to0$)

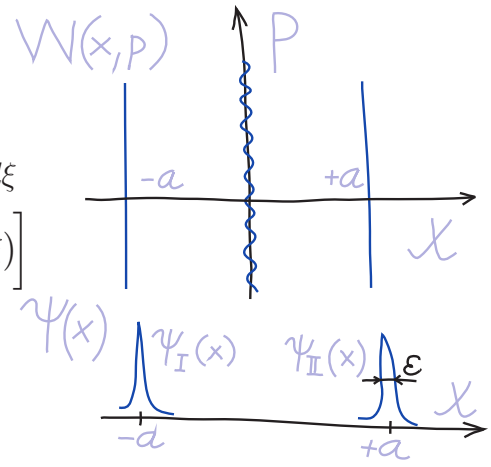
$$\rho(x,x')\approx\tfrac12\big[\delta_\epsilon(x{+}a)\delta_\epsilon(x'{+}a)+\delta_\epsilon(x{-}a)\delta_\epsilon(x'{-}a)+\delta_\epsilon(x{+}a)\delta_\epsilon(x'{-}a)+\delta_\epsilon(x{-}a)\delta_\epsilon(x'{+}a)\big]$$

Probability distribution: $\rho(x,x)\approx \underbrace{\tfrac12\frac{1}{\sqrt{2\pi\epsilon^2}}e^{-\frac{(x+a)^2}{2\epsilon^2}}}_{\to\delta(x+a)}+\underbrace{\tfrac12\frac{1}{\sqrt{2\pi\epsilon^2}}e^{-\frac{(x-a)^2}{2\epsilon^2}}}_{\to\delta(x-a)}+\underbrace{\frac{1}{\sqrt{2\pi\epsilon^2}}e^{-\frac{x^2+a^2}{2\epsilon^2}}}_{\to0\quad\text{for }\epsilon\to0}$

Wigner quasiprobability distribution:

$$W_\rho(x,p)=\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\rho(x+\tfrac{\xi}{2},x-\tfrac{\xi}{2})e^{-\frac{i}{\hbar}\xi p}d\xi$$

$$\approx\frac{1}{2\pi\hbar}\frac{1}{2\sqrt{2\pi\epsilon^2}}\Big[\Big(e^{-\frac{(x+a)^2}{2\epsilon^2}}+e^{-\frac{(x-a)^2}{2\epsilon^2}}\Big)\int_{-\infty}^{+\infty}e^{-\frac{\xi^2}{8\epsilon^2}-\frac{i}{\hbar}\xi p}d\xi$$
$$+e^{-\frac{x^2}{2\epsilon^2}}\Big(\int_{-\infty}^{+\infty}e^{-\frac{(a+\xi/2)^2}{2\epsilon^2}-\frac{i}{\hbar}\xi p}d\xi+\int_{-\infty}^{+\infty}e^{-\frac{(a-\xi/2)^2}{2\epsilon^2}-\frac{i}{\hbar}\xi p}d\xi\Big)\Big]$$



Using the Gaussian integral formula

$$\int_{-\infty}^{+\infty}e^{-(Ax^2+Bx+C)}dx=\sqrt{\tfrac{\pi}{A}}e^{\frac{B^2}{4A}-C}\quad\text{for Re}A{>}0$$

we arrive to:

$$W_\rho(x,p)\approx\frac{1}{2\pi\hbar}\Big(e^{-\frac{(x+a)^2}{2\epsilon^2}}+e^{-\frac{(x-a)^2}{2\epsilon^2}}+2e^{-\frac{x^2}{2\epsilon^2}}\cos\frac{2ap}{\hbar}\Big)e^{-\frac{p^2}{2(\hbar/2\epsilon)^2}}\quad\gtrless0$$

This distribution (satisfying $\iint W_\rho(x,p)\,dx\,dp=1$) consists of two factorized Gaussian peaks of widths $\sigma_x=\epsilon$ and $\sigma_p=\frac{\hbar}{2\epsilon}$ centerred at $(x,p)=(\mp a,0)$ and an oscillatory pattern (taking both positive and negative values) with the same factorized Gaussian envelope centerred at $(x,p)=(0,0)$. The oscillatory pattern does not fade away as $\epsilon\to0$. It indicates the coherence of both components in the superposition state $\psi(x)$.

(b) Statistical mixture $\boxed{\rho(x,x')=\tfrac12\,\delta_\epsilon(x{+}a)\delta_\epsilon(x'{+}a)+\tfrac12\,\delta_\epsilon(x{-}a)\delta_\epsilon(x'{-}a)}$

Probability distribution: $\rho(x,x)\approx\frac12\frac{1}{\sqrt{2\pi\epsilon^2}}e^{-\frac{(x+a)^2}{2\epsilon^2}}+\frac12\frac{1}{\sqrt{2\pi\epsilon^2}}e^{-\frac{(x-a)^2}{2\epsilon^2}}$

Wigner distribution: $W_\rho(x,p)\approx\frac{1}{2\pi\hbar}\Big(e^{-\frac{(x+a)^2}{2\epsilon^2}}+e^{-\frac{(x-a)^2}{2\epsilon^2}}\Big)e^{-\frac{p^2}{2(\hbar/2\epsilon)^2}}\quad\geq0$

(the oscillatory pattern is gone!) can be interpreted as a classical probability density in the phase space. The two components of $\rho(x,x')$ are incoherently mixed and do not interfere.

■ Density operator and decoherence for a two-state system

The rest of this section is devoted to the familiar spin-$\frac12$ system — a qubit. A general pure or mixed state of this system can be visualized in a simple unified way. We examine a qubit in equilibrium with a thermal bath and

illustrate the process of decoherence, which can be generated even by a very gentle interaction with some environment.

▶ Parametrization of general $d = 2$ density matrix

$$\hat{\rho} = \tfrac{1}{2}\left[\hat{I} + \vec{b}\cdot\hat{\vec{\sigma}}\right] = \tfrac{1}{2}\begin{pmatrix} 1+b_3 & b_1 - ib_2 \\ b_1 + ib_2 & 1-b_3 \end{pmatrix}$$

$\vec{b} \equiv (b_1, b_2, b_3)$ is a vector of parameters
$\Rightarrow$ normalization $\mathrm{Tr}\,\hat{\rho} = 1$ satisfied

$$\mathrm{Tr}\,\hat{\rho}^2 = \tfrac{1}{4}\,\mathrm{Tr}\left[\hat{I} + 2(\vec{b}\cdot\hat{\vec{\sigma}}) + \underbrace{(\vec{b}\cdot\hat{\vec{\sigma}})^2}_{|\vec{b}|^2\hat{I}}\right] = \frac{1+|\vec{b}|^2}{2} \begin{cases} = 1 \\ < 1 \end{cases} \text{ for } \begin{array}{ll} |\vec{b}| = 1 & \textbf{pure state} \\ |\vec{b}| < 1 & \textbf{mixed state} \end{array}$$

$$(\vec{b}\cdot\hat{\vec{\sigma}})^2 = \tfrac{1}{2}\sum_{ij} b_i b_j \underbrace{\left(\hat{\sigma}_i\hat{\sigma}_j + \hat{\sigma}_j\hat{\sigma}_i\right)}_{2\delta_{ij}\hat{I}} = |\vec{b}|^2\hat{I}$$

▶ Spin polarization

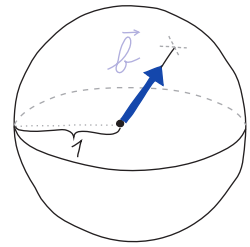
The average values of the 3 spin components:

$$\hat{\vec{S}} \equiv \tfrac{\hbar}{2}\hat{\vec{\sigma}} \quad \Rightarrow \quad \langle S_i\rangle_\rho = \mathrm{Tr}\,(\hat{S}_i\hat{\rho}) = \tfrac{\hbar}{4}\,\mathrm{Tr}\left[\hat{\sigma}_i + (\vec{b}\cdot\hat{\vec{\sigma}})\hat{\sigma}_i\right] = \tfrac{\hbar}{4}\sum_j b_j \overbrace{\mathrm{Tr}(\hat{\sigma}_j\hat{\sigma}_i)}^{2\delta_{ij}} = \tfrac{\hbar}{2}\,b_i$$

$$\boxed{\langle \vec{S}\rangle_\rho = \tfrac{\hbar}{2}\,\vec{b}}$$

average polarization vector

Geometric interpretation with the **Bloch sphere**: mixed states lie inside the sphere, pure states are on the surface.



(cf. the stereographic projection of spin states in Sec. 2b)

▶ Thermal ensemble

General Hamiltonian: $\boxed{\hat{H} = \hbar\omega_0\,\hat{I} + \hbar\,\vec{\omega}\cdot\hat{\vec{\sigma}}}$ with $|\vec{\omega}| \equiv \omega$

To get $e^{-\beta\hat{H}}$, we use the same trick as when calculating the evolution operator (Sec. 5b), but now for imaginary time $t = i\hbar\beta$:

$$e^{-\beta\hat{H}} = e^{-\beta\hbar\omega_0}\sum_{k=0}^{\infty}\frac{(-\beta\hbar\omega)^k}{k!}\left(\frac{\vec{\omega}}{\omega}\cdot\hat{\vec{\sigma}}\right)^k = e^{-\beta\hbar\omega_0}\left[\underbrace{\sum_{k=0,2,4\ldots}\frac{(-\beta\hbar\omega)^k}{k!}}_{\frac{e^{+\beta\hbar\omega}+e^{-\beta\hbar\omega}}{2}}\hat{I} + \underbrace{\sum_{k=1,3,5\ldots}\frac{(-\beta\hbar\omega)^k}{k!}}_{-\frac{e^{+\beta\hbar\omega}-e^{-\beta\hbar\omega}}{2}}\left(\frac{\vec{\omega}}{\omega}\cdot\hat{\vec{\sigma}}\right)\right]$$

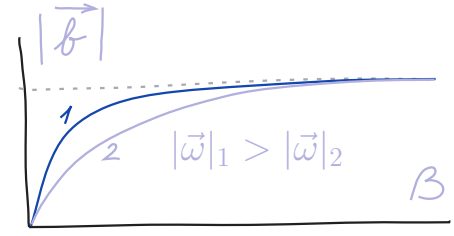
$$= e^{-\beta\hbar\omega_0}\left[\cosh(\beta\hbar\omega)\hat{I} - \sinh(\beta\hbar\omega)\left(\frac{\vec{\omega}}{\omega}\cdot\hat{\vec{\sigma}}\right)\right]$$

The partition function: $\mathrm{Tr}\,e^{-\beta\hat{H}} = \boxed{2e^{-\beta\hbar\omega}\cosh(\beta\hbar\omega) = Z(\beta)}$

The canonical density matrix:

$$\hat{\rho}_\beta = \tfrac{1}{Z(\beta)}e^{-\beta\hat{H}} = \tfrac{1}{2}\left[\hat{I} - \tanh(\beta\hbar\omega)\left(\frac{\vec{\omega}}{\omega}\cdot\hat{\vec{\sigma}}\right)\right]$$

$$\boxed{\vec{b}_\beta = -\tanh(\beta\hbar\omega)\frac{\vec{\omega}}{\omega}}$$



The average spin polarization $\langle\vec{S}\rangle_\beta = \tfrac{\hbar}{2}\,\vec{b}_\beta$ is oriented along the direction of the unit vector $\vec{n} = -\frac{\vec{\omega}}{\omega}$ and with a decreasing temperature $T \to 0$ it increases to the maximal size $\left|\langle\vec{S}\rangle_\beta\right| = \frac{\hbar}{2}$ associated with the (pure) ground state of $\hat{H}$.

▶ Dynamics of qubit coupled to environment

Bases in the spin & environment Hilbert spaces: $\overbrace{\{|\uparrow\rangle,|\downarrow\rangle\}}^{\mathcal{H}_1}\otimes\overbrace{\{|e_i\rangle\}_i}^{\mathcal{H}_2}$

We assume evolution of the qubit-environment system over time t defined by:

$$\boxed{\begin{array}{l}|\uparrow\rangle|e_i\rangle\xrightarrow{t}|\uparrow\rangle|e_{i\uparrow}(t)\rangle\\ |\downarrow\rangle|e_i\rangle\xrightarrow{t}|\downarrow\rangle|e_{i\downarrow}(t)\rangle\end{array}}$$

where $|e_{i\uparrow}(t)\rangle, |e_{i\downarrow}(t)\rangle\in\mathcal{H}_2$ stand for some states of the environment which in general overlap:

$$\langle e_{i\downarrow}(t)|e_{i\uparrow}(t)\rangle\neq 0$$

This represents a rather special evolution, which conserves the z component of spin. So one may think that the influence of the environment on a general pure spin state $|\psi\rangle=\alpha|\uparrow\rangle+\beta|\downarrow\rangle$ should be small. However, as shown below, the evolution quickly changes the above pure state to a mixed one.

Separable initial state:

$$\boxed{\hat\rho_{12}(0)=\underbrace{|\psi\rangle\langle\psi|}_{\hat\rho_1(0)}\otimes\underbrace{\left(\sum_i w_i|e_i\rangle\langle e_i|\right)}_{\hat\rho_2(0)}}$$

$$|\psi\rangle=\alpha|\uparrow\rangle+\beta|\downarrow\rangle$$

$$\boxed{\hat\rho_1(0)=\begin{pmatrix}|\alpha|^2 & \alpha\beta^*\\ \alpha^*\beta & |\beta|^2\end{pmatrix}}$$

Evolution:

$$\hat\rho_{12}(t)=\sum_i w_i\big[|\alpha|^2|e_{i\uparrow}(t)\rangle|\uparrow\rangle\langle\uparrow|\langle e_{i\uparrow}(t)|+\alpha\beta^*|e_{i\uparrow}(t)\rangle|\uparrow\rangle\langle\downarrow|\langle e_{i\downarrow}(t)|+$$
$$\alpha^*\beta|e_{i\downarrow}(t)\rangle|\downarrow\rangle\langle\uparrow|\langle e_{i\uparrow}(t)|+|\beta|^2|e_{i\downarrow}(t)\rangle|\downarrow\rangle\langle\downarrow|\langle e_{i\downarrow}(t)|\big]$$

Evolved spin state:

$$\hat\rho_1(t)=\mathrm{Tr}_2\hat\rho_{12}(t)=$$
$$|\alpha|^2|\uparrow\rangle\langle\uparrow|\underbrace{\left[\sum_{ij}w_i\langle e_j|e_{i\uparrow}(t)\rangle\langle e_{i\uparrow}(t)|e_j\rangle\right]}_{1}+\alpha\beta^*|\uparrow\rangle\langle\downarrow|\underbrace{\left[\sum_{ij}w_i\langle e_j|e_{i\uparrow}(t)\rangle\langle e_{i\downarrow}(t)|e_j\rangle\right]}_{\sum_i w_i\langle e_{i\downarrow}(t)|e_{i\uparrow}(t)\rangle\equiv\ D(t)}$$
$$+\alpha^*\beta|\downarrow\rangle\langle\uparrow|\underbrace{\left[\sum_{ij}w_i\langle e_j|e_{i\downarrow}(t)\rangle\langle e_{i\uparrow}(t)|e_j\rangle\right]}_{\sum_i w_i\langle e_{i\uparrow}(t)|e_{i\downarrow}(t)\rangle\equiv\ D(t)^*}+|\beta|^2|\downarrow\rangle\langle\downarrow|\underbrace{\left[\sum_{ij}w_i\langle e_j|e_{i\downarrow}(t)\rangle\langle e_{i\downarrow}(t)|e_j\rangle\right]}_{1}$$

$$\boxed{\hat\rho_1(t)=\begin{pmatrix}|\alpha|^2 & \alpha\beta^*D(t)\\ \alpha^*\beta D(t)^* & |\beta|^2\end{pmatrix}}\quad\text{where}\quad\boxed{|D(t)|\le\sum_i w_i\overbrace{|\langle e_{i\downarrow}(t)|e_{i\uparrow}(t)\rangle|}^{\le 1}\le 1}$$

▶ Spin decoherence

The evolved spin state is most probably mixed:

$$\mathrm{Tr}\,\hat\rho_1(t)^2=\mathrm{Tr}\begin{pmatrix}|\alpha|^4+|\alpha|^2|\beta|^2|D(t)|^2 & (|\alpha|^2+|\beta|^2)\alpha\beta^*D(t)\\ (|\alpha|^2+|\beta|^2)\alpha^*\beta D(t)^* & |\alpha|^2|\beta|^2|D(t)|^2+|\beta|^4\end{pmatrix}=|\alpha|^4+2|\alpha|^2|\beta|^2|D(t)|^2+|\beta|^4$$
$$=\underbrace{(|\alpha|^2+|\beta|^2)^2}_{1}-\underbrace{\big[1-|D(t)|^2\big]}_{\in[0,1]}\underbrace{2|\alpha|^2|\beta|^2}_{\in[0,1]}\begin{cases}=1 & \text{for } |D(t)|=1 \text{ or } \alpha\beta=0\\ <1 & \text{for } |D(t)|<1 \text{ and } \alpha\beta\neq 0\end{cases}$$

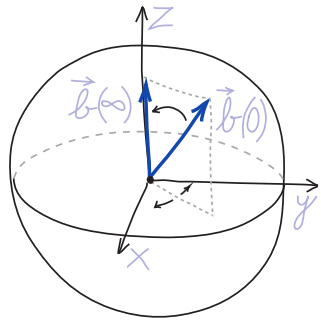
For a large environment, $|D(t)|$ is usually a very *quickly decreasing* function $\Rightarrow$

$$\left.\begin{array}{r}\text{pure state}\\ |\psi\rangle=\alpha|\uparrow\rangle+\beta|\downarrow\rangle\end{array}\right\}\xrightarrow{t}\left\{\begin{array}{l}\text{mixed state, for } t\to\infty:\\ \hat\rho_1=|\alpha|^2|\uparrow\rangle\langle\uparrow|+|\beta|^2|\downarrow\rangle\langle\downarrow|\end{array}\right.$$

This process of changing the coherent superposition of spin $|\uparrow\rangle, |\downarrow\rangle$ states at $t = 0$ to a statistical mixture of these states in asymptotic times represents decoherence of the spin/qubit system. It is caused by the entanglement of the spin with the environment, which records the spin states into almost orthogonal (distinguishable) states of the environment. It is essentially the same situation as in the double-slit experiment when the path of the particle is somehow (anyhow) recorded — the coherence of the particle wavefunction is destroyed and the interference pattern must disappear.

▶ Evolution of polarization vector

Spin initially along direction $\vec{n} = \begin{pmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{pmatrix}$: $|\psi\rangle = \underbrace{\overbrace{e^{-i\varphi}\cos\tfrac{\vartheta}{2}}^{\alpha}|\uparrow\rangle + \overbrace{\sin\tfrac{\vartheta}{2}}^{\beta}|\downarrow\rangle}_{|s_{\vec{n}}=+\frac{\hbar}{2}\rangle}$



The decoherence paramneter: $D(t) = |D(t)|e^{i\chi(t)}$

$$\boxed{\vec{b}(t) = \begin{pmatrix} |D(t)|\sin\vartheta\cos[\varphi - \chi(t)] \\ |D(t)|\sin\vartheta\sin[\varphi - \chi(t)] \\ \cos\vartheta \end{pmatrix}}$$

$\Rightarrow \quad \vec{b}(0) = \vec{n} \quad \overset{t\to\infty}{\longrightarrow} \quad \cos\vartheta\,\vec{n}_z = \vec{b}(\infty)$

dephasing of the xy-projection of $\vec{b}(t)$

7a. QUANTUM MEASUREMENT

Besides spontaneous evolution, described by the nonstationary Schrödinger equation, quantum mechanics assumes also another type of dynamics — a sudden change of the state vector induced by a measurement performed on the system. In contrast to classical physics, where measurements just specify states of the system without essentially disturbing them (in an ideal case, the influence of measurement can be reduced to zero), quantum physics needs a special treatment of measurements. Their impact on the system is irreducible and rather dramatic! This "sector" of QM has quite unusual consequences and is a permanent subject of a vivid debate.

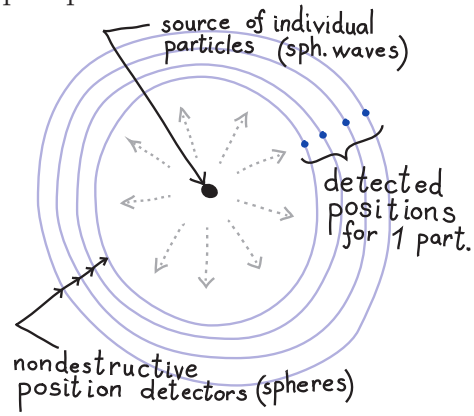
■ State vector reduction

The spontaneous quantum evolution is smooth and deterministic (in the sense of uniqueness of the evolved state vector in the Hilbert space). We may call this motion "**process U**", which emphasizes its unitary character. In contrast, the evolution induced by quantum measurement — at least in the form assumed by conventional quantum theory — is abrupt and indeterministic. Following R. Penrose, we can abbreviate this reduction of the state vector as "**process R**". We have to admit that the exact nature of this process is still partly unclear.

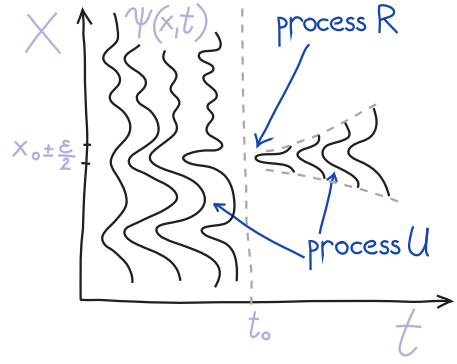
▶ Why do we need process R ?

Without the process R, the theory would not be able to explain correlations of results obtained in **repeated measurements** of the same quantity on the same system. Assume that we measure quantity A twice, first at time t_0 and then at time $t_1 = t_0 + \Delta t$. The conditional probability to measure eigenvalue a_j of $\hat{A}$ at t_1 given the result at t_0 was a_i reads as: $\mathfrak{p}(a_j t_1 | a_i t_0) = \langle \bar{\psi} | \hat{U}^\dagger(\Delta t) \hat{P}_{a_j} \hat{U}(\Delta t) | \bar{\psi} \rangle$, where $|\bar{\psi}\rangle \equiv \{$ state vector immediately after the first measurement. For $\Delta t \to 0$ the second measurement must yield the same outcome as the first one: $\lim_{\Delta t \to 0} \mathfrak{p}(a_j t_1 | a_i t_0) = \delta_{ij}$, so $\boxed{|\bar{\psi}\rangle = |a_i\rangle}$

Example: repeated position measurement on a particle with wavefunction given by an isotropic spherical wave



Sketch of the U and R evolutions for a position measurement:



▶ Measurement postulate

This leads us to the postulate on the instantenous evolution of a general quantum system induced by a measurement of an arbitrary observable A:

$$|\psi\rangle \xrightarrow{\text{measurement of quantity } A} |\bar{\psi}\rangle \equiv \hat{R}_A|\psi\rangle = \begin{cases} |a_1\rangle & \textit{iff } a_1 \text{ measured, prob. } \mathfrak{p}_\psi(a_1) = \langle\psi|\hat{P}_{a_1}|\psi\rangle \\ |a_2\rangle & \textit{iff } a_2 \text{ measured, prob. } \mathfrak{p}_\psi(a_2) = \langle\psi|\hat{P}_{a_2}|\psi\rangle \\ \vdots & \end{cases}$$

$$\boxed{\hat{R}_A|\psi\rangle \overset{a_i}{=} \frac{1}{\sqrt{\langle\psi|\hat{P}_{a_i}|\psi\rangle}} \hat{P}_{a_i}|\psi\rangle}$$

where $\overset{a_i}{=}$ means conditional equality, which holds *iff* the outcome of the measurement is equal to a_i.

This process is called either the "state vector **reduction**", or more dramatically the "**collapse** of wavefunction". We stress that the term "collapse" does not mean here the "end of wavefunction", but just its instantenous localization to a certain subspace of the Hilbert space. After the measurement, the wavefunction continues its evolution according to ordinary Schrödinger equation.

▶ Properties of the reduction operator $\hat{R}_A$

non-deterministic: one knows only probabilities of possible outputs

non-linear: $\left.\begin{matrix}\hat{R}_A|a_1\rangle=|a_1\rangle\\ \hat{R}_A|a_2\rangle=|a_2\rangle\end{matrix}\right\}$ but $\hat{R}_A\big(\alpha|a_1\rangle+\beta|a_2\rangle\big)=\left\{\begin{matrix}|a_1\rangle\\ |a_2\rangle\end{matrix}\right\}\neq\alpha\hat{R}_A|a_1\rangle+\beta\hat{R}_A|a_2\rangle$

non-unitary: $\left.\begin{matrix}|\psi\rangle=\alpha|a_1\rangle+\beta|a_2\rangle\\ |\psi'\rangle=\alpha'|a_1\rangle+\beta'|a_2\rangle\end{matrix}\right\}\xrightarrow{\hat{R}_A}\left\{\begin{matrix}\langle|a_1\rangle\\ \langle|a_2\rangle\end{matrix}\right.\quad\Rightarrow\quad\underbrace{\langle\psi|\psi'\rangle}_{\text{arbitrary}}\xrightarrow{\hat{R}_A}\underbrace{\langle\bar{\psi}|\bar{\psi}'\rangle}_{0\text{ or }1}$

"**non-local**","**acausal**": $\psi(\vec{x},t)$ collapses simultaneously in the whole space. This indicates that R *in the present form* is not real but only an *effective* process — a shortcut for a so far unknown physics or ontology (see below).

◄ Historical remark

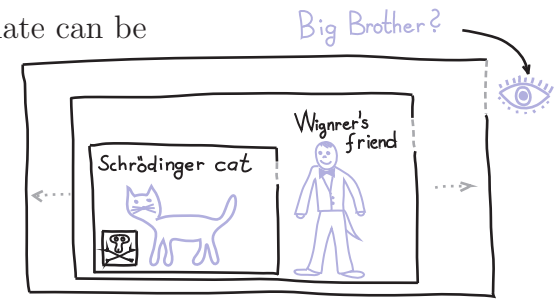
1927: Werner Heisenberg first explicitly considers the wavefunction collapse
1932: John von Neumann includes the reduction postulate into the mathematical formulation of QM and discusses its properties

► The unknown nature of process R

Numerous solutions of the quantum measurement problem (and the emergence of the "classical world") have been proposed, but none of them can be declared as the final answer. We do not aim here at the interpretation issues, so we only briefly outline basic directions in which various interpretations operate:
(a) *Classical answer*: R is an unavoidable and irreducible consequence of interaction between a "quantum system" and a "classical apparatus". This early-day answer is not considered satisfactory as everything is made of quantum constituents: Where ends the quantum domain and starts the classical one?
(b) *Metaphysical answers*: R "happens" on the interface between the quantum world and (human?) consciousness. The hard form of this idea (consciousness having an impact on physical reality) seems inadmissible, but a softer form looks acceptable: the state vector is not the "reality" itself but just a maximal (ultimate?) "information on reality". R captures a sudden change of this information and thus does not have to conform with "materialistic" forms of causality. Another answer of this type was given by the so-called "many-worlds" interpretation, in which the observer, identified with one of the possible recorded observation sequences, becomes a part of the physical description.
(c) *Logical answers*: R is avoided in the very formulation of QM. Example: formulation in terms of the path integral or quantum histories. The notion of state vector, hence also its reduction, is eliminated from the formalism. The theory is considered as a mere "machinery" to compute observable results.
(d) *Physical answers*: R results from a so far unknown, but completely natural process, which happens spontaneously when the "amount of matter" involved in unitary quantum evolution becomes "macroscopic". Examples: spontaneous-localization hypothesis, hypothesis of gravitationally-induced collapse (to be elaborated within the future theory of quantum gravity).

The vagueness of the reduction postulate can be illustrated by the celebrated paradox of **Schrödinger's cat** and its various extensions. The cat is, by a genuinely quantum mechanism (such as a decay of a single unstable nucleus), brought to a superposition state

$$\boxed{|\psi\rangle = \tfrac{1}{\sqrt{2}}|\text{dead}\rangle + \tfrac{1}{\sqrt{2}}|\text{alive}\rangle}$$



If the situation is observed by multiple observers, who of them causes the wavefunction collapse?

◀ Historical remark

1926-9: N. Bohr & W. Heisenberg put cornerstones of "Copenhagen interpretation"
1930's: J. von Neumann & E. Wigner consider consciousness-induced collapse
1935: E. Schrödinger points out oddities of QM description of macroscopic objects
1957: H. Everett proposes the "many-worlds" (relative-state) interpretation
1960's: E. Wigner writes about quantum paradoxes and introduces the "friend"
1980's-90's: attempts to introduce R as a spontaneous process (G.C. Ghirardi *et al.*, R. Penrose) and to explain R from the decoherence theory (W. Zurek)
1990's: attempts to formulate collapse-free QM (R.B. Griffiths, M. Gell-Mann)

■ System–apparatus interaction

We should quickly descend to a more physical level. Let us consider a schematic model of the measurement process, involving a specific interaction between the measured system and any kind of measuring "apparatus". We will see that a correctly performed measurement induces the system–apparatus entanglement expressed in the basis of the measured quantity. Both subsystems are then described by statistical ensembles involving alternative measurement outcomes.

▶ A model of measurement

The measured system S and the instrument I form a pair with the total Hilbert space $\mathcal{H} = \mathcal{H}_\mathrm{S} \otimes \mathcal{H}_\mathrm{I}$. The I space $\overline{\mathcal{H}}_\mathrm{I}$ (within the rigged space) is spanned by continuous position vectors $|x\rangle_\mathrm{I}$ (where x may define a "pointer" position). The S-I interaction is taken in the form $\boxed{\hat{H}_\mathrm{int} = \kappa(\hat{A} \otimes \hat{P})}$ where κ is an interaction strength, $\hat{A}$ is the quantity to be measured on S, with eigenvalues a_i and the corresponding eigenvectors $|a_i\rangle_\mathrm{S}$, and $\hat{P}$ is the momentum operator of I. We neglect self-Hamiltonians of both S & I, and consider an initial factorized state $|\Psi(0)\rangle = \left(\sum_i \alpha_i |a_i\rangle_\mathrm{S}\right) \otimes |x_0\rangle_\mathrm{I}$, where α_i are arbitrary coefficients (normalization assumed) and x_0 is a fixed initial position of I. The evolution leads to:

$$e^{-\frac{i}{\hbar}\hat{H}_\mathrm{int}t}|\Psi(0)\rangle = \sum_i \alpha_i\, |a_i\rangle_\mathrm{S} \otimes \underbrace{\left[e^{-\frac{i}{\hbar}\kappa t a_i \hat{P}}|x_0\rangle_\mathrm{I}\right]}_{\substack{\text{translation} \\ x_0 \to x_0 + \kappa t a_i}} = \boxed{\sum_i \alpha_i\, |a_i\rangle_\mathrm{S} |x_0 + \underbrace{\kappa t a_i}_{\Delta x_i}\rangle_\mathrm{I} = |\Psi(t)\rangle}$$

This is the Schmidt form of an entangled state, therefore both S & I partial density matrices are diagonal in the given bases (see bellow).

► States of the system & apparatus

The state of S & I after the interaction:

$$\hat\rho_{\rm S}(t)={\rm Tr}_{\rm I}|\Psi(t)\rangle\langle\Psi(t)|=\sum_{i,i'}\alpha_i\alpha_{i'}^*|a_i\rangle_{\rm S}\langle a_{i'}|\overbrace{\int dx\,\langle x|x_0{+}\Delta x_i\rangle_{\rm I}\langle x_0{+}\Delta x_{i'}|x\rangle}^{\delta(\Delta x_i-\Delta x_{i'})}$$

$$\hat\rho_{\rm I}(t)={\rm Tr}_{\rm S}|\Psi(t)\rangle\langle\Psi(t)|=\sum_{i,i'}\alpha_i\alpha_{i'}^*\underbrace{\sum_j\langle a_j|a_i\rangle_{\rm S}\langle a_{i'}|a_j\rangle}_{\delta_{ii'}}|x_0{+}\Delta x_i\rangle_{\rm I}\langle x_0{+}\Delta x_{i'}|$$

The resulting reduced density operators

$$\boxed{\hat\rho_{\rm S}(t)=\sum_i|\alpha_i|^2|a_i\rangle_{\rm S}\langle a_i|}\quad\text{and}\quad\boxed{\hat\rho_{\rm I}(t)=\sum_i|\alpha_i|^2|x_0{+}\Delta x_i\rangle_{\rm I}\langle x_0{+}\Delta x_i|}$$

are diagonal in the given bases and express statistical mixtures of all possible orthogonal measurement outcomes with probabilities $|\alpha_i|^2$ corresponding to the expression of the initial state of S. In this formulation of the measurement process, the reduction postulate represents just *drawing one particular state* from the pool of states contained in the statistical mixture $\hat\rho_{\rm S}(t)$ or $\hat\rho_{\rm I}(t)$.

► Imperfect (weak) measurement

Instead of the localized initial state $|x_0\rangle_{\rm I}$ of the instrument in the above model, consider a non-ideal initial state given by a Gaussian wavefunction of width σ, so

$\boxed{\psi_{\rm I}(x)=\frac{1}{(2\pi\sigma^2)^{1/4}}e^{-x^2/4\sigma^2}}$ and the initial state is $|\Psi(0)\rangle=\big(\sum_i\alpha_i|a_i\rangle_{\rm S}\big)\otimes\psi_{\rm I}(x)$

The system S evolves evolves from the state before the measurement

$${\rm Tr}_{\rm I}|\Psi(0)\rangle\langle\Psi(0)|=\sum_{i,i'}\alpha_i\alpha_{i'}^*\,|a_i\rangle_{\rm S}\langle a_{i'}|=\hat\rho_{\rm S}(0)$$

to the state after the measurement:

$${\rm Tr}_{\rm I}|\Psi(t)\rangle\langle\Psi(t)|=\sum_{i,i'}\alpha_i\alpha_{i'}^*\,|a_i\rangle_{\rm S}\langle a_i'|\tfrac{1}{\sqrt{2\pi\sigma^2}}\int dx\,e^{-\frac{(x-\Delta x_i)^2+(x-\Delta x_{i'})^2}{4\sigma^2}}=$$

$$=\ \text{(with the aid of Gaussian integration)}\ =\ \boxed{\sum_{i,i'}\alpha_i\alpha_{i'}^*\,e^{-\frac{1}{2\sigma^2}\left(\frac{\Delta x_i-\Delta x_{i'}}{2}\right)^2}|a_i\rangle_{\rm S}\langle a_{i'}|=\hat\rho_{\rm S}(t)}$$

Limiting cases:

$$\left.\begin{array}{l}\sigma=0\\ \text{ideal measurement}\end{array}\right\}\Rightarrow\ \hat\rho_{\rm S}(t)=\sum_i|\alpha_i|^2|a_i\rangle_{\rm S}\langle a_i|\qquad{\rm Tr}\hat\rho_{\rm S}^2(t)=\sum_i|\alpha_i|^4<1$$

$$\left.\begin{array}{l}\sigma=\infty\\ \text{no measurement}\end{array}\right\}\Rightarrow\ \hat\rho_{\rm S}(t)=\sum_{i,i'}\alpha_i\alpha_{i'}^*\,|a_i\rangle_{\rm S}\langle a_{i'}|=\hat\rho_{\rm S}(0)\quad{\rm Tr}\hat\rho_{\rm S}^2(t)=\big(\sum_i|\alpha_i|^2\big)^2=1$$

The intermediate case $\sigma\in(0,\infty)$ corresponds to a measurement with a limited accuracy (some shifts $\Delta x_i=\kappa t a_i$ of the pointer cannot be distinguished because of the pointer uncertainty σ). The final state $\hat\rho_{\rm S}(t)$ is between the pure initial

state and the maximally damaged (mixed) final state of an ideal measurement, yielding an intermediate purity $\mathrm{Tr}\hat{\rho}_{\mathrm{S}}^2(t)=\sum_{i,i'}|\alpha_i|^2|\alpha_{i'}|^2 e^{-\left(\frac{\Delta x_i-\Delta x_{i'}}{2\sigma}\right)^2}\in\left(\sum_i|\alpha_i|^4,1\right)$.

■ Repeated measurements

Altering considerably the state of a quantum system, the measurement becomes an important constituent of the evolution. We will briefly consider what happens when we measure one or two observables in a quick succession.

► Quantum Zeno effect

Repeated measurements of the same quantity **slow down**, or even completely stop (in the limiting case of infinite measurement frequency) the evolution.

Define a **binary quantity** ("yes/no" outcomes) $\boxed{\hat{A}\equiv 1|\psi\rangle\langle\psi|+0\sum_i|\phi_i^\perp\rangle\langle\phi_i^\perp|}$
where $|\psi\rangle \equiv$ an arbitrary selected state $\in\mathcal{H}$,
$\{|\phi_i^\perp\rangle\}_i \equiv$ a basis in the orthogonal complement $\mathcal{H}_\psi^\perp$ to $|\psi\rangle$ in $\mathcal{H}$.

If the system at $t=0$ is prepared in the state $|\psi(0)\rangle=|\psi\rangle$, the **survival probability** of the spontaneously evolving system for small times t reads as:

$\mathfrak{p}_0(t)=|\langle\psi(0)|\psi(t)\rangle|^2\approx 1-\left(\frac{t}{\tau}\right)^2+\ldots$ where $\tau=\sqrt{\langle\langle E^2\rangle\rangle_\psi}/\hbar$

Periodic measurement of $\hat{A}$ with time interval $\delta t=\frac{t}{n}\to 0$ leads to a modified (larger) survival amplitude:

$$\mathfrak{p}_0'(t)=\left[\mathfrak{p}_0\left(\tfrac{t}{n}\right)\right]^n\approx\left[1-\left(\tfrac{t}{n\tau}\right)^2\right]^n=\overbrace{\left(1-\tfrac{t}{n\tau}\right)^n}^{\to e^{-t/\tau}}\overbrace{\left(1+\tfrac{t}{n\tau}\right)^n}^{\to e^{+t/\tau}}\xrightarrow{n\to\infty}1$$

Note: for an exponential decay, in contrast, the measurement has no effect:

$$\mathfrak{p}_0'(t)=[e^{-\lambda\frac{t}{n}}]^n=e^{-\lambda t}=\mathfrak{p}_0(t)$$

► Description via system–apparatus interaction

Although it seems that the role of the collapse in the quantum Zeno effect is essential, an equivalent result can be obtained in a collapse-free formulation. Assume that at each time $t_k=k\frac{t}{n}$ with $k=1,2,...,n$, the state of the system is measured by an instrument $\mathrm{I}_k\in\{\mathrm{I}_k\}_{k=1}^n$ and recorded in its state $|1\rangle_k$ (intact system) or $|0\rangle_k$ (decayed system). The $\delta t=\frac{t}{n}$ evolution of the system can be written as $\boxed{|\psi\rangle_{\mathrm{S}}\overset{\delta t}{\to}\sqrt{1-\epsilon}\,|\psi\rangle_{\mathrm{S}}+\epsilon\,|\psi_1^\perp\rangle_{\mathrm{S}}}$ where ϵ is a small number and $|\psi_1^\perp\rangle_{\mathrm{S}}$ is a state from the orthogonal complement $\mathcal{H}_\psi^\perp$. We assume $\mathcal{H}_\psi^\perp$ so large that it confines any evolving state for a very long time, so that we can write $|\psi_1^\perp\rangle_{\mathrm{S}}\overset{\delta t}{\to}|\psi_2^\perp\rangle_{\mathrm{S}}\overset{\delta t}{\to}\ldots\overset{\delta t}{\to}|\psi_n^\perp\rangle_{\mathrm{S}}$, with $\{|\psi_k^\perp\rangle_{\mathrm{S}}\}_{k=1}^n$ being a sequence of states in $\mathcal{H}_\psi^\perp$.

$\Rightarrow$ After time t the composite system is in a state:

$$|\Psi(t)\rangle=(1-\epsilon)^{\frac{n}{2}}|\psi\rangle_{\mathrm{S}}\otimes\left(|1\rangle_1...|1\rangle_{n-1}|1\rangle_n\right)_{\mathrm{I}}+(1-\epsilon)^{\frac{n-1}{2}}\epsilon^{\frac{1}{2}}|\psi_1^\perp\rangle_{\mathrm{S}}\otimes\left(|1\rangle_1...|1\rangle_{n-1}|0\rangle_n\right)_{\mathrm{I}}$$
$$+(1-\epsilon)^{\frac{n-2}{2}}\epsilon^{\frac{2}{2}}|\psi_2^\perp\rangle_{\mathrm{S}}\otimes\left(|1\rangle_1...|0\rangle_{n-1}|0\rangle_n\right)_{\mathrm{I}}+\cdots+\epsilon^{\frac{n}{2}}|\psi_n^\perp\rangle_{\mathrm{S}}\otimes\left(|0\rangle_1...|0\rangle_{n-1}|0\rangle_n\right)_{\mathrm{I}}$$

We see that the term recording the measurement history $\left(|1\rangle_1...|1\rangle_{n-1}|1\rangle_n\right)_{\mathrm{I}}$ dominates for small δt, the other terms vanishing in the limit $\delta t\to 0$.

◄ Historical remark
1977: G. Sudarshan & B. Misra theoretically describe the quantum Zeno effect
1989-present: exp. evidences of the measurement-induced slowdown of evolution

► Consecutive measurements of incompatible observables

The reduction postulate has also a striking consequence for measurements of incompatible observables: Statistical distributions of outcomes of successive measurements of such observables depend on the order of measurements.

Measurement of quantities A and B in sequences (A, B) and (B, A) performed at times t_0 and $t_0+\Delta t$ with $\Delta t \to 0$ on an initial state $|\psi(t_0)\rangle \equiv |\psi\rangle$
Joint probabilities of results $A=a$ and $B=b$: $\underbrace{\mathfrak{p}_\psi(a,b)}_{\text{joint}} = \underbrace{\mathfrak{p}_\psi(b|a)}_{\text{conditional}}\, \mathfrak{p}_\psi(a)$

(i) Order A-B: $\mathfrak{p}_\psi^{(AB)}(a,b) = \langle\bar{\psi}|\hat{P}_b|\bar{\psi}\rangle\langle\psi|\hat{P}_a|\psi\rangle$
$= \frac{\langle\psi|\hat{P}_a\hat{P}_b\hat{P}_a|\psi\rangle}{\langle\psi|\hat{P}_a|\psi\rangle}\langle\psi|\hat{P}_a|\psi\rangle = \langle\psi|\hat{P}_a\hat{P}_b\hat{P}_a|\psi\rangle$

(ii) Order B-A: $\mathfrak{p}_\psi^{(BA)}(b,a) = \cdots\cdots\cdots = \langle\psi|\hat{P}_b\hat{P}_a\hat{P}_b|\psi\rangle$

Compatible versus incompatible observables:

$[\hat{A},\hat{B}] = 0 = [\hat{P}_a,\hat{P}_b] \quad \Rightarrow \quad \boxed{\mathfrak{p}_\psi^{(AB)}(a,b) = \mathfrak{p}_\psi^{(BA)}(b,a)}$ order independent

$[\hat{A},\hat{B}] \neq 0 \neq [\hat{P}_a,\hat{P}_b] \quad \Rightarrow \quad \boxed{\mathfrak{p}_\psi^{(AB)}(a,b) \neq \mathfrak{p}_\psi^{(BA)}(b,a)}$ order dependent

Statistical dependence of results
The reduction postulate trivially implies that the results of subsequent A & B measurements are in general statistically dependent. The correlation between results exists for both incompatible and compatible observables.

$$\mathfrak{p}_\psi(a|b) \neq \mathfrak{p}_\psi(a)$$
$$\mathfrak{p}_\psi(b|a) \neq \mathfrak{p}_\psi(b)$$
$$\mathfrak{p}_\psi(a,b) \neq \mathfrak{p}_\psi(a)\mathfrak{p}_\psi(b)$$

■ Measurements on entangled states

A real puzzle arises when we start thinking about the effects of quantum measurements on coupled systems. If such a system is in an entangled state, any local measurement on one of the subsystems can alter the potential outcomes of local measurements on the second subsystem. This is independent of how large is the spatial separation of both subsystems.

► Local measurements on a coupled system

A system composed of two subsystems, with total Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$
Local observables defined separately on both subsystems: $\begin{cases} \hat{A} \equiv \hat{A}_1 \otimes \hat{I}_2 \\ \hat{B} \equiv \hat{I}_1 \otimes \hat{B}_2 \end{cases}$
We trivially have $[\hat{A},\hat{B}] = 0 \quad \Rightarrow$ **compatible observables**

The statistical dependence of the results of subsequent measurements of these local observables appears only for *entangled* states. It generates a possibility to influence subsystem 2 by a local action on 1 and vice versa:

Effect of $\left\{ \begin{array}{c} A \\ B \end{array} \right\}$ measurements in $\mathcal{H}$: $\boxed{\hat{R}_k \propto \left\{ \begin{array}{ll} (\hat{R}_A)_1 \otimes \hat{I}_2 & k=1 \\ \hat{I}_1 \otimes (\hat{R}_B)_2 & k=2 \end{array} \right.}$

Factorized state $\boxed{|\Psi\rangle = |\psi_1\rangle_1 |\psi_2\rangle_2}$ $\Rightarrow$ $\hat{R}_k|\Psi\rangle = \left\{ \begin{array}{ll} |a\rangle_1|\psi_2\rangle_2 & k=1 \\ |\psi_1\rangle_1|b\rangle_2 & k=2 \end{array} \right.$

$\Rightarrow$ measurement on subsystem 1 has no consequence on 2 and vice versa, hence the results are statistically independent

Entangled state $\boxed{|\Psi\rangle = \sum_{i,j} \gamma_{ij} |\phi_i\rangle_1 |\phi_j\rangle_2}$ $\Rightarrow$ $\hat{R}_k|\Psi\rangle = \begin{cases} \mathcal{N}_1 \sum_{ij} \gamma_{ij} \langle a|\phi_i\rangle_1 |a\rangle_1 |\phi_j\rangle_2 & k=1 \\ \mathcal{N}_2 \sum_{ij} \gamma_{ij} \langle b|\phi_j\rangle_2 |\phi_i\rangle_1 |b\rangle_2 & k=2 \end{cases}$

$\mathcal{N}_1 = (\sum_{ii'j} \gamma^*_{ij} \gamma_{i'j} \langle \phi_i|\hat{P}_a|\phi_{i'}\rangle_1)^{-1/2}$ and $\mathcal{N}_2 = \cdots$ are normalization factors

$\Rightarrow$ both measurements change the state from entangled to separable

$\Rightarrow$ measurement on subsystem 1 generally alters probabilities of measurement outcomes for subsystem 2 and vice versa:

Before: $\mathfrak{p}_\Psi(b) = \langle \Psi|\hat{I} \otimes \hat{P}_b|\Psi\rangle = \sum_{ijj'} \gamma^*_{ij} \gamma_{ij'} \langle \phi_j|\hat{P}_b|\phi_{j'}\rangle_2$

After: $\mathfrak{p}_{\hat{R}_1\Psi}(b) = \langle \hat{R}_1\Psi|\hat{I} \otimes \hat{P}_b|\hat{R}_1\Psi\rangle = \mathcal{N}_1^2 \sum_{ii'jj'} \gamma^*_{ij} \gamma_{i'j'} \langle \phi_i|\hat{P}_a|\phi_{i'}\rangle_1 \langle \phi_j|\hat{P}_b|\phi_{j'}\rangle_2 \neq \mathfrak{p}_\Psi(b)$

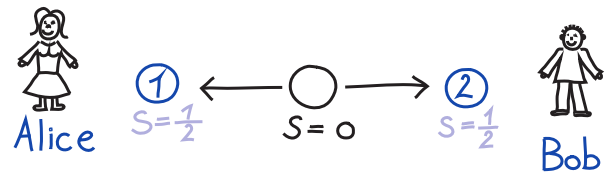
$\Rightarrow$ local measurements on entangled states have **non-local effects!** However, the nature of these effects must prevent any possibility of causality violation.

▶ EPR situation

The paradoxical consequences of measurements on entangled systems were first noticed by Einstein, Podolsky and Rosen, so the corresponding situation is often referred to by the acronym "EPR". The original EPR thought experiment was later reformulated in terms of the **spin singlet state** of an entangled pair of spin-$\frac{1}{2}$ particles. Essentially the same results can be obtained with other types of maximally entangled states, e.g., polarization states of a pair of photons.

$\boxed{|\Psi_{\rm EPR}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2)}$

It is assumed that particle 1 goes to observer A (named Alice) and particle 2 to observer B (named Bob).



Since $|\Psi_{\rm EPR}\rangle$ is the state with total spin $s = 0$ (see Sec. 3b), it may originate from the decay of a spin-0 object to a pair of spin-$\frac{1}{2}$ particles. The $|\Psi_{\rm EPR}\rangle$ state is naturally **invariant under arbitrary rotations** $\hat{R}_{\vec{n}\phi} = \hat{U} \otimes \hat{U}$, where $\hat{U} \equiv \mathbf{S}_{\vec{n}\phi} = \begin{pmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{pmatrix}$ with $\alpha,\beta \equiv$ normalized coefficients:

$\hat{R}_{\vec{n}\phi}|\Psi_{\rm EPR}\rangle = \frac{1}{\sqrt{2}} \Big[\big(\alpha|\Uparrow\rangle_1 + \beta|\Downarrow\rangle_1\big) \big(-\beta^*|\Uparrow\rangle_2 + \alpha^*|\Downarrow\rangle_2\big) - \big(-\beta^*|\Uparrow\rangle_1 + \alpha^*|\Downarrow\rangle_1\big) \big(\alpha|\Uparrow\rangle_2 + \beta|\Downarrow\rangle_2\big) \Big] = \overbrace{(|\alpha|^2 + |\beta|^2)}^{|\alpha|^2+|\beta|^2=1} |\Psi_{\rm EPR}\rangle$

So, we can use any of the infinite number of equivalent expressions:
$|\Psi_{\rm EPR}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2) = \frac{1}{\sqrt{2}}(|\nearrow\rangle_1|\swarrow\rangle_2 - |\swarrow\rangle_1|\nearrow\rangle_2) = \frac{1}{\sqrt{2}}(|\nwarrow\rangle_1|\searrow\rangle_2 - |\searrow\rangle_1|\nwarrow\rangle_2) = \cdots\cdots$

► Local spin measurements

Due to the invariance of $|\Psi_{\rm EPR}\rangle$ under rotations, the *a priori* probabilities of individual spin projections before any measurement are all the same:
$\mathfrak{p}(\uparrow_1) = \mathfrak{p}(\uparrow_2) = \mathfrak{p}(\downarrow_1) = \mathfrak{p}(\downarrow_2) = \mathfrak{p}(\nearrow_1) = \mathfrak{p}(\nearrow_2) = \mathfrak{p}(\swarrow_1) = \mathfrak{p}(\swarrow_2) = \cdots\cdots = \frac{1}{2}$

This changes once Alice makes the measurement on particle 1 in any spin basis:
Alice measures particle 1, e.g., in the basis $\{|\uparrow\rangle_1, |\downarrow\rangle_1\}$:

$$|\Psi_{\rm EPR}\rangle \xrightarrow{\text{Alice}} \hat{R}_1|\Psi_{\rm EPR}\rangle = \begin{cases} |\uparrow\rangle_1|\downarrow\rangle_2 & \textit{iff } \uparrow_1 \text{ measured} \quad \ldots \text{case (a)} \\ |\downarrow\rangle_1|\uparrow\rangle_2 & \textit{iff } \downarrow_1 \text{ measured} \quad \ldots \text{case (b)} \end{cases}$$

Bob then measures particle 2 **in the same basis** $\{|\uparrow\rangle_2, |\downarrow\rangle_2\}$:

$$\begin{bmatrix} \mathfrak{p}(\uparrow_2) \\ \mathfrak{p}(\downarrow_2) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \text{ in case (a)}, \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ in case (b)} \quad \neq \begin{cases} \text{probabilities before} \\ \text{Alices}'\text{s measurement} \end{cases}$$

The same holds for any basis $\{|\nearrow\rangle_1, |\swarrow\rangle_1\}$, $\{|\nwarrow\rangle_1, |\searrow\rangle_1\}$ ... chosen by Alice as long as Bob uses the *same* basis. In fact, **Bob's particle is always polarized** (either up, or down) **in the basis selected by Alice!**

◄ Historical remark

1935: Albert Einstein, Boris Podolsky, Nathan Rosen publish the EPR paper, questioning "completeness" of the quantum description
1951: David Bohm reformulates the "EPR paradox" to the spin language

► Description via density matrices

The reduced density operators of particles 1 & 2 in the entangled state $|\psi_{\rm EPR}\rangle$:

$$\hat{\rho}_1 = {\rm Tr}_2|\Psi_{\rm EPR}\rangle\langle\Psi_{\rm EPR}| = \sum_{\bullet=\uparrow,\downarrow} \tfrac{1}{2}\big(|\uparrow\rangle_1\langle\bullet|\downarrow\rangle_2 - |\downarrow\rangle_1\langle\bullet|\uparrow\rangle_2\big)\big(\langle\downarrow|\bullet\rangle_2\langle\uparrow|_1 - \langle\uparrow|\bullet\rangle_2\langle\downarrow|_1\big)$$
$$= \boxed{\tfrac{1}{2}|\uparrow\rangle_1\langle\uparrow| + \tfrac{1}{2}|\downarrow\rangle_1\langle\downarrow| = \tfrac{1}{2}\hat{I}_1 = \hat{\rho}_1}$$

$$\hat{\rho}_2 = {\rm Tr}_1|\Psi_{\rm EPR}\rangle\langle\Psi_{\rm EPR}| = \sum_{\bullet=\uparrow,\downarrow} \tfrac{1}{2}\big(\langle\bullet|\uparrow\rangle_1|\downarrow\rangle_2 - \langle\bullet|\downarrow\rangle_1|\uparrow\rangle_2\big)\big(\langle\downarrow|_2\langle\uparrow|\bullet\rangle_1 - \langle\uparrow|_2\langle\downarrow|\bullet\rangle_1\big)$$

$\hat{\rho}_1$ & $\hat{\rho}_2$ are obviously invariant under any spin basis transformation.

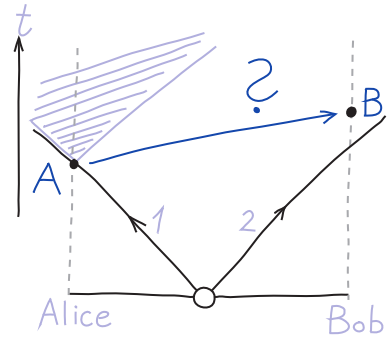
$$= \boxed{\tfrac{1}{2}|\uparrow\rangle_2\langle\uparrow| + \tfrac{1}{2}|\downarrow\rangle_2\langle\downarrow| = \tfrac{1}{2}\hat{I}_2 = \hat{\rho}_2}$$

Let t_0 be the time of the pair emission, t_1 the time of Alice's measurement, and t_2 the time when Bob learns (by some classical means) about Alice's results. In the language of reduced density matrices the evolution is described as follows:

time	particle 1	particle 2	
$t \in [t_0, t_1)$	$\hat{\rho}_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$	$\hat{\rho}_2 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$	quantum uncertainty (Alice & Bob)
$t \in [t_1, t_2)$	$\hat{\rho}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$	$\hat{\rho}_2 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$	purely statistical uncertainty (Bob)
$t \in [t_2, \infty)$	$\hat{\rho}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$	$\hat{\rho}_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ or $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, resp.	

In the first line, the states are those calculated from $|\psi_{\rm EPR}\rangle$. In the second line, Alice already has either the $|\uparrow\rangle_1$ or $|\downarrow\rangle_1$ state, but Bob does not know which one it actually is, so he has to use the density matrix to account for this statistical uncertainty. In the third line, the information about Alice's result arrives to Bob who therefore modifies (in his mind) the state of particle 2 accordingly.

▶ Impossibility of superluminal communication



The fact that the density matrix of particle 2 remains in the basis-invariant form $\hat\rho_2=\frac{1}{2}\hat I_2$ until $t=t_2$ shows that **no local measurement** on particle 2 in time interval $t\in[t_1,t_2)$ can reconstruct the result or the spin basis of Alice's measurement. For instance, imagine that in repeated emissions of particles 1 & 2 in state $|\psi_{\rm EPR}\rangle$ Alice always performs her measurement in the bases $\left\{\begin{smallmatrix}\{|\nearrow\rangle_1,|\swarrow\rangle_1\}\\ \{|\nwarrow\rangle_1,|\searrow\rangle_1\}\end{smallmatrix}\right\}$ to communicate the $\{\begin{smallmatrix}0\\1\end{smallmatrix}\}$ bit value to Bob. The basis used by Alice is indeed imprinted in the state of particle 2, but Bob cannot determine it as both up and down orientations of spin in this basis are equally probable. The situation would change if Bob can somehow make a number of identical copies of the particle-2 state. Having e.g., a sample of $n\gg1$ particles in states $|\swarrow\rangle_2|\swarrow\rangle_3\ldots|\swarrow\rangle_{n+1}$, he would be able to deduce on a high level of certainty that Alice is sending the bit value 0. However, this is not possible!

No-cloning theorem: it is impossible to copy the state vector to more carriers as the ideal "cloning" transformation $|\psi\rangle_1|\bullet\rangle_2\mapsto|\psi\rangle_1|\psi\rangle_2\ \forall|\psi\rangle$ violates linearity:

$$\left.\begin{array}{l}|\psi_a\rangle_1|\phi\rangle_2\mapsto|\psi_a\rangle_1|\psi_a\rangle_2\\ |\psi_b\rangle_1|\phi\rangle_2\mapsto|\psi_b\rangle_1|\psi_b\rangle_2\end{array}\right\}\Rightarrow\underbrace{(\alpha|\psi_a\rangle_1+\beta|\psi_b\rangle_1)}_{|\psi\rangle_1}|\phi\rangle_2\mapsto\underbrace{\alpha|\psi_a\rangle_1|\psi_a\rangle_2+\beta|\psi_b\rangle_1|\psi_b\rangle_2}_{\neq|\psi\rangle_1|\psi\rangle_2}$$

In can be proven rigorously that the **EPR setup cannot be used to send information out of the light cone**. Note that the treatment of the EPR problem would remain the same even within the relativistic QM formulation.

▶ Order of measurements

Alice's and Bob's measurements can be off the light cone. We know that the time order of such events can be reversed by a suitable Lorentz transformation ⇒ In the new frame, Bob can make his measurement (and the state reduction) first. Which picture is true? Both pictures are equivalent as they yield the same probabilities of measurement outcomes. This follows from mutual compatibility of local measurements on subsystems 1 & 2 (see above), which implies independence of the joint probabilities on the succession of measurements.

■ Quantum nonlocality, Bell inequalities

The EPR thought experiment challenges the assumption of locality, which — since the formulation of Einsten's relativity — represents an untouchable ingredient of any ultimate physical theory. From the above explanations it seems that the locality is rescued. Indeed, we saw that even with entangled states and the reduction postulate, the quantum description of EPR-like systems does not allow for superluminal communications and remains local on the operational level. However, there is a subtle consequence of quantum theory which goes *beyond the classical version of locality*. To show this, we use the same EPR setup but allow Alice and Bob to select spin bases of their respective measurements differently, independently from each other. With different spin bases, Alice's and Bob's results are no more strictly anticorrelated. Nevertheless, it turns out that the correlation is stronger than might be expected from any classical consideration satisfying the locality assumption. This subtle type of "nonlocality" is the real mystery of quantum theory.

▶ Hidden variables

Historically, the aim of EPR was to demonstrate incompleteness of QM. A complete theory was assumed to be classical-like ("realistic"), although possibly indeterministic, based on some so far unknown parameters called "hidden variables". Can the entire QM be replaced by a hidden-variable theory? A hidden-variable description of some special situations can be easily developed.

Example: the EPR situation when Alice & Bob perform their measurements in the *same fixed spin basis*, e.g., $\{|\uparrow\rangle, |\downarrow\rangle\}$. At each emission of the pair of particles, a random hidden variable $\kappa = \begin{cases} 0 & \text{probability } 50\% \\ 1 & \text{probability } 50\% \end{cases}$ decides whether the pair is emitted in the state $\uparrow_1\downarrow_2$ (e.g., when $\kappa=0$) or $\downarrow_1\uparrow_2$ (when $\kappa=1$).

A hidden-variable description can be formulated even if the basis is varied but remains the same for both Alice's & Bob's measurement. However, it was shown (see below) that once Alice & Bob are allowed to chose their bases independently, the corresponding hidden-variable theory reproducing the QM predictions would have to be nonlocal.

▶ EPR via hidden variables

We assume a classical-like, but probabilistic description of the EPR situation. Let us introduce all relevant quantities:

(a) **outputs** of Alice's & Bob's measurements: $a,\ \ b \in \{\overbrace{+1}^{\uparrow}, \overbrace{-1}^{\downarrow}\}$

(b) **rotation angles** of Alice's & Bob's spin bases: Φ_A, Φ_B

(c) **hidden variables** sorted to 3 groups:

$\left.\begin{matrix} \alpha \equiv \{\alpha_1 \dots\} \\ \beta \equiv \{\beta_1 \dots\} \end{matrix}\right\}$ related to particles $\left\{\begin{matrix} 1 \\ 2 \end{matrix}\right\}$ and the corresponding measurements,

$\gamma \equiv \{\gamma_1 \dots\}$ related to the emitted pair 1 & 2 as a whole.

Scheme:

$$\left.\begin{matrix}+1\\-1\end{matrix}\right\} = a \quad \overbrace{\underbrace{\boxed{\text{Alice}} \xleftarrow[\text{particle 1}]{} \boxed{\text{EPR source}}}_{\text{hidden variables } \alpha}}^{\text{angle } \Phi_A} \quad \overbrace{\underbrace{\boxed{\text{EPR source}} \xrightarrow[\text{particle 2}]{} \boxed{\text{Bob}}}_{\text{hidden variables } \beta}}^{\text{angle } \Phi_B} \quad b = \left\{\begin{matrix}+1\\-1\end{matrix}\right.$$

$$\text{hidden variables } \gamma$$

Probabilities

Conditional probabilities of outputs
Conditional & apriori probabilities of hidden variables

$$\left.\begin{matrix}\mathfrak{p}_{\Phi_A}(a|\alpha\gamma) & \mathfrak{p}_{\Phi_B}(b|\beta\gamma)\\ \mathfrak{p}_{\Phi_A}(\alpha|\gamma) & \mathfrak{p}_{\Phi_B}(\beta|\gamma)\end{matrix}\right\} \text{ conditional}$$

$$\mathfrak{p}(\gamma) \quad \text{apriori}$$

Here we assume that output a cannot depend on b, β, Φ_B (similarly b cannot depend on a, α, Φ_A), hidden variable α cannot depend on β, Φ_B (similarly β cannot depend on α, Φ_A), and variable γ cannot depend on any other quantity. This follows from the required locality of the hidden-variable description.

▶ Consequences of locality

A less obvious consequence of the required locality is the factorization of the joint probability of outputs a & b:

$$\boxed{\mathfrak{p}_{\Phi_A\Phi_B}(ab|\alpha\beta\gamma) = \mathfrak{p}_{\Phi_A}(a|\alpha\gamma)\mathfrak{p}_{\Phi_B}(b|\beta\gamma)}$$

This follows from statistical independence of variables $\{a, \alpha\}$ on $\{b, \beta\}$ and vice versa, and from no influence of angles $\left\{\begin{matrix}\Phi_A\\ \Phi_B\end{matrix}\right\}$ on probabilities related to $\left\{\begin{matrix}\text{Bob}\\ \text{Alice}\end{matrix}\right\}$:

$$\mathfrak{p}_{\Phi_A\Phi_B}(ab|\alpha\beta\gamma) = \frac{\mathfrak{p}_{\Phi_A\Phi_B}(ab\alpha\beta\gamma)}{\mathfrak{p}_{\Phi_A\Phi_B}(\alpha\beta\gamma)} = \frac{\mathfrak{p}_{\Phi_A\Phi_B}(a|b\alpha\beta\gamma)\mathfrak{p}_{\Phi_A\Phi_B}(b\alpha\beta\gamma)}{\mathfrak{p}_{\Phi_A\Phi_B}(\alpha\beta\gamma)} = \mathfrak{p}_{\Phi_A\cancel{\Phi_B}}(a|\cancel{b}\alpha\beta\gamma)\mathfrak{p}_{\cancel{\Phi_A}\Phi_B}(b|\cancel{a}\alpha\beta\gamma)$$

$\Rightarrow$ For fixed $\{\gamma, \Phi_A, \Phi_B\}$, the average $\langle ab\rangle_{\Phi_A\Phi_B\gamma} = \iint \sum_{a,b=-1}^{+1} ab\, \mathfrak{p}_{\Phi_A\Phi_B}(ab|\alpha\beta\gamma)\, d\alpha\, d\beta$

factorizes: $\boxed{\langle ab\rangle_{\Phi_A\Phi_B\gamma} = \langle a\rangle_{\Phi_A\gamma}\langle b\rangle_{\Phi_B\gamma}}$

Variable γ is out of our control, so we evaluate the observable correlation coefficient between A & B measurement outcomes as $\langle ab\rangle_{\Phi_A\Phi_B} = \int \langle ab\rangle_{\Phi_A\Phi_B\gamma} P(\gamma) d\gamma$

We finally consider the following 4-angle combination of correlation coefficients:

$$\boxed{\mathcal{B}(\Phi_A, \Phi'_A, \Phi_B, \Phi'_B) \equiv \langle ab\rangle_{\Phi_A\Phi_B} + \langle ab\rangle_{\Phi_A\Phi'_B} + \langle ab\rangle_{\Phi'_A\Phi_B} - \langle ab\rangle_{\Phi'_A\Phi'_B}} =$$

$$\int \left[\langle ab\rangle_{\Phi_A\Phi_B\gamma} + \langle ab\rangle_{\Phi_A\Phi'_B\gamma} + \langle ab\rangle_{\Phi'_A\Phi_B\gamma} - \langle ab\rangle_{\Phi'_A\Phi'_B\gamma}\right] \mathfrak{p}(\gamma) d\gamma =$$

$$\int \underbrace{\left[\langle a\rangle_{\Phi_A\gamma}\langle b\rangle_{\Phi_B\gamma} + \langle a\rangle_{\Phi_A\gamma}\langle b\rangle_{\Phi'_B\gamma} + \langle a\rangle_{\Phi'_A\gamma}\langle b\rangle_{\Phi_B\gamma} - \langle a\rangle_{\Phi'_A\gamma}\langle b\rangle_{\Phi'_B\gamma}\right]}_{\in[-2,+2] \quad \Leftarrow \quad \langle a\rangle,\langle b\rangle\in[-1,+1]} \mathfrak{p}(\gamma) d\gamma \in [-2, +2]$$

The last constraint follows from the fact that $xy + xy' + x'y - x'y' \in [-2, +2]$ for $x, x', y, y' \in [-1, +1]$. Hence the locality requirements restrict $\mathcal{B}$ so that

$$\boxed{-2 \le \mathcal{B}(\Phi_A, \Phi'_A, \Phi_B, \Phi'_B) \le +2}$$

Bell inequalities
(one of their forms)

These inequalities represent necessarily conditions to be satisfied by *any local* classical-like theory that aspires to fully describe the EPR experiment.

▶ Quantum factorized states satisfy Bell inequalities

General factorized state $|\Psi\rangle = \underbrace{\big(\alpha|\uparrow\rangle_1 + \alpha'|\downarrow\rangle_1\big)}_{|\varphi\rangle_1}\underbrace{\big(\beta|\uparrow\rangle_2 + \beta'|\downarrow\rangle_2\big)}_{|\chi\rangle_2}$ (with $\alpha,\alpha'\beta,\beta' \equiv$ normalized coefficients)

For this state we have $\langle ab\rangle_{\Phi_A\Phi_B} = \langle\varphi|\hat{A}_{\Phi_A}|\varphi\rangle\langle\chi|\hat{B}_{\Phi_B}|\chi\rangle = \overbrace{\langle a\rangle_{\Phi_A}}^{\in[-1,+1]}\overbrace{\langle b\rangle_{\Phi_B}}^{\in[-1,+1]}$, where $\left\{\begin{smallmatrix}\hat{A}_{\Phi_A}=\hat{U}_{\Phi_A}\hat{\sigma}_z\hat{U}^{-1}_{\Phi_A}\\ \hat{B}_{\Phi_B}=\hat{U}_{\Phi_B}\hat{\sigma}_z\hat{U}^{-1}_{\Phi_B}\end{smallmatrix}\right\}$ is the spin operator of particle $\left\{\begin{smallmatrix}1\\2\end{smallmatrix}\right\}$ in $\left\{\begin{smallmatrix}\text{Alice's}\\ \text{Bob's}\end{smallmatrix}\right\}$ basis.

$\Rightarrow \quad \mathcal{B} = \langle a\rangle_{\Phi_A}\langle b\rangle_{\Phi_B} + \langle a\rangle_{\Phi_A}\langle b\rangle_{\Phi'_B} + \langle a\rangle_{\Phi'_A}\langle b\rangle_{\Phi_B} - \langle a\rangle_{\Phi'_A}\langle b\rangle_{\Phi'_B} \in [-2,+2]$

▶ Quantum entangled states violate Bell inequalities

The average $\langle ab\rangle_{\Phi_A\Phi_B}$ for entangled state like $|\Psi_{\text{EPR}}\rangle$ does *not* factorize!

Spinor transformation between measuring frames (y-axis rotation by $\Phi_\bullet$): $\begin{pmatrix}|\nearrow\rangle_k\\ |\swarrow\rangle_k\end{pmatrix} = \underbrace{\begin{pmatrix}\cos\frac{\Phi_\bullet}{2} & \sin\frac{\Phi_\bullet}{2}\\ -\sin\frac{\Phi_\bullet}{2} & \cos\frac{\Phi_\bullet}{2}\end{pmatrix}}_{\hat{U}_{\Phi_\bullet}}\begin{pmatrix}|\nearrow_{\Phi_\bullet}\rangle_k\\ |\swarrow_{\Phi_\bullet}\rangle_k\end{pmatrix}$ $\begin{smallmatrix}k=1,\bullet=A\\ k=2,\bullet=B\end{smallmatrix}$

The $|\psi_{\text{EPR}}\rangle$ in rotated bases is expressed as:

$$\underbrace{\tfrac{1}{\sqrt{2}}\big(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\big)}_{|\Psi_{\text{EPR}}\rangle} = \underbrace{\tfrac{\sin\frac{\Phi_A}{2}\cos\frac{\Phi_B}{2} - \cos\frac{\Phi_A}{2}\sin\frac{\Phi_B}{2}}{\sqrt{2}}}_{\mathfrak{a}_{++}(\Phi_A,\Phi_B)}\underbrace{|\nearrow_{\Phi_A}\rangle_1|\nearrow_{\Phi_B}\rangle_2}_{ab=+1} + \underbrace{\tfrac{\sin\frac{\Phi_A}{2}\sin\frac{\Phi_B}{2} + \cos\frac{\Phi_A}{2}\cos\frac{\Phi_B}{2}}{\sqrt{2}}}_{\mathfrak{a}_{+-}(\Phi_A,\Phi_B)}$$
$$\times$$
$$\underbrace{|\nearrow_{\Phi_A}\rangle_1|\swarrow_{\Phi_B}\rangle_2}_{ab=-1} + \underbrace{\tfrac{-\sin\frac{\Phi_A}{2}\sin\frac{\Phi_B}{2} - \cos\frac{\Phi_A}{2}\cos\frac{\Phi_B}{2}}{\sqrt{2}}}_{\mathfrak{a}_{-+}(\Phi_A,\Phi_B)}\underbrace{|\swarrow_{\Phi_A}\rangle_1|\nearrow_{\Phi_B}\rangle_2}_{ab=-1} + \underbrace{\tfrac{\sin\frac{\Phi_A}{2}\cos\frac{\Phi_B}{2} - \cos\frac{\Phi_A}{2}\sin\frac{\Phi_B}{2}}{\sqrt{2}}}_{\mathfrak{a}_{--}(\Phi_A,\Phi_B)}\underbrace{|\swarrow_{\Phi_A}\rangle_1|\swarrow_{\Phi_B}\rangle_2}_{ab=+1}$$

$$\langle ab\rangle_{\Phi_A\Phi_B} = |\mathfrak{a}_{++}(\Phi_A,\Phi_B)|^2 - |\mathfrak{a}_{+-}(\Phi_A,\Phi_B)|^2 - |\mathfrak{a}_{-+}(\Phi_A,\Phi_B)|^2 + |\mathfrak{a}_{--}(\Phi_A,\Phi_B)|^2$$
$$= \cdots \text{ with a little push } \cdots = -\cos(\Phi_A - \Phi_B)$$

$$\mathcal{B} = -\cos(\Phi_A - \Phi_B) - \cos(\Phi_A - \Phi'_B) - \cos(\Phi'_A - \Phi_B) + \cos(\Phi'_A - \Phi'_B)$$

$$\boxed{-2\sqrt{2} \le \mathcal{B}(\Phi_A, \Phi'_A, \Phi_B, \Phi'_B) \le +2\sqrt{2}}$$

Bell inequalities violated, replaced by wider "quantum inequalities"

For example, with $\Phi_A = 0°, \Phi'_A = 45°, \Phi_B = 112.5°, \Phi'_B = 67.5°$ we get $\mathcal{B} = +2\sqrt{2}$

$\Rightarrow$ Predictions of QM differ from those of a general local hidden-variable theory

Conclusion: "Quantum nonlocality" does *not* exist in the sense of an *exploitable* superluminal communication. Nevertheless, a trace of nonlocality lies in correlations between Alice's & Bob's results in the generalized EPR situation. These correlations are stronger than possible classical ones if locality is required in the classical description $\Rightarrow$ The following soft form of nonlocality is valid: **Quantum mechanics cannot be replaced by any classical-like local theory!**

◀ Historical remark

1964: John Bell derives the first version of his inequalities
1969: J. Clauser *et al.* derive the most common form of Bell's inequalities
1981: A. Aspect *et al.* provide the first reliable experimental test confirming the violation of Bell's inequalities; discussion continues about potential "loopholes"
1990's-present: many more experimental tests, including "loophole-free" ones

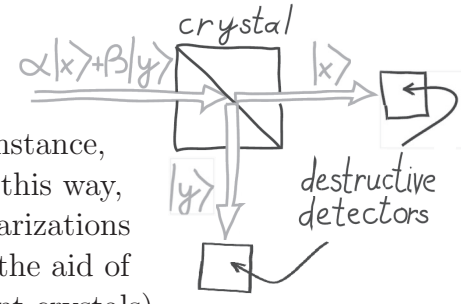
7b. EXAMPLES OF QUANTUM MEASUREMENTS

In the previous section we have introduced the universal process of quantum measurement in a rather abstract, mathematical way. But how can any real measurement of tiny quantum objects be actually performed?

■ Destructive & nondestructive measurements

The collapse postulate, describing what happens with the wavefunction of a quantum system in an ideal measurement, does not apply in all cases. Real measurements often completely destroy the measured object. The cases, when the object is preserved and its wavefunction "collapses", are usually connected with indirect measurements based on the entanglement of the measured system with some other pieces of matter.

▶ Destructive measurements

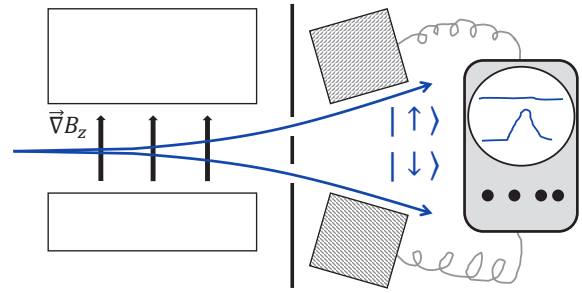


The measured system (a particle) is often destroyed in the measurement process. For instance, the detection of photons goes *almost* always this way, both for the measurements of tracks and polarizations of photons (the latter being performed with the aid of polarizing beam splitters based on birefringent crystals).

▶ Nondestructive measurements

These are most commonly based on an entanglement of the measured system with another system, on which the actual measurement takes place. Examples:
(a) Tracks (positions) of charged particles: These can be detected through the ionization caused by the particle in the surrounding material. Schematically the instantaneous state of the particle + surrounding can be written as:

$$|\Psi\rangle = \int d\vec{x}\ \psi(\vec{x})\ |\,{}^{\text{ionization}}_{\text{around}\,\vec{x}}\,\rangle$$

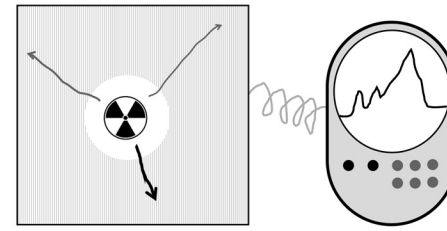


Spin orientations of charged particles can be nondestructively measured using the Stern-Gerlach type of instrument, in which different spin orientations lead to different deflections of the magnetic dipole in inhomogeneous magnetic field. If $\left\{ {}^{\psi_\uparrow(\vec{x})}_{\psi_\downarrow(\vec{x})} \right\}$ is the shifted wavefunction corresponding to $\left\{ {}^{|\uparrow\rangle}_{|\downarrow\rangle} \right\}$ spin-$\frac{1}{2}$ state, we schematically write:

$$|\Psi\rangle = \alpha|\uparrow\rangle \int d\vec{x}\ \psi_\uparrow(\vec{x})\ |\,{}^{\text{ionization}}_{\text{around}\,\vec{x}}\,\rangle + \beta|\downarrow\rangle \int d\vec{x}\ \psi_\downarrow(\vec{x})\ |\,{}^{\text{ionization}}_{\text{around}\,\vec{x}}\,\rangle,$$

where we assume negligible overlap of components $\psi_\uparrow(\vec{x})$ and $\psi_\downarrow(\vec{x})$.

(b) Decay processes: To measure whether the "parent" system (an excited atom, an unstable nucleus or particle...) has decayed to a "daughter" system, we usually detect the emitted particles (photons, α-particles, electrons...).



Schematically, the instantaneous state of the entire system can be written as

$$|\Psi\rangle = \alpha|\psi_{\text{parent}}\rangle|0\rangle + \beta|\psi_{\text{daughter}}\rangle|\chi\rangle,$$

$\left\{\begin{smallmatrix}|0\rangle\\|\chi\rangle\end{smallmatrix}\right\}$ denoting states in the Fock space of decay products with products $\left\{\begin{smallmatrix}\text{absent}\\\text{present}\end{smallmatrix}\right\}$

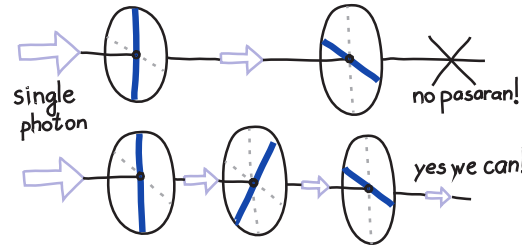
▶ Partially destructive measurements – filters

Another type of measurement arises if the measured system is destroyed only for a certain subset of possible measurement outcomes. Imagine the above example of the photon polarization measurement with one of the destructive detectors removed: Each time when the photon enters the device and there is no signal from the remaining detector, the photon is in the other arm of the beam splitter and has the corresponding polarization.

In general, for this type of measurement we can write

$$\hat{R}_A|\psi\rangle = \begin{cases} \times & \text{probability} = \langle\psi|\hat{P}_{a_1}|\psi\rangle \quad \Rightarrow \text{ result } a_1 \text{ measured} \\ \mathcal{N}(\hat{I}-\hat{P}_{a_1})|\psi\rangle & \text{probability} = 1-\langle\psi|\hat{P}_{a_1}|\psi\rangle \Rightarrow \text{ result } \neq a_1 \text{ deduced} \end{cases}$$

A partially destructive instrument acts as a filter. We stress that a quantum filter changes the state of the system (unlike the classical filter, which only lets some states through). This is illustrated by the **problem of three polarizers**: Two polarization filters with $\varphi = 0°$ & $90°$ stop every photon. The third filter with $\varphi = 45°$ inserted between the two changes the photon polarization state to $|\psi\rangle = \frac{1}{\sqrt{2}}|x\rangle + \frac{1}{\sqrt{2}}|y\rangle$ (see below) and hence enables some photons to pass through the whole device.



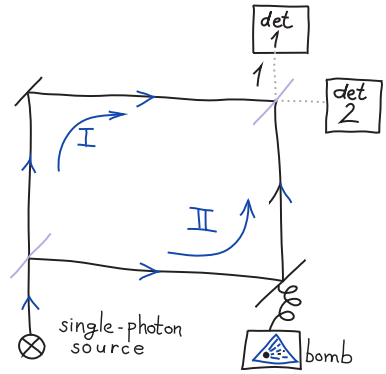
▶ "Interaction-free" measurements

The class of measurements, in which a certain outcome is deduced just from the absence of the measured particle in the branches of the instrument corresponding to the remaining outcomes, is sometimes cast as "interaction-free". Consider a two-path interferometer, in which one of the paths contains the detector. If the detector is silent, the particle is localized on the other path, which prevents the two-path interference from occurring. So once we observe the particle propagating in the forbidden direction, in which the interference

would be destructive, we can say that the *measurement was successful*, but — at the same time — the *particle went along the path with no detector!*

Example: **Bomb testing problem**

Mach-Zehnder photon interferometer: The photon beam is split on the first beam splitter (BS1) to paths I and II, which both after a normal-mirror reflection merge at the second beam splitter (BS2) followed by detectors 1 & 2. A symbolic expression of the evolving photon state reads as:



$$|1\rangle \xrightarrow{\text{BS1}} \tfrac{1}{\sqrt{2}}(|\text{I}\rangle + i|\text{II}\rangle) \xrightarrow{\text{mirrors}} \tfrac{i}{\sqrt{2}}(|\text{I}\rangle + i|\text{II}\rangle) \equiv |\psi\rangle$$

$$\left.\begin{array}{l} |\text{I}\rangle \xrightarrow{\text{BS2}} \tfrac{1}{\sqrt{2}}(|2\rangle + i|1\rangle) \\ |\text{II}\rangle \xrightarrow{\text{BS2}} \tfrac{1}{\sqrt{2}}(|1\rangle + i|2\rangle) \end{array}\right. \text{ with } \left\{\begin{matrix}|1\rangle \\ |2\rangle\end{matrix}\right\} \equiv \text{two exit directions} \Bigg\} \quad \Rightarrow \quad |\psi\rangle \xrightarrow{\text{BS2}} -|1\rangle \equiv |1\rangle.$$

The photon goes only to detector 1, so an interference occurs. Now assume that a bomb with a trigger sensitive to a *single-photon* reflection is placed, e.g., in arm II. The bomb acts as a which-path detector, reducing the photon state as follows: $\frac{1}{\sqrt{2}}(|\text{I}\rangle + i|\text{II}\rangle) \xrightarrow{\hat{R}} \left\{\begin{matrix}|\text{I}\rangle & 50\,\% \\ |\text{II}\rangle & 50\,\%\end{matrix}\right.$. In both cases, the photon can then exit in either of states $\left\{\begin{matrix}|1\rangle \\ |2\rangle\end{matrix}\right\}$. The sequence $|1\rangle \to \cdots \xrightarrow{\hat{R}} |\text{I}\rangle \xrightarrow{\text{BS2}} |2\rangle$ (with probability 25 %) indicates functionality of the bomb *without causing its explosion*! Note that more sophisticated setups have been described in which the efficiency of the "bomb detection" may increase arbitrarily close to 100 %

■ Production & measurement of entangled states

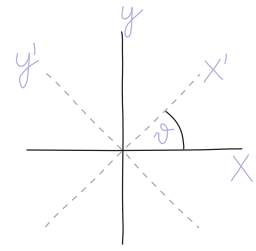
An increasingly important role in QM is played by measurements that are able to distinguish various entangled states of some elementary objects (like qubits). Such measurements are often performed on photons, so we first outline some facts about the photon polarization.

▶ Photon polarization as spin-1 projection

All kinds of light polarization are manifestations of the photon spin $s = 1$. We start from the basis states $\{|x\rangle, |y\rangle\}$ of linear polarization, where the directions $\vec{n}_x \perp \vec{n}_y \perp$ photon flight direction $\vec{n}_c = \frac{\vec{c}}{c}$

Rotated linear polarization basis: $\boxed{\begin{pmatrix}|x'\rangle \\ |y'\rangle\end{pmatrix} = \begin{pmatrix}\cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta\end{pmatrix}\begin{pmatrix}|x\rangle \\ |y\rangle\end{pmatrix}}$

Circular polarization basis: $\boxed{\begin{pmatrix}|L\rangle \\ |R\rangle\end{pmatrix} \equiv \begin{pmatrix}|\to_{\vec{n}_c}\rangle \\ |\leftarrow_{\vec{n}_c}\rangle\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i \\ 1 & +i\end{pmatrix}\begin{pmatrix}|x\rangle \\ |y\rangle\end{pmatrix}}$



Here we introduced spin-1 projection states in the photon flight direction:
$|\rightarrow_{\vec{n}_c}\rangle \equiv |s=1, m_{\vec{n}_c}=+1\rangle$ & $|\leftarrow_{\vec{n}_c}\rangle \equiv |s=1, m_{\vec{n}_c}=-1\rangle$.
Note that state $|s=1, m_{\vec{n}_c}=0\rangle$ does *not* exist for massless ($v=c$) particles.

▶ Bell states

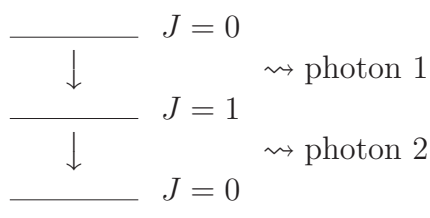
The EPR experiment is most commonly realized not with spin-$\frac{1}{2}$ particles, but with photons, the photon polarization states playing the role of spin-$\frac{1}{2}$ projections. Since the EPR particles represent essentially a pair of qubits, we proceed with the qubit-basis notation $|0\rangle, |1\rangle$. The basis in the 2-qubit Hilbert space can be taken factorized, as well as entangled:

$$\left\{\begin{array}{l} |0\rangle_1|0\rangle_2 \\ |0\rangle_1|1\rangle_2 \\ |1\rangle_2|0\rangle_2 \\ |1\rangle_1|1\rangle_2 \end{array}\right\} \overset{\text{unitary transf. } \hat{U}}{\longrightarrow} \left\{\begin{array}{l} \frac{1}{\sqrt{2}}\left(|0\rangle_1|1\rangle_2 + |1\rangle_1|0\rangle_2\right) \equiv |\Psi^+\rangle \\ \frac{1}{\sqrt{2}}\left(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2\right) \equiv |\Psi^-\rangle \\ \frac{1}{\sqrt{2}}\left(|0\rangle_1|0\rangle_2 + |1\rangle_1|1\rangle_2\right) \equiv |\Phi^+\rangle \\ \frac{1}{\sqrt{2}}\left(|0\rangle_1|0\rangle_2 - |1\rangle_1|1\rangle_2\right) \equiv |\Phi^-\rangle \end{array}\right\} \quad \begin{array}{l}\text{orthonormal} \\ \textbf{Bell basis}\end{array}$$

Bell states show **maximal entanglement** as the entanglement entropy of both partial density matrices for any of these states is maximal $S_1 = S_2 = \ln 2$. The violation of Bell inequalities is the same for any state of the Bell basis.

▶ Production of Bell states

At present, various entangled states of pairs of photons are prepared with the aid of so-called parametric down conversion, which is a nonlinear optical process in some crystals. We mention here an older method based on a two-step cascade of electromagnetic transitions in atoms:



The total angular momentum of both emitted photons must be 0, so the photon spin state is:

$$\frac{1}{\sqrt{2}}\left(|\rightarrow\rangle_1|\leftarrow\rangle_2 + |\leftarrow\rangle_1|\rightarrow\rangle_2\right) =$$
$$= \boxed{\frac{1}{\sqrt{2}}\left(|x\rangle_1|x\rangle_2 + |y\rangle_1|y\rangle_2\right) \equiv |\Phi^+\rangle}$$

▶ Measurement in the Bell basis

The identification of Bell states is equivalent to an ideal measurement of a suitable quantity composed of these states, e.g.:
$\hat{A} = 1|\Psi^+\rangle\langle\Psi^+| + 2|\Psi^-\rangle\langle\Psi^-| + 3|\Phi^+\rangle\langle\Phi^+| + 4|\Phi^-\rangle\langle\Phi^-|$
The problem is that the resolution of all 4 Bell states is possible only with measurements that simultaneously affect both qubits. Alternatively, one can perform an inverse of the above unitary transformation (which involves mutual interaction of both qubits) and perform local measurements on both qubits.

$$\left\{\begin{array}{l} |\Psi^+\rangle \\ |\Psi^-\rangle \\ |\Phi^+\rangle \\ |\Phi^-\rangle \end{array}\right\} \overset{\hat{U}^{-1}}{\longrightarrow} \left\{\begin{array}{l} |0\rangle_1|0\rangle_2 \text{ ... output 1} \\ |0\rangle_1|1\rangle_2 \text{ ... output 2} \\ |1\rangle_1|0\rangle_2 \text{ ... output 3} \\ |1\rangle_1|1\rangle_2 \text{ ... output 4} \end{array}\right\}$$

◀ **Historical remark**
1922.: O. Stern & W. Gerlach perform the first spin-projection measurement
1970-90's: development of techniques to produce photon pairs in entangled states
1993: A. Elitzur & L. Vaidman present the bomb testing problem
1990-present: rapid progress in controlling & measurements of simple quantum systems on various experimental platforms (S. Haroche, D. Wineland, A. Zeilinger...)

8. LINKS BETWEEN QUANTUM AND CLASSICAL

This is a breaking point of our journey. In Secs. 1a–7a we have constructed the basic formalism of quantum theory and in Secs. 1b–7b we have have demonstrated some of its elementary applications. This stage is now finished. Before proceeding to some more complex applications of QM in the forthcoming sections, we need to specify under which circumstances the new quantum description gives rise the familiar classical laws. It turns out that the land on the border between quantum and classical physics contains a rather inaccessible and sometimes hardly passable terrain. Genuinely quantum structures often hide classical roots, and conversely, our classical word has to emerge from purely quantum substrate. I dare to say that the quantum-classical correspondence belongs to the most interesting topics in physics.

■ Classical limit of quantum theory

When quantum dynamics becomes approximately classical? We will see that even for classical-like initial states, which seem to guarantee an almost perfectly classical description of the system, the classical-like dynamics tends to become invalid after a certain finite time (not tremendously long even for really large systems). Quantum-classical correspondence at these time scales can be maintained only due to decoherence — the process in which quantum attributes of the system get lost though interactions with any kind of "environment". The role of decoherence seems really substantial as it is also the main suspect in the matter of selecting the ultimate basis of alternative states in which the classical world emerges. On the other hand, to answer the final question "who selects the actually realized alternative?" is probably only an issue of interpretation, which may forever remain outside the competences of physics.

▶ Singular limit $\hbar \to 0$

A general physical theory can be subject to a limiting procedure: the variation of its essential constant to the limit in which a particular approximate theory takes the reins. Familiar examples are the limits $c \to \infty$ (or $\frac{v}{c} \to 0$), when special relativity changes to classical mechanics, and $N \to \infty$, when statistical physics becomes thermodynamics. It turns out that the limit $\hbar \to 0$ (or

$\frac{\Delta S}{\hbar} \to \infty$), in which quantum mechanics should crossover to classical mechanics, is rather tricky — we may even say singular.

Example I: harmonic-oscillator eigenstates

Classical motion with period $T = \frac{2\pi}{\omega}$ is given by: $x(t) = \underbrace{\sqrt{\frac{2E}{M\omega^2}}}_{x_{\max}(E)} \sin \omega t$

Probability density for finding the oscillator at position x in random time:

$$\rho_{\rm clas}(x)_E dx = \frac{2}{T} \underbrace{\left|\frac{dt}{dx}\right|}_{1/|\dot{x}|} dx = \frac{1}{\pi} \frac{1}{x_{\max}(E)|\cos \omega t|} dx \quad \Rightarrow \quad \boxed{\rho_{\rm clas}(x)_E \equiv \frac{1}{\pi} \frac{1}{\sqrt{x_{\max}(E)^2 - x^2}}}$$

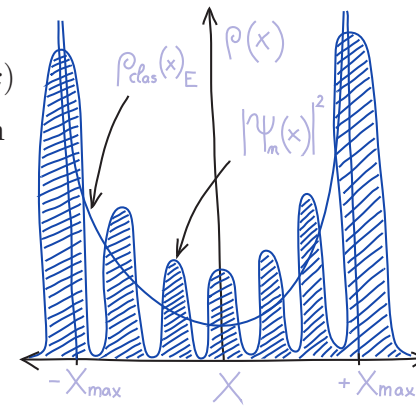
Is there any link to the quantum probability density $\boxed{\rho_{\rm quant}(x)_{E_n} \equiv |\psi_n(x)|^2}$?

To keep $E_n \equiv E = \text{const}$ for $\hbar \to 0$, we need $n \to \infty \quad \Rightarrow$ infinitely dense oscillations of $\psi_n(x)$

We introduce a smoothed quantum distribution

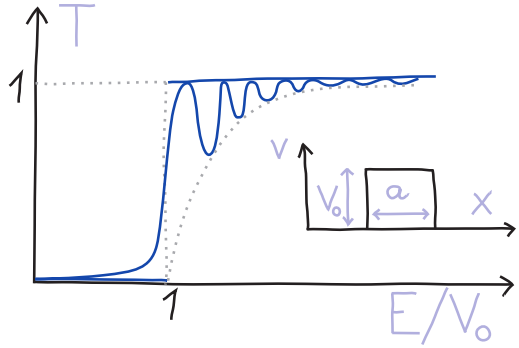
$$\bar{\rho}_{\rm quant}(x)_{E_n} \equiv \frac{1}{dx} \int_{x-\frac{dx}{2}}^{x+\frac{dx}{2}} |\psi_n(x')|^2 dx' \xrightarrow{n\to\infty} \rho_{\rm clas}(x)_E$$

which gets close to the classical one for $n \gg 1$. Therefore, the limit $\hbar \to 0$ reproduces the classical case only if **smoothing** of $|\psi_n(x)|^2$ is performed along with the limiting procedure.



Example II: potential-barrier transmission probability

We consider the square potential barrier of width a and height V_0. The reflection & transmission of quantum waves on this barrier depends on a dimensionless barrier parameter $\gamma = \frac{1}{\hbar}\sqrt{2MV_0a^2}$ and dimensionless energy $\epsilon = \frac{E}{V_0}$. The use of the method of probability currents (see Sec. 5a) yields the quantum transmission coefficient (probability to get to the other side of the barrier):



$$\underbrace{T_{\rm quant}(\epsilon)}_{\mathfrak{p}_{\rm trans}(\epsilon)} = \begin{cases} \frac{1}{1+\frac{1}{4\epsilon(1-\epsilon)}\sinh^2(\gamma\sqrt{1-\epsilon})} & \epsilon < 1 \\ \frac{1}{1+\frac{1}{4\epsilon(\epsilon-1)}\sin^2(\gamma\sqrt{\epsilon-1})} & \epsilon \geq 1 \end{cases}$$

What is the link to the classical transmission coefficient

$$T_{\rm clas}(\epsilon) = \begin{cases} 0 & \epsilon < 1 \\ 1 & \epsilon \geq 1 \end{cases}$$

for $\hbar \to 0 \Rightarrow \gamma \to \infty$?

(a) $\epsilon < 1$: $\lim\limits_{\gamma\to\infty} T_{\rm quant}(\epsilon) = 0 = T_{\rm clas}(\epsilon)$

(b) $\epsilon \geq 1$: $\lim\limits_{\gamma\to\infty} T_{\rm quant}(\epsilon)$ shows infinitely-dense oscillations within the interval $[\frac{1}{1+1/4\epsilon(\epsilon-1)}, 1]$. This is not $T_{\rm clas} = 1$. To get to the classical result, we need **two types of smoothening**:

(i) of the potential: $\bar{V}(x) \equiv \frac{1}{dx}\int_{x-\frac{dx}{2}}^{x+\frac{dx}{2}} V(x')^2 dx'$ (which smooths out the edge),

(ii) of the transmission coefficient: $\bar{T}_{\rm quant}(\epsilon) \equiv \frac{1}{d\epsilon}\int_{\epsilon-\frac{d\epsilon}{2}}^{\epsilon+\frac{d\epsilon}{2}} T_{\rm quant}(\epsilon')d\epsilon'$.

▶ Problem of long times

Limitations of the Ehrenfest theorem: We consider a particle moving in a potential field. The Ehrenfest theorem (see Sec. 5b) seems to guarantee the correspondence between the classical dynamics and the quantum evolution of the average position and momentum for initially well localized wavepackets. A good example are coherent states of the harmonic oscillator, which evolve in close correspondence with classical trajectories. However, for a vast majority of systems, such a correspondence is limited to not too long times. The **spreading of wavepackets** (in almost all potentials) implies that the semiclassical description ceases to apply at times $t \gtrsim \tau_{\rm Q}$, in which the variance of the force across the wavepacket spread becomes comparable with (or larger than) the force average. This leads to a criterion: $\mathrm{Max}_j \left\langle \left| \frac{\partial^2 V}{\partial x_j x_i} \right| \right\rangle_{\psi(\tau_{\rm Q})} \Delta x_j(\tau_{\rm Q}) \approx \left\langle \left| \frac{\partial V}{\partial x_i} \right| \right\rangle_{\psi(\tau_{\rm Q})}$, where $\Delta x_j(\tau_{\rm Q})$ is the spread along direction x_j at $t = \tau_{\rm Q}$.

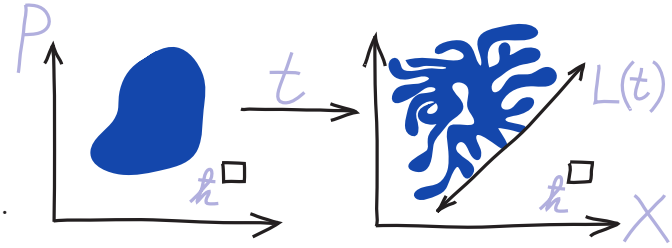
Phase-space description: Consider an initial $t=0$ state of a general system represented by a non-negative Wigner quasiprobability distribution $W(\vec{x},\vec{p},0)$ in the $2f$-dimernsional phase space, equivalent with a classical probability distribution $\rho(\vec{x},\vec{p},0)$. The support $\mathcal{S}_\rho(0)$ of the initial distribution is a simple compact domain of volume $\Omega_\rho(0)$. The semiclassical approximation holds if $W(\vec{x},\vec{p},t)$ evolved by quantum dynamics roughly coincides with $\rho(\vec{x},\vec{p},t)$ evolved by classical dynamics.

$$\begin{array}{ccc} W(\vec{x},\vec{p},0) & \xrightarrow{\text{quantum evolution}} & W(\vec{x},\vec{p},t) \\ \equiv & & \overset{?}{\equiv} \\ \rho(\vec{x},\vec{p},0) & \xrightarrow{\text{classical evolution}} & \rho(\vec{x},\vec{p},t) \end{array}$$

The classical dynamics conserves the *volume*, so $\Omega_\rho(t) = \Omega_\rho(0)$, but makes the *shape* of $\mathcal{S}_\rho(t)$ more and more complicated with increasing time. Its maximal linear size grows typically as $L_\rho(t) \approx L_\rho(0) e^{t/\tau_{\rm chaos}}$, where $\tau_{\rm chaos}^{-1}$ is the maximal Lyapunov exponent characterizing sensitivity of dynamics to initial conditions. Semiclassical behavior ends when **fine structures** of $\mathcal{S}_\rho(t)$ reach the size $\hbar^f$ of the **quantum cells** deduced from the uncertainty principle. A rough estimate of this time:

$$\boxed{\tau_{\rm Q} \approx \tau_{\rm chaos} \ln \frac{\Omega_\rho(0)}{\hbar^f}}$$

At $t \sim \tau_{\rm Q}$, the distribution $W(\vec{x},\vec{p},t)$ develops negative domains $\Rightarrow$ gets non-classical.



▶ The effects of decoherence

Even a maximally isolated system interacts with omnipresent matter (relict radiation, solar photons, dark matter...) or with some internal degrees of freedom is most likely out of control. This has important consequences:

Semiclassical behavior in long times: On the classical level, interactions of the system with some environment show up as **random noise** which prevents the distribution $\rho(\vec{x},\vec{p},t)$ from developing the $\sim\hbar^f$ fine structures. Hence for classical-like initial states, predictions of (a) classical theory with noise and (b) quantum theory with decoherence are usually consistent up to long times.

"Einselection": A quantum system S interacts with some environment E. The total Hilbert space is $\mathcal{H}=\mathcal{H}_{\rm S}\otimes\mathcal{H}_{\rm E}$. Assume a basis $\{|a_k\rangle\}_k$ of $\mathcal{H}_{\rm S}$ formed by eigenvectors of an observable $\hat{A}$ (we neglect possible degeneracies) and a general basis $\{|e_i\rangle\}_i$ of $\mathcal{H}_{\rm E}$. As in the spin example in Sec. 6b, we start from a factorized S+E state $\hat{\rho}(0)$ at $t=0$, in which the system is in a pure state $|\psi\rangle_{\rm S}$, and end in a generally non-separable mixed state $\hat{\rho}(t)$ at $t>0$.

$$\boxed{|\psi\rangle_{\rm S}=\sum_k \alpha_k|a_k\rangle}$$

We assume that the quantity $\hat{A}$ is **conserved** (it commutes with the total Hamiltonian including the S-E interaction), so the evolution of basis states reads as:

$$\boxed{|a_k\rangle|e_i\rangle \xrightarrow{t} |a_k\rangle|e_{ki}(t)\rangle}$$

where $|e_{ki}(t)\rangle$ are some states of the environment.

This leads to the following evolution of the whole S+E system:

$$\hat{\rho}(0)=\underbrace{|\psi\rangle\langle\psi|}_{\sum_{k,k'}\alpha_k\alpha_{k'}^*|a_k\rangle\langle a_{k'}|}\otimes\underbrace{\Big(\sum_i w_i|e_i\rangle\langle e_i|\Big)}_{\hat{\rho}_{\rm E}(0)}\xrightarrow{t}\sum_i w_i\sum_{k,k'}\alpha_k\alpha_{k'}^*|a_k\rangle|e_{ki}(t)\rangle\langle e_{k'i}(t)|\langle a_{k'}|=\hat{\rho}(t)$$

$$\Rightarrow\quad \hat{\rho}_{\rm S}(t)=\mathrm{Tr}_{\rm E}\,\hat{\rho}(t)=\sum_{k,k'}\alpha_k\alpha_{k'}^*\Big(\sum_i w_i\langle e_{k'i}(t)|e_{ki}(t)\rangle\Big)|a_k\rangle\langle a_{k'}|$$

We may assume that for $t>\tau_{\rm decoh}$, where the decoherence time $\tau_{\rm decoh}$ quickly decreases with an increasing size of the environment, we obtain $\langle e_{k'i}(t)|e_{ki}(t)\rangle\approx\delta_{kk'}$ $\forall i$ (the scalar product approximately factorizes to the overlap integrals in all individual degrees of freedom of E). Then we have:

$$\boxed{\hat{\rho}_{\rm S}(t)\approx\sum_k|\alpha_k|^2|a_k\rangle\langle a_k|}$$

$\Rightarrow$ the state of system S expressed in variable a_k is a *classical-like statistical mixture* of alternatives. The basis diagonalizing $\hat{\rho}_{\rm S}(t)$, in which the system becomes classical, is *selected by the S-E interaction*, which conserves $\hat{A}$. This process is sometimes called "einselection", or "environmentally-induced superselection" (of "classical" basis).

◀ Historical remark

1913: N. Bohr discusses the quantum-classical correspondence within the "old QM"
1920's-present: research of various aspects of quasiclassical quantum mechanics
1970's-90's: M. Berry points out the singularity of the $\hbar\to 0$ limit
1970-90's: H.D. Zeh and W. Zurek consider environmentally-induced decoherence as an effective mechanism for quantum-to-classical transition

■ Feynman integral

When the classical trajectories of particles were replaced by quantum wavefunctions, people might believe that trajectories became irretrievably outmoded. However, they returned in all their glory in a later reformulation of quantum theory in terms of path integration. This brilliant approach further elucidates the link between quantum and classical, but also serves as a computational tool for some more advanced problems of quantum theory. Here we just take a little taste of this powerful technique.

► Infinitesimal single-particle propagator

Free-particle propagator: $G_0^+[(\vec{x}+\Delta\vec{x})(t+\Delta t)|\vec{x}t] = \left(\frac{M}{2i\pi\hbar\Delta t}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\overbrace{\frac{M}{2}\frac{(\Delta\vec{x})^2}{\Delta t}}^{\mathcal{L}_0\left(\vec{x},\frac{\Delta\vec{x}}{\Delta t}\right)\Delta t = dS_0}}$

Infinitesimal $\Delta t \to 0$ propagator of **particle in potential** $V(\vec{x})$:

$\mathcal{L}\left(\vec{x},\frac{\Delta\vec{x}}{\Delta t}\right) = \frac{M}{2}\left(\frac{\Delta\vec{x}}{\Delta t}\right)^2 - V(\vec{x})$

$$\boxed{G^+[(\vec{x}+\Delta\vec{x})(t+\Delta t)|\vec{x}t] = \left(\tfrac{M}{2i\pi\hbar\Delta t}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\overbrace{\mathcal{L}\left(\vec{x},\frac{\Delta\vec{x}}{\Delta t}\right)\Delta t}^{dS}}}$$

$$= G_0^+[(\vec{x}+\Delta\vec{x})(t+\Delta t)|\vec{x}t]\; e^{-\frac{i}{\hbar}V(\vec{x})\Delta t} \approx \left(\tfrac{M}{2i\pi\hbar\Delta t}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\frac{M}{2}\frac{(\Delta\vec{x})^2}{\Delta t}} \left[1 - \tfrac{i}{\hbar}V(\vec{x})\Delta t\right]$$

It must be so since the $\Delta t \to 0$ limit of evolution operator factorizes:

$$\hat{U}(\Delta t) = e^{-\frac{i}{\hbar}\left[-\frac{\hbar^2}{2M}\vec{\nabla}^2 + V(\vec{x})\right]\Delta t} \approx \underbrace{e^{-\frac{i}{\hbar}\left[-\frac{\hbar^2}{2M}\vec{\nabla}^2\right]\Delta t}}_{\hat{U}_0(\Delta t)} e^{-\frac{i}{\hbar}V(\vec{x})\Delta t} \quad (\text{from } \left[\hat{T}\Delta t, \hat{V}\Delta t\right] \sim \mathcal{O}(\Delta t^2) \to 0)$$

► Finite single-particle propagator

Since any finite time interval can be split to a sequence of infinitesimal intervals, we can compose a finite-time propagator from the infinitesimal ones. We proceed in the Heisenberg representation, in which the propagator represents the scalar product of time-dependent position eigenvectors: $\boxed{G^+(\vec{x}t|\vec{x}_0t_0) \equiv \langle \vec{x}t|\vec{x}_0t_0\rangle}$

$|\vec{x}t\rangle \equiv$ eigenvector of $\hat{\vec{X}}_{\mathrm{H}}(t)$

$$G^+(\vec{x}t|\vec{x}_0t_0) = \int \overbrace{\langle \vec{x}t|\vec{x}_1t_1\rangle}^{G^+(\vec{x}t|\vec{x}_1t_1)} \overbrace{\langle \vec{x}_1t_1|\vec{x}_0t_0\rangle}^{G^+(\vec{x}_1t_1|\vec{x}_0t_0)} d\vec{x}_1 =$$

$$\int\ldots\int \underbrace{G^+(\vec{x}t|\vec{x}_nt_n)}_{\left(\frac{M}{2i\pi\hbar\Delta t_n}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\mathcal{L}\left(\vec{x}_n,\frac{\Delta\vec{x}_n}{\Delta t_n}\right)\Delta t_n}} \ldots \underbrace{G^+(\vec{x}_{k+1}t_{k+1}|\vec{x}_kt_k)}_{\left(\frac{M}{2i\pi\hbar\Delta t_k}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\mathcal{L}\left(\vec{x}_k,\frac{\Delta\vec{x}_k}{\Delta t_k}\right)\Delta t_k}} \ldots \underbrace{G^+(\vec{x}_1t_1|\vec{x}_0t_0)}_{\left(\frac{M}{2i\pi\hbar\Delta t_0}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\mathcal{L}\left(\vec{x}_0,\frac{\Delta\vec{x}_0}{\Delta t_0}\right)\Delta t_0}} d\vec{x}_n \ldots d\vec{x}_k \ldots d\vec{x}_1$$

Assume $\Delta t_k \equiv \Delta t = \frac{t-t_0}{n+1}$

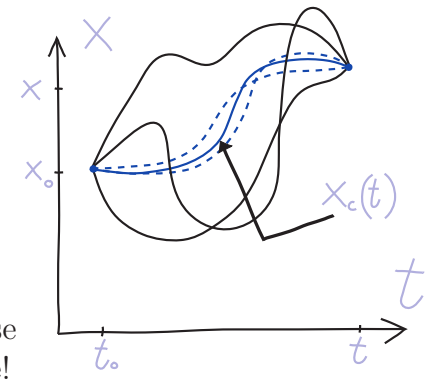
$$\Rightarrow G^+(\vec{x}t|\vec{x}_0t_0) = \overbrace{\int\ldots\int d\vec{x}_n\ldots d\vec{x}_1 \left[\frac{M}{2i\pi\hbar(\Delta t)}\right]^{\frac{3}{2}(n+1)}}^{\overset{n\to\infty}{\longrightarrow} \int \mathcal{D}[\vec{x}(t)]} e^{\frac{i}{\hbar}\overbrace{\sum_{k=0}^{n}\mathcal{L}\left(\vec{x}_k,\frac{\vec{x}_{k+1}-\vec{x}_k}{\Delta t}\right)\Delta t}^{\overset{n\to\infty}{\longrightarrow} \int \mathcal{L}\left(\vec{x},\dot{\vec{x}}\right)dt \;\equiv\; S[\vec{x}(t)]}}$$

$(\vec{x}',t') \equiv (\vec{x}_{n+1},t_{n+1})$

Path integral:

$$\boxed{G^+(\vec{x}t|\vec{x}_0t_0) = \int \mathcal{D}[\vec{x}(t)]\; e^{\frac{i}{\hbar}S[\vec{x}(t)]}}$$

$\equiv$ functional integral over the space of **all possible trajectories** $\vec{x}(t)$ satisfying $\vec{x}(t_0)=\vec{x}_0 \longrightarrow \vec{x}=\vec{x}(t)$



Note: the functional integration is in fact a very complicated procedure, whose technical aspects we do not explore here!

▶ Classical correspondence

The contribution to the functional integral is most significant for trajectories in a vicinity of the **classical trajectory** $\vec{x}_c(t)$, for which $\boxed{\delta S = 0}$ (these trajectories contribute "in phase" while the others tend to cancel each other). This effect in general increases as we approach to the classical limit $\hbar \to 0$.

Example: **free particle**

$$G_0^+(\vec{x}t|\vec{x}_0t_0) = \left[\frac{M}{2\pi i\hbar(t-t_0)}\right]^{\frac{3}{2}} e^{\frac{i}{\hbar}\overbrace{\frac{M}{2}\frac{(\vec{x}-\vec{x}_0)^2}{t-t_0}}^{S_0[\vec{x}_c(t)]}}$$

$\Rightarrow$ non-classical trajectories cancel out perfectly even for $\hbar > 0$

▶ Path-integral formulation of the double-slit interference

To see the path integration in action, we try to apply it to the double-slit experiment from Introduction. Let us stress, however, that the calculations in this and the following paragraphs are rather schematic.

We consider the usual scheme:

$$\text{Emitter } \vec{x}_0 \equiv (\underbrace{-s}_{\to-\infty}, 0) \longrightarrow \text{Slits} \left\{ \begin{array}{l} \vec{x}_A \equiv (0, +\frac{d}{2}) \\ \vec{x}_B \equiv (0, -\frac{d}{2}) \end{array} \right\} \longrightarrow \text{Screen } \vec{x} \equiv (l, y)$$

We assume the initial state ($t\to-\infty$) as a Gaussian wavepacket with average momentum $\vec{p}=(Mv,0)$ and width $\sqrt{\sigma_p}\equiv\Delta p \ll p$. $\Rightarrow$ On the slit plane we get an approximately planar wave with almost a sharp de Broglie wavelength $\lambda_B = \frac{h}{Mv}$.

We divide the trajectories to two disjunct subsets $\{\vec{x}_A(t)\}$ & $\{\vec{x}_B(t)\}$ passing the slits A & B:

$$G^+(\vec{x}t|\vec{x}_0t_0) = \int \mathcal{D}[\vec{x}_A(t)]\; e^{\frac{i}{\hbar}S[\vec{x}_A(t)]} + \int \mathcal{D}[\vec{x}_B(t)]\; e^{\frac{i}{\hbar}S[\vec{x}_B(t)]}$$

Assume that only classical trajectories contribute to almost free propagation:

$$G^+(\vec{x}t|\vec{x}_0t_0) \propto \left[e^{\frac{i}{\hbar}S_A} + e^{\frac{i}{\hbar}S_B}\right] = e^{\frac{i}{\hbar}\frac{S_A+S_B}{2}}\left[e^{+\frac{i}{\hbar}\frac{S_A-S_B}{2}} + e^{-\frac{i}{\hbar}\frac{S_A-S_B}{2}}\right] \propto \cos\tfrac{S_A-S_B}{2\hbar}$$

$$\frac{S_A-S_B}{2\hbar} = \underbrace{\frac{M}{2\hbar}\frac{v_A+v_B}{2}}_{\frac{\pi}{\lambda_B}}\underbrace{\Delta\text{path}}_{\approx\frac{y}{l}d} \Rightarrow \boxed{\rho_{scr}(y) \propto \cos^2\left(\tfrac{\pi}{\lambda_B}\tfrac{d}{l}y\right)} \Rightarrow \Delta y = \tfrac{l}{d}\lambda_B \text{ interval between two minima/maxima}$$

The approximations of Δpath and the constant prefactor are valid only for small y, and the real interference pattern disappears outside a limited domain.

▶ Aharonov-Bohm effect

A bonus of the path-integral treatment of the double-slit experiment is an elegant explanation of the so-called Aharonov-Bohm effect. Consider an ideal electric coil placed in between both slits A & B. The coil is oriented perpendicularly to the plane defined by emitter & both slits, with the section area S. Magnetic flux $\Phi = B_\perp S$ is confined inside the coil. The area S can be made arbitrarily small and the coil can be shielded against the passage of particles, so that the particles have no chance to experience the field $B_\perp$. Yet the field has a strong impact on the interference pattern! The reason for this surprising behavior is that the vector potential, which appears in the Schrödinger equaition, may take nonvanishing values $\vec{A}(\vec{x})\neq 0$ even in the spatial domains, where the field induction vanishes, $\vec{B}(\vec{x})=0$.

For a cylindrical coil of radius R: $\vec{A}(\vec{x}) = \begin{cases} \frac{1}{2}Br\vec{e}_\varphi & r<R \text{ (region of } B\neq 0) \\ \frac{1}{2}BR^2\frac{1}{r}\vec{e}_\varphi & r\geq R \text{ (region of } B=0) \end{cases}$

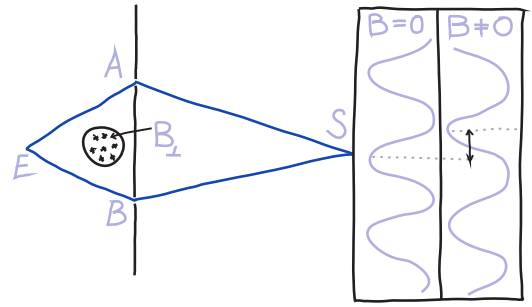
Lagrangian of a charged particle: $\boxed{\mathcal{L}(\vec{x},\dot{\vec{x}}) \longrightarrow \mathcal{L}(\vec{x},\dot{\vec{x}}) + q\dot{\vec{x}}\cdot\vec{A}(\vec{x})}$

$$G^+(\vec{x}t|\vec{x}_0t_0) \propto \left[e^{\frac{i}{\hbar}\left(S_{\rm A}^{(0)}+q\int\limits_{\rm A}\vec{v}_{\rm A}\cdot\vec{A}_{\rm A}dt\right)} + e^{\frac{i}{\hbar}\left(S_{\rm B}^{(0)}+q\int\limits_{\rm B}\vec{v}_{\rm B}\cdot\vec{A}_{\rm B}dt\right)}\right] \propto \cos\left[\frac{1}{\hbar}\left(S_{\rm A}^{(0)}-S_{\rm B}^{(0)}+\frac{q\Phi}{2}\right)\right]$$

where $S_{\rm A}^{(0)}, S_{\rm B}^{(0)}$ are actions for zero field and where we used the relation:

$$\int\limits_{\rm A}\vec{v}_{\rm A}\cdot\vec{A}_{\rm A}\,dt - \int\limits_{\rm B}\vec{v}_{\rm B}\cdot\vec{A}_{\rm B}\,dt = \oint\limits_{\rm AB}\vec{A}\cdot d\vec{x}$$
$$= \int\limits_S(\vec{\nabla}\times\vec{A})\cdot d\vec{S} = B_\perp S = \Phi$$

$$\Rightarrow \boxed{\rho_{\rm scr}(y) \propto \cos^2\left(\frac{\pi}{\lambda_{\rm B}}\frac{d}{l}\,y + \frac{q\Phi}{2\hbar}\right)}$$



The interference pattern is shifted although the particle *cannot enter* the region with $\vec{B}(\vec{x})\neq 0$. So what affects quantum dynamics of charged particles seems to be rather the field of the vector potential $\vec{A}(\vec{x})$ than the field of $\vec{B}(\vec{x})$. Nevertheless, as we saw, the observable shift of the interference pattern depends only on the flux Φ, which is *independent of the gauge*—a particular choice of $\vec{A}(\vec{x})$ consistent with the given $\vec{B}(\vec{x})$.

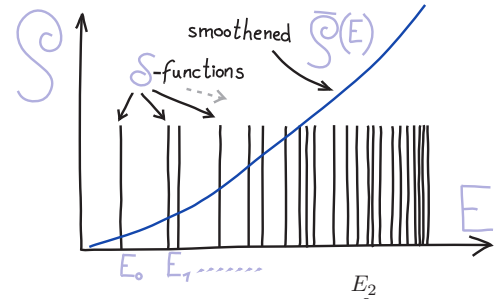
▶ Application of path integral to level density

Despite the quantization of energy in bound quantum systems is considered as a genuinely quantum attribute of such systems, it turns out that the key properties of energy spectra follow from classical dynamics. To show this, we first relate the density of energy spectrum to the evolution operator of the system and then use the Feynman integral.

Level density (cf. Sec. 6a)

$$\boxed{\varrho(E) = \sum_k \delta(E - E_k)}$$

contains complete information on the system's discrete energy spectrum $\{E_k\}$. The unit of $\varrho(E)$ is $(\text{energy})^{-1}$ and the number of levels in any energy interval $[E_1, E_2]$ is given by $N_{[E_1,E_2]} = \int_{E_1}^{E_2} \varrho(E)\, dE$.



The exact level density can be smoothed by any weight function $\delta_\sigma(x) \geq 0$ satisfying $\int \delta_\sigma(x)\, dx = 1$, $\int x\delta_\sigma(x)\, dx = 0$ and $\int x^2\delta_\sigma(x)\, dx = \sigma^2$:

$$\overline{\varrho}_\sigma(E) = \int \delta_\sigma(E - E')\varrho(E')\, dE' = \sum_k \delta_\sigma(E - E_k).$$

If the width $\sigma > \langle E_{k+1} - E_k \rangle$ (average level spacing), the smoothed density $\overline{\varrho}_\sigma(E)$ does not show individual levels but the main trends of the spectrum.

The link to the evolution operator is obvious from the relations:

$$\operatorname{Tr}\hat{U}(t) = \sum_k \langle E_k|\hat{U}(t)|E_k\rangle = \sum_k e^{-\frac{i}{\hbar}E_k t} = \int \varrho(E) e^{-\frac{i}{\hbar}Et} dE \qquad \text{Fourier transformation}$$

$$\varrho(E) = \tfrac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \operatorname{Tr}\hat{U}(t) e^{+\frac{i}{\hbar}Et} dt = \tfrac{1}{\pi\hbar}\operatorname{Re} \int_0^{+\infty} \operatorname{Tr}\hat{U}(t) e^{+\frac{i}{\hbar}Et} dt \qquad \text{inverse Fourier transformation}$$

$$= \tfrac{1}{\pi\hbar}\operatorname{Re} \int_0^{+\infty} \operatorname{Tr}\hat{G}(t) e^{+\frac{i}{\hbar}Et} dt$$

In the $\vec{x}$-representation:

$$\boxed{\varrho(E) = \tfrac{1}{\pi\hbar} \operatorname{Re} \int d\vec{x} \int_0^{+\infty} dt\; G^+(\vec{x}\, t \,|\, \vec{x}\, 0)\; e^{+\frac{i}{\hbar}Et}}$$

$\vec{x} \xrightarrow{t} \vec{x}$ propagator

$\langle \vec{x}|\hat{G}^+(t,0)|\vec{x}\rangle \equiv G^+(\vec{x}t|\vec{x}0)$

$\Rightarrow$ The path integral method for $G^+(\vec{x}t|\vec{x}_0 0)$ can be also used to evaluate $\varrho(E)$

▶ Oscillatory level density via classical periodic orbits

It turns out that the main features of the level density can be determined from **periodic orbits** (the $\vec{x} \xrightarrow{t} \vec{x}$ orbits which also satisfy $\vec{p} \xrightarrow{t} \vec{p}$). While the classical periodic orbits determine the so-called oscillatory component of the level density, the most trivial nonclassical orbits of zero length determine the smooth part of the level density. So we assume a decomposition:

$$\boxed{\varrho(E) \;=\; \underbrace{\overline{\varrho}(E)}_{\text{smooth}} \;+\; \underbrace{\widetilde{\varrho}(E)}_{\text{oscillatory}} \qquad \text{components}}$$

where $\overline{\varrho}(E)$ can approximated by the above $\overline{\varrho}_\sigma(E)$, but is precisely defined by the zero-length orbit calculation below.

The oscillatory component is given in the form of so-called Berry-Tabor (for integrable systems) or Gutzwiller (for chaotic systems) formulas. We do not derive these formulas here, but just give their general form using a sum over all classical periodic orbits of the system:

$$\boxed{\widetilde{\varrho}(E)=\tfrac{1}{\pi\hbar}\sum_{o}\sum_{r=1}^{\infty}\tfrac{\tau_o}{|\boldsymbol{M}_o|}\cos\left[\tfrac{1}{\hbar}\,r S_o(E)+\phi_o\right]}$$

where $\left\{\begin{array}{l} o\equiv \text{ identifier of periodic orbit}\\ r\equiv \text{ number of repetitions of } o\\ \tau_o\equiv \text{ basic time period of } o\\ |\boldsymbol{M}_o|\equiv \text{ a stability measure of } o\\ S_o(E)\equiv \text{ action along } o\\ \phi_o\equiv \text{ a phase connected with } o\end{array}\right.$

For a "cavity" (a compact spatial domain with $V=0$ surrounded by inaccessible complementary domain with $V=\infty$):

$$\tfrac{1}{\hbar}S_o(E)=\tfrac{1}{\hbar}\oint\vec{p}\cdot d\vec{x}=\tfrac{1}{\hbar}\sqrt{2ME}\,l_o=\underbrace{\tfrac{2}{\hbar}\,\tau_o(E)}_{2\pi/\Delta_o(E)}E$$

$\left\{\begin{array}{l} l_o\equiv \text{ geometric length of orbit } o\\ \tau_o(E)\equiv \text{ its time period at energy } E\\ \Delta_o(E)\equiv \text{ variable wavelength of the energy oscillation: } \Delta_o(E)=\tfrac{\pi\hbar}{\tau_o(E)}\end{array}\right.$

$\left.\begin{array}{l}\text{Long } (l_o\gg L)\\ \text{Short } (l_o\approx L)\end{array}\right\}$ periodic orbits ($L\equiv$ cavity linear size) cause $\left\{\begin{array}{l}\text{short}\\ \text{long}\end{array}\right\}$ oscillations of $\varrho(E)$.

Very long orbits, yielding $\Delta_o\lesssim \mathrm{Min}(E_{k+1}-E_k)$, can be cut off. The summed oscillatory density $\widetilde{\varrho}(E)$ typically exhibits "beating patterns" which result from interfering terms caused by several most relevant stable orbits. This generates thickenings & dilutions of energy spectra with respect to the slowly-varying smooth level density. Such phenomena are relevant for the stability of some quantum systems (cf. various shell effects in atoms or metallic clusters).

▶ Smooth level density via zero-length orbits

The smooth level density $\overline{\varrho}(E)$ can be derived from the contribution $G^{+}_{l=0}$ of zero-length orbits to the path-integral expression of $G^{+}(\vec{x}\,t\,|\,\vec{x}\,0)$. For single-particle applications, these "orbits" correspond to the particle remaining at rest, which for nonzero potentials is not a classical behavior.

In the single-particle case we get: $G^{+}_{l=0}(\vec{x}\,t\,|\,\vec{x}\,0)=\lim\limits_{\Delta\vec{x}\to 0}\left(\tfrac{M}{2i\pi\hbar\,t}\right)^{\frac{3}{2}}e^{\frac{i}{\hbar}\left[\frac{M}{2}\frac{\Delta\vec{x}^2}{t}-V(\vec{x})\,t\right]}$

$$\overline{\varrho}(E)=\tfrac{1}{\pi\hbar}\,\mathrm{Re}\left\{\int\limits_0^{+\infty}G^{+}_{l=0}(\vec{x}\,t\,|\,\vec{x}\,0)\;e^{+\frac{i}{\hbar}Et}\;dt\,d\vec{x}\right\}=$$

$$=\tfrac{1}{\pi\hbar}\lim_{\Delta\vec{x}\to 0}\mathrm{Re}\left\{\left(\tfrac{M}{2i\pi\hbar}\right)^{\frac{3}{2}}\int\limits_0^{+\infty}\underbrace{t^{-\frac{3}{2}}\,e^{\frac{i}{\hbar}\left[\frac{M}{2}\frac{\Delta\vec{x}^2}{t}\right]}}_{*}e^{\frac{i}{\hbar}[E-V(\vec{x})]t}\,dt\,d\vec{x}\right\}=\ldots$$

Trick: $\quad *=\left(\tfrac{i}{2\pi\hbar M}\right)^{\frac{3}{2}}\int e^{\frac{i}{\hbar}\left[\vec{p}\cdot\Delta\vec{x}-\frac{\vec{p}^2}{2M}\,t\right]}d\vec{p}\qquad$ (Gaussian integral)

$$\cdots=\tfrac{1}{\pi\hbar}\tfrac{1}{(2\pi\hbar)^3}\lim_{\Delta\vec{x}\to 0}\mathrm{Re}\left\{\iint\limits_0^{+\infty}e^{\frac{i}{\hbar}\left[\vec{p}\cdot\Delta\vec{x}-\frac{\vec{p}^2}{2M}\,t\right]}e^{\frac{i}{\hbar}[E-V(\vec{x})]t}\,dt\,d\vec{x}\,d\vec{p}\right\}$$

$$=\tfrac{1}{(2\pi\hbar)^3}\iint\lim_{\Delta\vec{x}\to 0}\underbrace{\tfrac{1}{\pi\hbar}\mathrm{Re}\left(\int\limits_0^{+\infty}e^{\frac{i}{\hbar}\left[E-\frac{\vec{p}^2}{2M}-V(\vec{x})\right]t}\,dt\right)}_{\delta\left(E-\frac{\vec{p}^2}{2M}-V(\vec{x})\right)}e^{\frac{i}{\hbar}\vec{p}\cdot\Delta\vec{x}}\,d\vec{x}\,d\vec{p}$$

$$\boxed{\overline{\varrho}(E)=\tfrac{1}{(2\pi\hbar)^3}\underbrace{\iint\delta\left[E-\tfrac{\vec{p}^2}{2M}-V(\vec{x})\right]d\vec{x}\,d\vec{p}}_{\frac{d}{dE}\Omega(E)}}$$

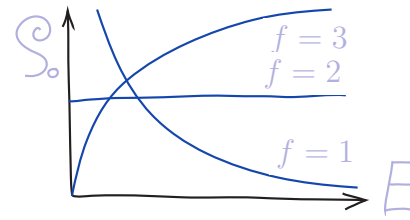
$\Omega(E)\equiv\iint\Theta\left[E-\tfrac{\vec{p}^2}{2M}-V(\vec{x})\right]d\vec{x}\,d\vec{p}$
$\equiv$ phase-space volume available for a particle with $\tfrac{\vec{p}^2}{2M}+V(\vec{x})\le E$

Example: **"Cavities" of general dimension** $f = \begin{cases} 1 \ldots \textbf{1D infinite square well} \\ 2 \ldots \textbf{2D billiard} \\ 3 \ldots \textbf{3D cavity} \end{cases}$

$$\frac{d}{dE}\Omega(E) = \iint \delta\left[E - \frac{\vec{p}^2}{2M}\right] d\vec{x}\, d\vec{p} = \underbrace{V_f}_{\substack{\text{space} \\ \text{volume}}} \int\int \underbrace{\delta\left[E - \frac{p^2}{2M}\right]}_{\frac{M}{p_0}\delta(p-p_0)} p^{f-1} dp \underbrace{f(\theta) d\theta}_{\substack{\text{polar/spher.} \\ \text{angle(s)}}} = V_f \frac{M}{p_0} \underbrace{S_f p_0^{f-1}}_{\substack{\text{sphere} \\ \text{surface}}}$$

$$p_0 = \sqrt{2ME}$$

$$\boxed{\overline{\varrho}(E) \propto E^{\frac{f-2}{2}} = \begin{cases} E^{-1/2} & f=1 \\ E^{0} & f=2 \\ E^{+1/2} & f=3 \end{cases}}$$



An analogous result, a generalized **Weyl formula**, is valid for general systems with $2f$-dimensional phase space (e.g., N-particle systems with $f = 3N$):

$$\boxed{\overline{\varrho}(E) = \frac{1}{(2\pi\hbar)^f} \frac{d}{dE}\Omega(E)}$$

$\Omega(E) \equiv \iint \Theta\left[E - H(\vec{p},\vec{x})\right] d\vec{x}\, d\vec{p}$ $\equiv$ **phase-space volume** available for the system with $H(\vec{p},\vec{x}) \le E$

$\Rightarrow N_{[E_0,E]} = \int_{E_0}^{E} \overline{\varrho}(E)\, dE = \frac{\Omega(E)}{(2\pi\hbar)^f} \equiv$ the phase-space volume for energy $\in [E_0, E]$ in units of the elementary quantum cell given by the uncertainty principle

◀ Historical remark

1912: Hermann Weyl derives a formula for the density of resonances in a cavity
1927-30's: development of semiclassical methods in the level-density evaluation
1948: Richard Feynman presents the path-integral formulation of QM
1959: Yakir Aharonov & David Bohm discover the effect of elmg. potentials in QM
1970's: M. Gutzwiller, M. Berry, M. Tabor *et al.* derive periodic-orbit formulas

■ Semiclassical approximation

Not only that the quantum-classical correspondence represents a problem of fundamental importance, its investigation also yields a class of powerfull approximation techniques. Here we present the so-called WKB theory.

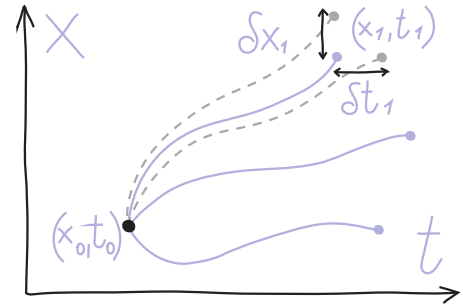
▶ Classical Hamilton-Jacobi theory

Classical mechanics can also be formulated in a "wave" form. The appearance of classical trajectories in this formulation is quite analogous to the way how rays of light arise from electromagnetic waves in geometrical optics.

We remind the action $S[\vec{x}(t)]_{t_0}^{t_1} = \int_{t_0}^{t_1} \mathcal{L}[\vec{x}(t), \dot{\vec{x}}(t)]dt$ of a structureless particle with Lagrangian $\mathcal{L}(\vec{x}, \dot{\vec{x}}) = \frac{M}{2}\dot{\vec{x}}^2 - V(\vec{x})$, represents a functional on the space of trajectories $\vec{x}(t)$. For a fixed initial point $\vec{x}(t_0) = \vec{x}_0$ and a fixed final point $\vec{x}(t_1) = \vec{x}_1$ the classical equations of motion select the trajectory $\vec{x}_c(t)$ satisfying the variational principle $\delta S[\vec{x}_c(t)]_{t_0}^{t_1} = 0$

Consider a bunch of classical trajectories $\{\vec{x}_c(t)\}$ (satisfying $\delta S = 0$) leading from a *fixed initial point* $(\vec{x}_0, t_0)$ to *variable final point* $(\vec{x}_1, t_1)$. The action along these trajectories as a function of $(\vec{x}_1, t_1)$ is the central object of the H.-J. theory:

$$S(\vec{x}_1, t_1) = \int_{t_0}^{t_1} \mathcal{L}[\vec{x}_c(t), \dot{\vec{x}}_c(t)]dt$$



Differential equations for $S(\vec{x}_1, t_1)$:

(a) Space variation $(\vec{x}_1, t_1) \to (\vec{x}_1 + \delta\vec{x}_1, t_1)$
$\Rightarrow S \to (S + \delta S)$

$$\delta S = \int_{t_0}^{t_1} \Big(\frac{\partial \mathcal{L}}{\partial x_i}\delta x_i + \underbrace{\frac{\partial \mathcal{L}}{\partial \dot{x}_i}\delta \dot{x}_i}_{\frac{d}{dt}(\frac{\partial \mathcal{L}}{\partial \dot{x}_i}\delta x_i) - (\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_i})\delta x_i} \Big) dt$$

$$= \underbrace{\Big[\frac{\partial \mathcal{L}}{\partial \dot{x}_i}\delta x_i\Big]_{t_0}^{t_1}}_{\frac{\partial \mathcal{L}}{\partial \dot{x}_i}\delta x_{1i}} + \int_{t_0}^{t_1} \underbrace{\Big[\frac{\partial \mathcal{L}}{\partial x_i}\delta x_i - (\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_i})\delta x_i\Big]}_{0} dt \qquad \Rightarrow \quad \frac{\partial S(\vec{x}_1, t_1)}{\partial x_{1i}} = \overbrace{\frac{\partial \mathcal{L}(\vec{x}, \dot{\vec{x}})}{\partial \dot{x}_i}}^{p_i}\Big|_{\substack{\vec{x}=\vec{x}_c(t_1) \\ \dot{\vec{x}}=\dot{\vec{x}}_c(t_1)}}$$

$$\Rightarrow \boxed{\vec{\nabla}_{\vec{x}_1} S(\vec{x}_1, t_1) = \vec{p}_1}$$

(b) Time variation $(\vec{x}_1, t_1) \to (\vec{x}_1, t_1 + \delta t_1)$

$$\underbrace{\frac{dS}{dt_1}}_{\mathcal{L}[\vec{x}_c(t_1), \dot{\vec{x}}_c(t_1)]} = \frac{\partial S}{\partial t_1} + \underbrace{\frac{\partial S}{\partial x_{1i}}}_{p_{1i}} \underbrace{\dot{x}_{1i}}_{\dot{x}_{ci}(t_1)} \Rightarrow \frac{\partial S}{\partial t_1} = \underbrace{\Big[\mathcal{L} - \vec{p}\cdot\dot{\vec{x}}\Big]_{t=t_1}}_{-H(\vec{x}_1, \vec{p}_1, t_1)} \Rightarrow \boxed{\frac{\partial}{\partial t_1} S(\vec{x}_1, t_1) = -H(\vec{x}_1, \vec{p}_1, t_1)}$$

Both these equations together yield a single equation for $S(\vec{x}_1, t_1) \equiv S(\vec{x}, t)$:

$$\frac{\partial}{\partial t_1} S(\vec{x}_1, t_1) + H[\vec{x}_1, \vec{\nabla}_{\vec{x}_1} S(\vec{x}_1, t_1), t_1] = 0 \qquad \text{or shortly:} \quad \boxed{\frac{\partial}{\partial t} S + H(\vec{x}, \vec{\nabla} S, t) = 0}$$

Example: massive particle in a scalar potential $\boxed{\frac{\partial}{\partial t} S + \frac{1}{2M}(\vec{\nabla} S)^2 + V(\vec{x}) = 0}$

For a **time-independent Hamiltonian** the energy is conserved: $H = E = \text{const}$

$\Rightarrow \quad \frac{\partial}{\partial t} S = -E \quad \Rightarrow \quad \boxed{S(\vec{x}, t) = W(\vec{x}) - Et} \quad \Rightarrow \quad H(\vec{x}, \vec{\nabla} W) = E$

$\Rightarrow$ the generating function $W(\vec{x})$ can be determined from $\vec{\nabla} W = \vec{p}$

$\Rightarrow \quad \boxed{W(\vec{x}) = \int_{\vec{x}_0}^{\vec{x}} \vec{p}\cdot d\vec{x}'}$ contour integral along a classical trajectory from an arbitrary initial point $\vec{x}_0$ to the given point $\vec{x}$

If $S(\vec{x}, t)$ is a solution of the H-J equation, the momentum $\vec{p} = \vec{\nabla} S$ at each point is perpendicular to the surfaces $S(\vec{x}, t) = \text{const} \Rightarrow$ classical trajectories are like *rays* associated with a "wave" whose phase is represented by $S(\vec{x}, t)$.

▶ WKB equations for a single particle

In the language of so-called WKB equations (named after G. Wentzel, H.A. Kramers and L. Brillouin, who — among some others– formulated the related theory in the early days of QM), quantum description becomes related to the Hamilton-Jacobi theory. We will stick to the case of a single particle in a potential. Let us rewrite the Shrödinger equation $\Big[-\frac{\hbar^2}{2M}\vec{\nabla}^2 + V(\vec{x})\Big]\psi(\vec{x}, t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x}, t)$

with substitution $\boxed{\psi(\vec{x},t)=\sqrt{\rho(\vec{x},t)}e^{\frac{i}{\hbar}S(\vec{x},t)}}$ where $\rho(\vec{x},t)$ & $S(\vec{x},t)$ are some unknown functions:

$$-\tfrac{\hbar^2}{2M}\left[\Delta\sqrt{\rho}+\tfrac{2i}{\hbar}(\vec{\nabla}\sqrt{\rho})\cdot(\vec{\nabla}S)+\tfrac{i}{\hbar}\sqrt{\rho}\Delta S-\tfrac{1}{\hbar^2}\sqrt{\rho}(\vec{\nabla}S)^2\right]e^{\frac{i}{\hbar}S}+V\sqrt{\rho}e^{\frac{i}{\hbar}S}$$
$$=i\hbar\left[\tfrac{\partial\sqrt{\rho}}{\partial t}+\tfrac{i}{\hbar}\sqrt{\rho}\tfrac{\partial S}{\partial t}\right]e^{\frac{i}{\hbar}S}$$

$$\text{Separate}\begin{cases}\text{Re part}: & -\tfrac{\hbar^2}{2M}\Delta\sqrt{\rho}+\tfrac{1}{2M}\sqrt{\rho}(\vec{\nabla}S)^2+V\sqrt{\rho} &=& -\sqrt{\rho}\tfrac{\partial S}{\partial t}\\ \text{Im part}: & -\tfrac{\hbar}{M}(\vec{\nabla}\sqrt{\rho})\cdot(\vec{\nabla}S)-\tfrac{\hbar}{2M}\sqrt{\rho}\Delta S &=& \hbar\tfrac{\partial\sqrt{\rho}}{\partial t}\end{cases}$$

$2\sqrt{\rho}\times$ Im part $\Rightarrow$ $\tfrac{\partial\rho}{\partial t}+\tfrac{1}{M}\underbrace{\left[\rho\Delta S+(\vec{\nabla}\rho)\cdot(\vec{\nabla}S)\right]}_{\vec{\nabla}\cdot(\rho\vec{\nabla}S)}=0$ **continuity equation**

$\Rightarrow$ $\boxed{\tfrac{\partial\rho}{\partial t}+\vec{\nabla}\cdot\underbrace{\left(\rho\tfrac{\vec{\nabla}S}{M}\right)}_{\vec{j}=\rho\vec{v}}=0}$

Re part $\Rightarrow$

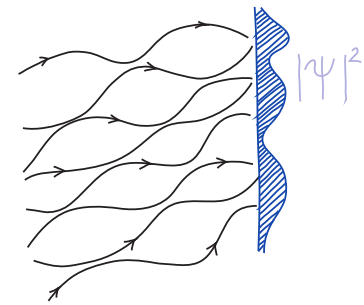
$$\boxed{\underbrace{-\tfrac{\hbar^2}{2M}\tfrac{1}{\sqrt{\rho}}\Delta\sqrt{\rho}}_{*}+\tfrac{1}{2M}(\vec{\nabla}S)^2+V+\tfrac{\partial S}{\partial t}=0}$$

Hamilton-Jacobi equation
+ quantum correction $*\propto\hbar^2$

In the **classical limit** $\hbar\to 0$, the quantum correction term $\boxed{*\to 0}$ $\Rightarrow$ one obtains a coupled pair of classical equations: (a) the Hamilton-Jacobi equation for $S(\vec{x},t)$ $\Rightarrow$ velocity field $\vec{v}(\vec{x},t)\equiv\frac{1}{M}\vec{\nabla}S(\vec{x},t)$, (b) the continuity equation for $\rho(\vec{x},t)$, given $\vec{v}(\vec{x},t)$ determined in step (a). These equations describe an **ensemble of classical particles** with initial space density $\rho(\vec{x},0)$ evolving in agreement with classical equations of motion.

▶ "Pilot-wave" picture of QM

In the quantum case, the correction term $*\ncong 0$ may be considered as an addition to the potential $V(\vec{x})$. Then the WKB equations may be interpreted in terms of classical trajectories of an ensemble of particles moving in a modified potential $\boxed{V_{\text{pilot}}(\vec{x},t)=V(\vec{x})-\underbrace{\tfrac{\hbar^2}{2M}\tfrac{1}{\sqrt{\rho}}\Delta\sqrt{\rho}}_{V_{\text{Q}}(\vec{x},t)}}$



The "quantum potential" $V_{\text{Q}}(\vec{x},t)$ depends on the solution of the quantum problem — on $|\psi(\vec{x},t)|^2$

$\Rightarrow$ The force $\vec{F}_{\text{pilot}}=-\vec{\nabla}V_{\text{pilot}}$ acts also at places where *no classical field* $\vec{F}_{\text{clas}}=-\vec{\nabla}V$ is present.

$\Rightarrow$ Quantum wavefunction $\psi(\vec{x},t)$ plays the role of a "pilot wave" which modulates individual particle trajectories.

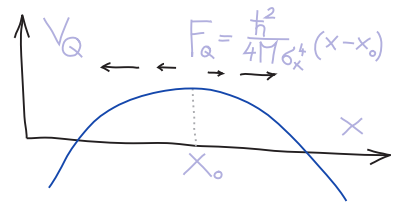
$\Rightarrow$ Quantum interference patterns can be explained without abandoning the concept of trajectories.

However, V_{Q} is a strange field (*not* an interaction with other particles of the ensemble $\Leftarrow$ acts even for 1 particle) which turns out to have explicitly **non-local** character ($\Rightarrow$ non-local hidden-variable theory equivalent to QM).

Example: Gaussian wavepacket of free particle: $\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma_x(t)^2}} e^{-\frac{[x-x_0(t)]^2}{2\sigma_x(t)^2}}$

$\Rightarrow V_{\rm Q}(x,t) = \frac{\hbar^2}{4M\sigma_x(t)^2}\left\{1 - \frac{[x-x_0(t)]^2}{2\sigma_x(t)^2}\right\}$

Force increasing with the wavepacket localization
$\Rightarrow$ consistent with the wavepacket spreading



▶ WKB approximation – conditions of use

Even with the actual value of the Planck constant, the quantum term in the WKB equations can sometimes be neglected. This is the essence of the semi-classical approximation in terms of the WKB theory. When the quantum term can be considered small? $* = -\frac{\hbar^2}{2M}\frac{1}{\sqrt{\rho}}\Delta\sqrt{\rho} \sim \mathcal{O}(\hbar^2) \overset{?}{\ll}$ terms $\sim \begin{cases}\mathcal{O}(\hbar^0)\\ \mathcal{O}(\hbar^1)\end{cases}$

For the sake of simplicity we assume the 1D case in the stationary regime:

Continuity eq. $\underbrace{\frac{\partial\rho}{\partial t}}_{0} + \frac{\partial}{\partial x}(\rho\frac{\partial S}{\partial x}) = 0 \;\Rightarrow\; \rho\frac{\partial S}{\partial x} = \text{const}$

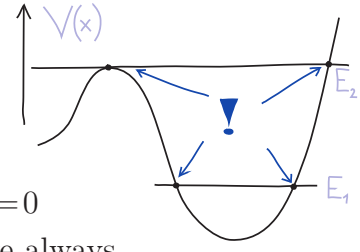
WKB eq. $-\frac{\hbar^2}{2M}\frac{\partial^2\sqrt{\rho}}{\partial x^2}\frac{1}{\sqrt{\rho}} + \frac{1}{2M}\left(\frac{\partial S}{\partial x}\right)^2 + V + \overbrace{\frac{\partial S}{\partial t}}^{-E} = 0 \;\Rightarrow\; \overbrace{-\frac{\hbar^2}{2M}\left[\frac{\partial^2\rho}{\partial x^2}\frac{1}{2\rho} - \frac{(\frac{\partial\rho}{\partial x})^2}{4\rho^2}\right]}^{*} + \frac{1}{2M}\left(\frac{\partial S}{\partial x}\right)^2 = E - V$

Substituting ρ from 1st to 2nd eq. and comparing the quantum & classical terms, we obtain the quasiclassicality condition:

So the relative momentum change at the distance of de Broglie wavelength must be negligible!

$$\left(\frac{\hbar\frac{\partial^2 S}{\partial x^2}}{(\frac{\partial S}{\partial x})^2}\right)^2 \ll 1 \;\Rightarrow\; \overbrace{\frac{\hbar}{p}}^{\lambda_{\rm B}}\frac{|\frac{\partial p}{\partial x}|}{p} \ll 1 \;\Rightarrow\; \boxed{\left|\frac{\Delta p}{p}\right|_{\Delta x=\lambda_{\rm B}} \ll 1}$$

This condition is usually satisfied for sufficiently high energy E except:
(a) "wild" (rapidly oscillating) potentials $V(x)$
(b) regions near **turning points** x_0 with $E = V(x_0)$
(c) regions near **stationary points** x_0 with $\frac{dV}{dx}(x_0) = 0$



In case (a), $\frac{\Delta p}{p}$ can be arbitrary, in cases (b) & (c) we always get $\frac{\Delta p}{p} \to \infty$ as x approaches to the return or stationary point x_0.

▶ Stationary WKB approximation around 1D turning point

From the stationary continuity equation we already know: $\rho(x)\frac{\partial S(x)}{\partial x} = \text{const}$

From the H.-J. theory: $W(x) = S(x,t) + Et = \int_{x_0}^{x} p\,dx = \pm\int_{x_0}^{x}\sqrt{2M[E-V(x')]}dx'$

$\Rightarrow$ $\boxed{\rho(x) \propto \frac{1}{\sqrt{2M[E-V(x)]}} \propto \frac{1}{|v_{\rm clas}(x)|}}$ in the classically available region $V(x) < E$

The WKB wavefunction on both sides of a turning point x_0 with $V(x_0) = E$:

$$\psi_{\rm I}(x,t)=\frac{\pm\mathcal{N}}{\Big(2M[E-V(x)]\Big)^{1/4}}e^{\pm\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2M[E-V(x')]}dx'-\frac{i}{\hbar}Et} \qquad \text{for } V(x)<E \quad \text{(region I)}$$

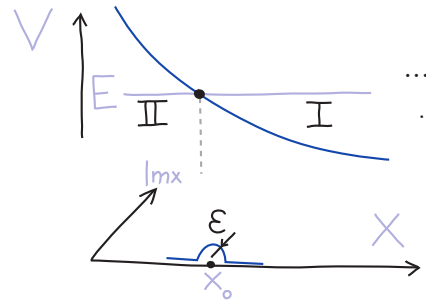
$$\psi_{\rm II}(x,t)=\frac{\pm\mathcal{N}}{\Big(2M[V(x)-E]\Big)^{1/4}}e^{\pm\frac{1}{\hbar}\int_{x}^{x_0}\sqrt{2M[V(x')-E]}dx'-\frac{i}{\hbar}Et} \qquad \text{for } V(x)>E \quad \text{(region II)}$$

How to connect these solutions at x_0 where the WKB approximation fails? Bypassing x_0 from II to I in the complex plane $x\in\mathbb{C}$ along a half-circle with radius ε:

starting in **region II**...

following $\underbrace{\Delta x}_{x-x_0}=-\varepsilon e^{i\phi}$ from ϕ=0...

$\underbrace{\left|\frac{dV}{dx}\right|_{x_0}}_{\approx V(-\varepsilon)-E}\varepsilon\, e^{i\phi}\;\to$



...arriving to **region I**

...to ϕ=π: $\underbrace{\Delta x}_{x-x_0}=-\varepsilon e^{i\pi}=+\varepsilon$

$\to\; e^{i\pi}\;\underbrace{\varepsilon\left|\frac{dV}{dx}\right|_{x_0}}_{\approx E-V(+\varepsilon)}$

$\Rightarrow$ the wavefunction prefactor, exponent and whole ψ change as follows:

$$\left.\begin{array}{r}\left.\dfrac{\mathcal{N}}{\Big(2M[V(x)-E)]\Big)^{1/4}}\right|_{x_0-\varepsilon}\approx\dfrac{\mathcal{N}}{\Big(2M\left|\frac{dV}{dx}\right|_{x_0}\varepsilon e^{i0}\Big)^{1/4}}\\ \int_{x_0-\varepsilon}^{x_0}\sqrt{2M[V(x')-E]}dx'\approx 0\\ \psi_{\rm II}(x,t)\big|_{x_0-\varepsilon}\end{array}\right\}\ {\rm II}\cong{\rm I}\ \left\{\begin{array}{l}\left.\dfrac{\mathcal{N}}{\Big(2M\left|\frac{dV}{dx}\right|_{x_0}\varepsilon e^{i\pi}\Big)^{1/4}}\approx\dfrac{e^{-i\pi/4}\,\mathcal{N}}{\Big(2M[E-V(x)]\Big)^{1/4}}\right|_{x_0+\varepsilon}\\ 0\approx\int_{x_0}^{x_0+\varepsilon}\sqrt{2M[E-V(x')]}dx'\\ e^{-i\pi/4}\,\psi_{\rm I}(x,t)\big|_{x_0+\varepsilon}\end{array}\right.$$

$\Rightarrow\psi_{\rm I}(x,t)$ given above receives an extra $\boxed{\text{phase factor } e^{-i\pi/4}}$

▶ Application to bound states in a potential well

2 classical turning points in the well:

II	x_{01}	I	x_{02}	II′
forbidden	↑	allowed	↑	forbidden

Wavefunction in the allowed region can be connected to the left or right forbidden region II or II':

$$\psi_{\rm I}(x)=\begin{cases}\pm\mathcal{N}\ (2M[E-V(x)])^{-1/4}\ e^{i\left[+\frac{1}{\hbar}\int_{x_{01}}^{x}\sqrt{2M[E-V(x')]}dx'-\frac{\pi}{4}\right]} & \text{using left return point } x_{01}\\ \pm\mathcal{N}\ (2M[E-V(x)])^{-1/4}\ e^{i\left[-\frac{1}{\hbar}\int_{x}^{x_{02}}\sqrt{2M[E-V(x')]}dx'+\frac{\pi}{4}\right]} & \text{using right return point } x_{02}\end{cases}$$

Consistency condition:

$$\left[+\tfrac{1}{\hbar}\int_{x_{01}}^{x}\sqrt{2M[E-V(x')]}dx'-\tfrac{\pi}{4}\right]-\left[-\tfrac{1}{\hbar}\int_{x}^{x_{02}}\sqrt{2M[E-V(x')]}dx'+\tfrac{\pi}{4}\right]=\pm n\pi \qquad n=0,1,2,3,...$$

$$\underbrace{2\int_{x_{01}}^{x_{02}}\sqrt{2M[E-V(x')]}dx'}_{\oint p\,dx}=\left(n+\tfrac{1}{2}\right)\underbrace{2\pi\hbar}_{h}$$

Bohr–Sommerfeld energy quantization (derived in old QM without the $\frac{1}{2}$ term)

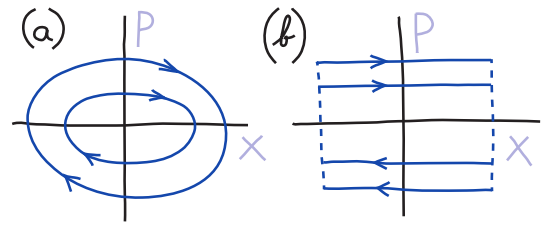
Examples in which the WKB energies reproduce the exact 1D QM results:

(a) **harmonic oscillator**

$\frac{1}{2M}p^2 + \frac{M\omega^2}{2}x^2 = E \quad \Rightarrow \quad$ ellipse $\left(\frac{x}{a}\right)^2 + \left(\frac{p}{b}\right)^2 = 1$ with area $S = \pi a\, b \equiv \oint p\, dx$

$= \pi\sqrt{\frac{2E}{M\omega^2}}\sqrt{2ME} = \left(n+\frac{1}{2}\right) h$

$\Rightarrow \qquad E = \left(n+\frac{1}{2}\right)\hbar\omega$



(b) **infinite well**

no access to region II

$\Rightarrow$ consistency condition reads as:

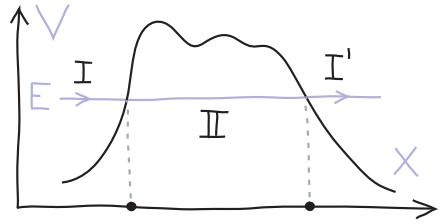
$+\frac{1}{\hbar}\int_{x_{01}}^{x} \sqrt{2ME}dx' + \frac{1}{\hbar}\int_{x}^{x_{02}} \sqrt{2ME}dx' = k\pi \quad$ with $k = 1, 2, 3, \ldots$

$\Rightarrow \qquad \oint p\, dx = 2\sqrt{2ME}\; L = kh \qquad \Rightarrow \quad E = \frac{(\pi\hbar)^2}{2ML^2}k^2$

► Application to tunneling through a potential barrier

2 turning points on both barrier sides:

I	x_{01}	II	x_{02}	I′
allowed	↑	forbidden	↑	allowed



The WKB method is applied to the wavefunction ansatz for scattering problems from Sec. 5a. We assume a wavefunction with the $x \to -\infty$ asymptotics of incoming & reflected waves, and the $x \to +\infty$ asymptotics of the transmitted wave. The WKB approximation of the transmission coefficient $T = \frac{j_{\text{trans}}}{j_0}$ is:

$$T_{\text{WKB}} \approx e^{-\frac{2}{\hbar}\int_{x_{01}}^{x_{02}} \sqrt{2M[V(x)-E]}dx}$$

◄ Historical remark

1913: Niels Bohr proposed a model of hydrogen based on semiclassical quantization
1919: Arnold Sommerfeld elaborates the semiclassical quantization ⇒ old QM
1926: G. Wentzel, H.A. Kramers, L. Brillouin (based on earlier work of A. Einsten, H. Jeffreys...) develop the WKB approximation for a single-particle Schrödinger eq.
1927: Louis de Broglie formulates the basis of the pilot wave theory
1928: George Gamow uses the WKB transmission coeff. to explain nuclear α-decay
1952: David Bohm uses the idea to formulate a hidden-variable alternative to QM

9. QUANTUM INFORMATION

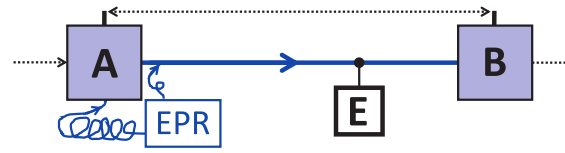
Having spent so much effort by building the foundations of quantum theory and developing the paths back to our classical world, we deserve now to see some genuine quantum miracles! Not just paradoxes, but practical applications of the strange and beautiful quantum laws — applications that may help us to design new magical

technologies and to impress friends! There are three main resources for such applications, namely the quantum superposition, quantum entanglement and quantum measurement. These new concepts actually revolutionized the information science.

■ Quantum information channel

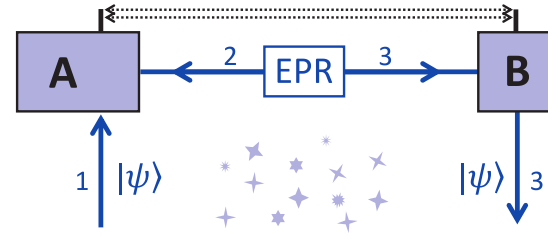
Classical information (bits 0 & 1) is often transmitted by means of quantum objects, like photons. However, the use of full quantum properties of the carrier particles tremendously enhances the capabilities of the transmission. Of course, this comes at a price of a much more demanding requirements upon the physical maintenance of the channel over which the particles are sent.

▶ Quantum cryptography



The measurement-induced collapse of wavefuction can, in principle, disclose any hidden measurement performed on the system. This can be used to detect an eavesdropper Eve (E) in secret quantum-channel communication between Alice (A) and Bob (B). It is assumed that A & B are also connected by a classical communication channel.
Protocol (i): Alice sends a binary sequence by individual photons in linear polarization states $\left.\begin{matrix}|x\rangle \\ |x'\rangle\end{matrix}\right\} \equiv 0$ and $\left.\begin{matrix}|y\rangle \\ |y'\rangle\end{matrix}\right\} \equiv 1$, selecting between 2 rotated polarization frames S & S′. Bob measures photon polarizations using *independent selection* of the *same* frames S & S′. If E is absent, the photons for which A & B frames coincide must yield the same A & B polarizations. Any violation of this rule, which is detected on a released sample of photons, indicates that the photon state was distorted during the transmission (Eve's measurement). If no eavesdropping is detected, the states of the remaining photons, for which A & B frames were the same, can be used as a private key.
Protocol (ii): The communication is repeatedly interrupted by test measurements, in which A & B probe the violation of Bell's inequalities on a sample of EPR pairs of entangled photons, one of which is sent through the quantum channel. Eve's local measurement makes the the state of the pair factorized, so in case of eavesdropping the A & B test measurements satisfy Bell's inequalities.

▶ Quantum teleportation



The teleportation means a transfer of the state of a given physical object to another carrier composed of different particles (possibly far away from the original particles). Quantum mechanics offers a way how this goal can be achieved using quantum

entanglement. It needs to be stressed that quantum teleportation is a **causal process** with no superluminal action!

We will demonstrate the teleportation of an **unknown single-qubit state** $|\psi\rangle$ of particle 1 (on Alice's side) to particle 3 (on Bob's side), which belongs to an entangled EPR pair of qubit particles 2 (going to Alice) and 3 (going to Bob). The unknown state of particle 1 is $\boxed{|\psi\rangle_1 = \alpha|0\rangle_1 + \beta|1\rangle_1 \equiv \binom{\alpha}{\beta}_1}$ and the pair of particles 2 & 3 is in any of the Bell states, e.g. $\boxed{|\Psi^-\rangle_{23} = \frac{1}{\sqrt{2}}\big(|0\rangle_2|1\rangle_3 - |1\rangle_2|0\rangle_3\big)}$ (like the spin-$\frac{1}{2}$ singlet state). The procedure is as follows:

Alice measures particles 1 & 2 in the entangled basis of 4 Bell states (Sec. 7b):

$$\left\{\begin{array}{ll} \#1 & |\Psi^+\rangle_{12}=\frac{1}{\sqrt{2}}(|0\rangle_1|1\rangle_2+|1\rangle_1|0\rangle_2) \\ \#2 & |\Psi^-\rangle_{12}=\frac{1}{\sqrt{2}}(|0\rangle_1|1\rangle_2-|1\rangle_1|0\rangle_2) \\ \#3 & |\Phi^+\rangle_{12}=\frac{1}{\sqrt{2}}(|0\rangle_1|0\rangle_2+|1\rangle_1|1\rangle_2) \\ \#4 & |\Phi^-\rangle_{12}=\frac{1}{\sqrt{2}}(|0\rangle_1|0\rangle_2-|1\rangle_1|1\rangle_2) \end{array}\right\}$$

This suggests the following decomposition of the initial 1 & 2 & 3 state:

$$\underbrace{(\alpha|0\rangle_1 + \beta|1\rangle_1)}_{|\psi\rangle_1}\underbrace{\tfrac{1}{\sqrt{2}}\,(|0\rangle_2|1\rangle_3 - |1\rangle_2|0\rangle_3)}_{|\Psi^-\rangle_{23}} =$$

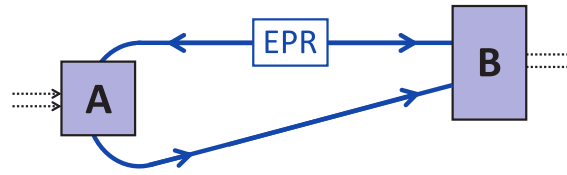
$$= \frac{1}{\sqrt{4}}\Big[|\Psi^+\rangle_{12}\overbrace{(-\alpha|0\rangle_3+\beta|1\rangle_3)}^{|\psi^{\#1}\rangle_3} + |\Psi^-\rangle_{12}\overbrace{(-\alpha|0\rangle_3-\beta|1\rangle_3)}^{|\psi^{\#2}\rangle_3} + |\Phi^+\rangle_{12}\overbrace{(\alpha|1\rangle_3-\beta|0\rangle_3)}^{|\psi^{\#3}\rangle_3} + |\Phi^-\rangle_{12}\overbrace{(\alpha|1\rangle_3+\beta|0\rangle_3)}^{|\psi^{\#4}\rangle_3}\Big]$$

Define: $\hat{U}^{\#1} = \left(\begin{smallmatrix} -1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ $\hat{U}^{\#2} = \left(\begin{smallmatrix} -1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ $\hat{U}^{\#3} = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ $\hat{U}^{\#3} = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$

In correlation with the result $\#k$ of Alice's measurement, Bob receives particle 3 in the state $|\psi^{\#k}\rangle_3$. Alice communicates the result $\#k$ of her measurement via the classical 2-bit channel to Bob, who then applies the corresponding unitary transformation $\hat{U}^{\#1}$ such that $\boxed{\hat{U}^{\#k}|\psi^{\#k}\rangle_3 = \binom{\alpha}{\beta}_3 = \alpha|0\rangle_3 + \beta|1\rangle_3 \equiv |\psi\rangle_3}$

The teleportation of the state $|\psi\rangle$ from particle 1 to particle 3 is completed.

▶ Quantum dense coding



Reception of one particle from an entangled pair enables Eve to send information to Bob in a compressed form. Assume that the entangled pair is in the Bell state $|\Psi^-\rangle$. Alice performs one of the above-defined unitary transformations $\hat{U}^{\#k}$ on particle 1 and sends this particle to Bob. Bob then receives the pair 1 & 2 in the corresponding Bell state: (up to the overall phase). By performing a measurement in the Bell basis, Bob can deduce which of the 4 transformations Alice applied. So Alice transfers to Bob 2 bits of classical information by sending him only a single 1-qubit particle. This can double the speed of the A→B information flow.

$$\left\{\begin{array}{l} |\Psi^+\rangle \text{ for } k{=}1 \\ |\Psi^-\rangle \text{ for } k{=}2 \\ |\Phi^+\rangle \text{ for } k{=}3 \\ |\Phi^-\rangle \text{ for } k{=}4 \end{array}\right.$$

■ Quantum computation

The use of quantum laws for a substantial speedup of some computational tasks would be the most spectacular practical application of QM. This field attracts

a lot of theoretical and experimental effort and public attention since 1990's, when fast quantum algorithms for crucial computational problems were designed, and has made tremendous progress since then. Possession of a powerful quantum computer might be a strategic advantage, so this is a race!

▸ From reversible to quantum computation

Thoughts about the role of QM in computation came as the size of electronic elements started approaching the atomic scale. Can the computation be performed by elementary physical constituents? An obvious obstacle is *irreversibility* of common computational procedures, which is in contrast to reversibility of fundamental physical processes. The irreversibility leads to the *production of entropy* ($\Rightarrow$ heat) and thus sets fundamental limits to macroscopic computers. Theoretical attempts to compose the computation of reversible steps grew into considerations whether the involvement of QM cannot have more substantial consequences. It was pointed out that the impossibility to replace QM by a local classical-like theory (Bell inequalities, see Sec. 7a) implies that *quantum dynamics cannot be simulated in parallel by a classical computer*. This then led to the question whether some types of *quantum evolution can be equivalent to the fast solution of some classical computational problems*. Yes, they can.

▸ Quantum computer

From Sec. 1b we know that the quantum generalization of the classical bit $b \in \{0,1\}$ is the qubit carrying any superposition of the 0,1 states, and that the generalization of an N-bit register $(b_0, b_1, ..., b_{N-1}) \equiv x = \sum_{i=0}^{N-1} b_i\, 2^i \in \{0, 1, ..., 2^N{-}1\}$ is the quantum register carrying any superposition of numbers x:

Qubit: $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$ with $\left\{ \begin{smallmatrix} \alpha_0,\alpha_1\in\mathbb{C} \\ |\alpha_0|^2+|\alpha_1|^2=1 \end{smallmatrix} \right.$,

Quantum register: $|\Psi\rangle = \sum_{x=0}^{2^N-1} \alpha_x |x\rangle$ with $\left\{ \begin{smallmatrix} \alpha_x\in\mathbb{C} \\ \sum_x |\alpha_x|^2=1 \end{smallmatrix} \right.$ $|x\rangle \equiv |b_0\rangle|b_1\rangle...|b_{N-1}\rangle \equiv$ separable basis in $\mathcal{H}=\mathcal{H}_0\otimes\mathcal{H}_1\otimes...\otimes\mathcal{H}_{N-1}$

Quantum computer is an N-qubit device that for a general state $|\Psi\rangle$ allows to perform (i) **controllable unitary operations** $\hat{U}$ (not necessarily all but a sufficiently large class of them) and (ii) **quantum measurements** (usually a class of local measurements on individual qubits).

▸ One- and two-qubit operations

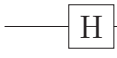
A general N-qubit unitary operation can be decomposed into a product of unitary operations acting only on single qubits or on pairs of qubits:

$$\boxed{\hat{U} = \hat{U}_M \hat{U}_{M-1} \ldots \hat{U}_2 \hat{U}_1 \quad \text{with } \hat{U}_k \in \left\{ \hat{U}_i^{(1)}, \hat{U}_{ij}^{(2)} \right\}} \quad \left\{ \begin{smallmatrix} \hat{U}_i^{(1)} \equiv \text{a 1qubit unitary op. on qubit } i \\ \hat{U}_{ij}^{(2)} \equiv \text{a 2qubit unitary op. on qubits } i,j \end{smallmatrix} \right.$$

With increasing N, the number M scales polynomially in favorable cases (which can be implemented as scalable quantum algorithms) or faster than polynomially in cases when quantum computation would not be scalable.

Examples of 1- and 2-qubit operations:

Hademard transformation: a 1-qubit unitary operation

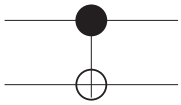


defined as $\big\{|0\rangle \to \frac{1}{\sqrt{2}}\big(|0\rangle+|1\rangle\big), \quad |1\rangle \to \frac{1}{\sqrt{2}}\big(|0\rangle-|1\rangle\big).\big\}$

This operation can be used to produce a uniform superposition of all $|x\rangle$ states:

$$\left(\bigotimes_i \hat{U}^{\rm H}\right)|0\rangle = \bigotimes_{i=0}^{N-1}\left(\hat{U}_i^{\rm H}|0\rangle_i\right) = \frac{1}{2^{N/2}}\sum_{x=0}^{2^N-1}|x\rangle$$

CNOT transformation (controlled NOT): a 2-qubit unitary operation



defined as $\left\{\begin{array}{ll} |0\rangle_a|0\rangle_b \to |0\rangle_a|0\rangle_b, & |0\rangle_a|1\rangle_b \to |0\rangle_a|1\rangle_b, \\ |1\rangle_a|0\rangle_b \to |1\rangle_a|1\rangle_b, & |1\rangle_a|1\rangle_b \to |1\rangle_a|0\rangle_b. \end{array}\right\}$

This operation generates entanglement between qubits:

$$\hat{U}_{ab}^{\rm CNOT}\big(\alpha|0\rangle_a+\beta|1\rangle_a\big)|0\rangle_b = \alpha|0\rangle_a|0\rangle_b + \beta|1\rangle_a|1\rangle_b$$

▶ Some many-qubit operations

Two important examples of unitary transformations acting on many qubits:

(i) **Quantum Fourier transformation**:

$$\boxed{\hat{U}^{\rm QPT}|x\rangle = \frac{1}{2^{N/2}}\sum_{y=0}^{2^N-1} e^{i\frac{2\pi xy}{2^N}}|y\rangle}$$

The unitarity follows from:

$$\langle\hat{U}^{\rm QPT}x|\hat{U}^{\rm QPT}x'\rangle = \frac{1}{2^N}\sum_{y=0}^{2^N-1}\sum_{y'=0}^{2^N-1} e^{i\frac{2\pi(x'y'-xy)}{2^N}}\langle y|y'\rangle = \frac{1}{2^N}\sum_{y=0}^{2^N-1} e^{i\frac{2\pi(x'-x)y}{2^N}} = \delta_{xx'}$$

There exists a 1- & 2-qubit decomposition with $M=\frac{N(N+1)}{2}$ (polynomially fast).

(ii) **Function evaluation**: The trivial transformation $|x\rangle \to |f(x)\rangle$, or rather $|x\rangle \to |f(x) \bmod 2^N\rangle$ (since $f(x)$ may exceed the capacity of the N-qubit register) would not work since for non-invertible functions $f(x)$ the operation would be irreversible ($\Rightarrow$ non-unitary). Instead, we split the whole register to part A with n qubis and part B with m qubits. The input x is realized on part A, the output $f(x)$ on part B. More precisely, the transformation reads as:

$$\boxed{\hat{U}^f|x\rangle_{\rm A}|y\rangle_{\rm B} \to |x\rangle_{\rm A}|[y+f(x)] \bmod 2^m\rangle_{\rm B}}$$

The unitarity follows from:

$$\langle\hat{U}^f xy|\hat{U}^f x'y'\rangle = \langle x|x'\rangle_{\rm A}\langle[y+f(x)] \bmod 2^m|[y'+f(x')] \bmod 2^m\rangle_{\rm B} = \delta_{xx'}\delta_{yy'}$$

The decomposition of $\hat{U}^f$ to 1- & 2-qubit operations depends on $f(x)$ and is *not* generally guaranteed to be polynomial.

▶ Quantum algorithms

Quantum algorithm is a particular sequence of 1- and 2-qubit unitary operations and a particular final quantum measurement to be performed on a properly initialized quantum register. It is usually assumed that the initial state of the register is the trivial factorized state $|0\rangle = |0\rangle_1|0\rangle_2...|0\rangle_{N-1}$. The same sequence of operations and measurements with the same initial state can be repeated K

times to yield a sufficiently large statistical sample of outputs. A common task is **finding properties of an unknown function $f(x)$** : $\underbrace{x}_{\in\{0,\ldots,2^n-1\}} \mapsto \underbrace{f(x)}_{\in\{0,\ldots,2^m-1\}}$

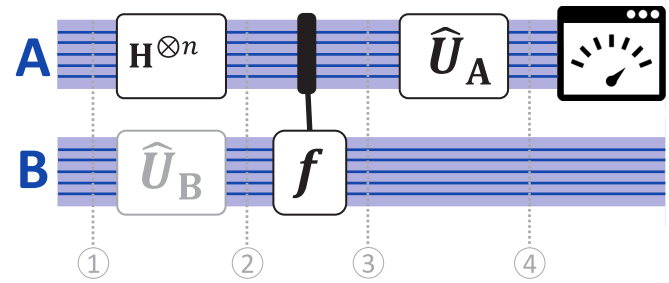
The usual scheme is this:

groups A & B with n & m qubits

$\mathrm{H}^{\otimes n} \equiv \bigotimes_{i=0}^{n-1} \hat{U}_i^{\mathrm{H}}$

$f \equiv$ evaluation of $f(x)$

$\hat{U}_{\mathrm{A}}, \hat{U}_{\mathrm{A}} \equiv$ unitary operations to be specified



Examples:

(i) **Deutsch-Jozsa algorithm**: A toy algorithm deciding whether an unknown (1-bit) $\mapsto$ (1-bit) function $f(x)$ is constant [cases (a) & (b)] or balanced [cases (c) & (d)] in a *single call* of the function-evaluation routine.

	$f(0)$	$f(1)$
(a)	0	0
(b)	1	1
(c)	0	1
(d)	1	0

Here $\boxed{n=m=1}$ and the unitary operations $\boxed{\hat{U}_{\mathrm{A}} = \hat{U}^{\mathrm{H}}}$ and $\boxed{\hat{U}_{\mathrm{B}} = \hat{U}^{\mathrm{H}}\hat{\sigma}_x}$ (where $\hat{\sigma}_x$ represents the 1-qubit NOT operation).

The state of the register at the indicated control points is as follows:

①	②	③	④	
$\lvert 0\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}$	$\frac{1}{2}(\lvert 0\rangle+\lvert 1\rangle)_{\mathrm{A}}(\lvert 0\rangle-\lvert 1\rangle)_{\mathrm{B}}$	$\frac{1}{2}(\lvert 0\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}-\lvert 0\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}}+\lvert 1\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}-\lvert 1\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}})$	$\frac{1}{\sqrt{2}}\lvert 0\rangle_{\mathrm{A}}(\lvert 0\rangle-\lvert 1\rangle)_{\mathrm{B}}$	(a)
		$\frac{1}{2}(\lvert 0\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}}-\lvert 0\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}+\lvert 1\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}}-\lvert 1\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}})$	$\frac{1}{\sqrt{2}}\lvert 0\rangle_{\mathrm{A}}(\lvert 1\rangle-\lvert 0\rangle)_{\mathrm{B}}$	(b)
		$\frac{1}{2}(\lvert 0\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}-\lvert 0\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}}+\lvert 1\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}}-\lvert 1\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}})$	$\frac{1}{\sqrt{2}}\lvert 1\rangle_{\mathrm{A}}(\lvert 0\rangle-\lvert 1\rangle)_{\mathrm{B}}$	(c)
		$\frac{1}{2}(\lvert 0\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}}-\lvert 0\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}+\lvert 1\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}-\lvert 1\rangle_{\mathrm{A}}\lvert 1\rangle_{\mathrm{B}})$	$\frac{1}{\sqrt{2}}\lvert 1\rangle_{\mathrm{A}}(\lvert 1\rangle-\lvert 0\rangle)_{\mathrm{B}}$	(d)

So the measurement on qubit A distinguishes the constant $\Rightarrow \lvert 0\rangle_{\mathrm{A}}$ and balanced $\Rightarrow \lvert 1\rangle_{\mathrm{A}}$ cases. Note that in the classical case one would necessarily need two calls of the function-evaluation procedure! This example illustrates the synergy of quantum superpositions (both inputs are simultaneously present in stage ②) and quantum entanglement (individual inputs are correleted with the corresponding outputs in stage ③). None of these ingredients can be absent in quantum computation.

(ii) **Shor algorithm**: It is the heart of Shor's factorization algorithm — its quantum part, which determines the **period r of a certain function** $f(x)$. In this case $\boxed{\hat{U}_{\mathrm{B}} = \hat{I}}$ (so this operation is absent) and $\boxed{\hat{U}_{\mathrm{A}} = \hat{U}^{\mathrm{QPT}}}$

①	②	③	④
$\lvert 0\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}$	$\frac{1}{\sqrt{2^n}}\sum_x \lvert x\rangle_{\mathrm{A}}\lvert 0\rangle_{\mathrm{B}}$	$\frac{1}{\sqrt{2^n}}\sum_x \lvert x\rangle_{\mathrm{A}}\lvert f(x)\rangle_{\mathrm{B}}$	$\frac{1}{2^n}\sum_x\sum_y e^{i\frac{2\pi xy}{2^n}}\lvert y\rangle_{\mathrm{A}}\lvert f(x)\rangle_{\mathrm{B}}$

The probability of a particular output y on subregister A is thus given by:

$$\mathfrak{p}_{\mathrm{A}}(y) = \frac{1}{2^{2n}}\sum_{x,x'} e^{i\frac{2\pi(x-x')y}{2^n}} \underbrace{\langle f(x')|f(x)\rangle}_{\substack{=1 \text{ for } x-x'=kr \\ =0 \text{ otherwise}}} = \frac{1}{2^{2n}}\sum_{k=0,\pm1,\ldots} e^{ik\frac{2\pi r}{2^n}y}$$

For large n, m, this probability is a periodic function of y sharply peaked around

values satisfying $\frac{2\pi r}{2^n}y = 2\pi l$ with $l = 0,1,2,...$, so $y = l\frac{2^n}{r}$. The period r (an integer number) is therefore deducible from a relatively small number of repeated runs of the procedure. Indeed, Shor's algorithm solves the factorization problem (finding a pair of prime factors P, Q of a given integer $I = PQ$) so that the computational complexity (the number of elementary operations performed in the solution) grows only polynomially with the number of digits of I (the best known classical algorithm exhibits an exponential growth of complexity).

▶ Correcting errors

The efficiency of quantum computation quickly fades away if interactions with any kind of environment induce decoherence of the computer. As such interactions are hardly preventable, the feasibility of a functioning quantum computer seems to be rather questionable. Fortunately, there exist methods for repeatadly correcting the state of the computer so that the effects of decoherence can be considerably slowed down. An unpleasant consequence is however a multiplication of the number of qubits needed for the computation.

Assume a single qubit with density operator $\hat{\rho}(0) = |\psi\rangle\langle\psi|$ corresponding to a pure initial state $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$. At $t > 0$, the qubit state $\hat{\rho}(t)$ is generally mixed because of decoherence. The density operator can be decomposed as $\hat{\rho}(t) = \sum_i \mathfrak{p}_i |\psi_i\rangle\langle\psi_i|$ to arbitrary 4 linearly independent states $|\psi_i\rangle$. We choose one specific decomposition yielding a clear **classification of errors**:

$$\hat{\rho}(t) = \mathfrak{p}_0(t)\underbrace{|\psi\rangle\langle\psi|}_{\text{no error}} + \mathfrak{p}_z(t)\underbrace{\hat{\sigma}_z|\psi\rangle\langle\psi|\hat{\sigma}_z}_{\text{phase error}} + \mathfrak{p}_x(t)\underbrace{\hat{\sigma}_x|\psi\rangle\langle\psi|\hat{\sigma}_x}_{\text{flip error}} + \mathfrak{p}_{xz}(t)\underbrace{\hat{\sigma}_x\hat{\sigma}_z|\psi\rangle\langle\psi|\hat{\sigma}_z\hat{\sigma}_x}_{\text{combined error}}$$

The probabilities are normalized, $\mathfrak{p}_0 + \mathfrak{p}_z + \mathfrak{p}_x + \mathfrak{p}_{xz} = 1$, and for small times $t = \delta t$ satisfy $\mathfrak{p}_0 \sim 1 - O(\delta t^2)$ and $\mathfrak{p}_x, \mathfrak{p}_y, \mathfrak{p}_{xz} \sim O(\delta t^2)$.

The quantum error correction proceeds as follows: Each logical qubit is represented by $k > 1$ physical qubits, the states being mapped as $\big[|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle\big] \mapsto \big[|\overline{\psi}\rangle = \alpha_0|\overline{0}\rangle + \alpha_1|\overline{1}\rangle\big]$. The whole quantum algorithm is performed on the logical instead of physical qubits. For a given number k it can be assumed that within a certain small time interval $\Delta t(k)$ only one (any) of the physical qubits is affected by an error. This yields a limited number of possible errors, which can be detected and fixed. Performing computation on N logical qubits with kN physical qubits, the correcting procedure on each logical qubit must be repeated with period $\Delta t(k)$. The correction of a **general single-qubit error** was shown to require redundancy $\boxed{k \geq 5}$

$$|0\rangle \mapsto |\overline{0}\rangle = \sum_{x=0}^{2^k-1} \alpha_x |x\rangle$$
$$|1\rangle \mapsto |\overline{1}\rangle = \sum_{x=0}^{2^k-1} \beta_x |x\rangle$$
$$\langle\overline{0}|\overline{0}\rangle = \langle\overline{1}|\overline{1}\rangle = 1,\ \langle\overline{0}|\overline{1}\rangle = 0$$

Example: correction of single-qubit **flip errors** with $k = 3$ encoding $\begin{cases} |\overline{0}\rangle = |000\rangle \\ |\overline{1}\rangle = |111\rangle \end{cases}$
Quantum measurement of a quantity $\hat{A} = \sum_{i=1}^{3} i\hat{P}_i$ on each logical qubit, with projectors $\hat{P}_i = \hat{\sigma}_x^{(i)}\big(|000\rangle + |111\rangle\big)\big(\langle 000| + \langle 111|\big)\hat{\sigma}_x^{(i)}$, yields as the

result a the number $i \in \{1,2,3\}$ of the flipped qubit (the result $a=0$ indicates no flip). This measurement does *not* destroy the superposition and entanglement of the logical qubit, so it keeps the logical state of the whole computer intact! The correction of the ith-qubit error on the given logical qubit is achieved simply by applying the operator $\hat{\sigma}_x^{(i)}$ on this qubit.

◀ Historical remark

1982: R. Feynman anticipates potential use of quantum systems for computation
1985: D. Deutsch defines quantum computing and seeks for quantum algorithms
1985: A. Peres proposes the method for correcting single-qubit flip errors
1984: C.H. Bennet & G. Brassard describe a protocol for quantum cryptography
1991: A. Ekert proposes entanglement-based method of quantum cryprography
1993: C.H. Bennett *et al.* describe a scheme for quantum teleportation
1994: P. Shor develops an efficient quantum algorithm for prime factorization
1995: P. Shor proposes the first general single-qubit error correction code
1997: first experimental realization of quantum teleportation by A. Zeilinger *et al.*
1995-present: massive effort to built the quantum computer on various platforms

10. STATIONARY APPROXIMATION METHODS

Application of quantum theory to realistic systems results in very complicated computational problems, which often cannot be solved exactly on the present-day computers. Not surprisingly, there exists a plethora of approximation techniques that help us to get close to exact solutions. Here we start with techniques used to approximate stationary states, i.e., eigenstates of a general Hamiltonian. We focus on the two main methods — the variational and perturbation method — and describe some applications of the latter (the variational method will come into play in Sec. 15).

■ Variational method

In classical physics, variational principles represent an autonomous formulation of the fundamental laws of nature. The role of these principles in nonrelativistic quantum mechanics is not as important. Nevertheless, they constitute a very useful approximation method.

▶ Dynamical variational principle

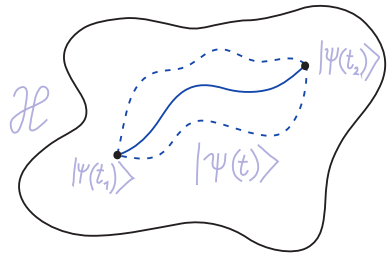
Let us start with a variational formulation of the dynamical Schrödinger equation. Trying to keep the formalism parallel to that of classical mechanics, we employ the notion of independent bra & ket variations. In particular, we search a quantum analog of classical variational principle:

$$\delta \int_{t_1}^{t_2} \mathcal{L}[\vec{x}(t), \dot{\vec{x}}(t)]\, dt = 0 \quad \text{with boundary conditions} \begin{cases} \delta\vec{x}(t_1) = 0 = \delta\vec{x}(t_2) \\ \delta\dot{\vec{x}}(t_1) \neq 0 \neq \delta\dot{\vec{x}}(t_2) \end{cases}$$

The quantum variational principle can be cast as:

$$\underbrace{\delta \int_{t_1}^{t_2} \left\langle \psi(t) \left| i\hbar\tfrac{d}{dt} - \hat{H} \right| \psi(t) \right\rangle dt}_{\int_{t_1}^{t_2} \left[\langle \delta\psi'(t)| i\hbar\frac{d}{dt} - \hat{H}|\psi(t)\rangle + \langle \psi(t)| i\hbar\frac{d}{dt} - \hat{H}|\delta\psi(t)\rangle \right] dt} = 0$$

with
- **ket variation** $|\delta\psi(t)\rangle$: $\boxed{|\delta\psi(t_1)\rangle = 0 = |\delta\psi(t_2)\rangle}$
- **bra variation** $\langle\delta\psi'(t)|$: $\boxed{\langle\delta\psi'(t_1)| \neq 0 \neq \langle\delta\psi'(t_2)|}$



We consider the variations of kets and bras independently, distinguishing 4 different entities:
$\langle\delta\psi(t)| \leftrightarrow |\delta\psi(t)\rangle$ & $\langle\delta\psi'(t)| \leftrightarrow |\delta\psi'(t)\rangle$
The only correlation between $|\delta\psi(t)\rangle$ and $\langle\delta\psi'(t)|$ is through the conserved normalization $\langle\psi|\psi\rangle = 1$

$$\Rightarrow \delta\langle\psi|\psi\rangle = \boxed{\langle\delta\psi'(t)|\psi(t)\rangle + \langle\psi(t)|\delta\psi(t)\rangle = 0}$$

Proof of the variational principle (we show that it implies Schrödinger eq.):

$$\int_{t_1}^{t_2} \Big[\langle\delta\psi'(t)|i\hbar\tfrac{d}{dt} - \hat{H}|\psi(t)\rangle + \underbrace{\langle\psi(t)|i\hbar\tfrac{d}{dt} - \hat{H}|\delta\psi(t)\rangle}_{\langle\delta\psi(t)|i\hbar\frac{d}{dt} - \hat{H}|\psi(t)\rangle^* + i\hbar\frac{d}{dt}\langle\psi|\delta\psi\rangle} \Big] dt$$

$$= \int_{t_1}^{t_2} \Big[\langle\delta\psi'(t)|i\hbar\tfrac{d}{dt} - \hat{H}|\psi(t)\rangle + \langle\delta\psi(t)|i\hbar\tfrac{d}{dt} - \hat{H}|\psi(t)\rangle^* \Big] dt + i\hbar \overbrace{[\langle\psi|\delta\psi\rangle]_{t_1}^{t_2}}^{0}$$

$\overset{!}{=} 0 \quad \forall\, \langle\delta\psi'(t)|$ & $\langle\delta\psi(t)|$ (with the above constraints) $\boxed{\Rightarrow \left(i\hbar\tfrac{d}{dt} - \hat{H}\right)|\psi(t)\rangle = 0}$

Note: If $\langle\delta\psi'(t)| = \langle\delta\psi(t)|$ (kets & bras varied in the same way), we would only get $\mathrm{Re}\langle\delta\psi(t)|i\hbar\frac{d}{dt} - \hat{H}|\psi(t)\rangle = 0$, which would not imply Schrödinger eq.
An alternative treatment of the variational principle (without independent bra & ket variations) is possible if the variation is performed only in kets (or bras):
$\delta\langle\psi|i\hbar\frac{d}{dt} - \hat{H}|\psi\rangle \equiv \langle\psi|i\hbar\frac{d}{dt} - \hat{H}|\delta\psi\rangle$

▶ Transition to stationary problems

The dynamical variational principle for nonrelativistic QM, derived in the previous paragraph, is not very impressive. Indeed, the Schrödinger equation can be recognized in it already before its formal derivation. On the other hand, the variational techniques are rather useful for stationary problems—in approximating the lowest eigenstates of complicated Hamiltonians.

Assume $|\psi(t)\rangle = e^{-\frac{i}{\hbar}Et}|\psi\rangle$ $\Rightarrow$ $\begin{cases} |\delta\psi(t)\rangle = e^{-\frac{i}{\hbar}Et}|\delta\psi\rangle \\ \langle\delta\psi'(t)| = e^{+\frac{i}{\hbar}Et}\langle\delta\psi'| \end{cases}$

$$\int_{t_1}^{t_2} \Big[\langle\delta\psi'(t)|i\hbar\tfrac{d}{dt} - \hat{H}|\psi(t)\rangle + \langle\psi(t)|i\hbar\tfrac{d}{dt} - \hat{H}|\delta\psi(t)\rangle \Big] dt$$

$$= \int_{t_1}^{t_2} \Big[\underbrace{\langle\delta\psi'|E - \hat{H}|\psi\rangle + \langle\psi|E - \hat{H}|\delta\psi\rangle}_{\delta\langle\psi|E-\hat{H}|\psi\rangle} \Big] dt = \underbrace{(t_2 - t_1)}_{\neq 0} \underbrace{\delta\langle\psi|E - \hat{H}|\psi\rangle}_{\overset{!}{=}0} = 0$$

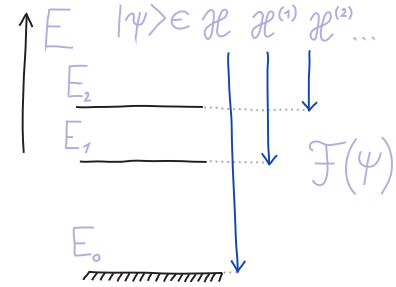
$$\boxed{\delta\langle\psi|\hat{H}-E|\psi\rangle = \delta\big[\langle\psi|\hat{H}|\psi\rangle - E\langle\psi|\psi\rangle\big] = 0} \quad \Leftrightarrow \quad \boxed{\delta\langle\psi|\hat{H}|\psi\rangle = 0 \;\&\; \langle\psi|\psi\rangle = 1}$$

with a Lagrange multiplier — with explicit normalization constraint

If the above variational conditions are applied in the whole Hilbert space $\mathcal{H}$, they yield the **ground state**. To obtain the first excited state, the conditions must be applied only within the orthogonal complement in $\mathcal{H}$ of the ground-state energy subspace. Increasing restrictions reveal higher excited states.

▶ Stationary variational principle

Define $\boxed{\mathcal{F}(|\psi\rangle) = \dfrac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}}$ ≡functional on $\mathcal{H}$



The **ground-state energy & eigenvector** correspond to the global minimum of $\mathcal{F}$:

$$\boxed{E_0 = \mathrm{Min}\,\{\mathcal{F}(|\psi\rangle)\}_{|\psi\rangle\in\mathcal{H}} = \mathcal{F}(|E_0\rangle)}$$

Proof: $|\psi\rangle = \sum_i \alpha_i |E_i\rangle \;\Rightarrow\; \mathcal{F}(|\psi\rangle) = \sum_i |\alpha_i|^2 E_i \geq E_0 = \mathcal{F}(|E_0\rangle)$

If $\mathcal{H}^{(1)}$ is the orthogonal complement of the ground-state subspace $\mathcal{H}_0$, the **1st excited-state energy & eigenvector** read as:

$$\boxed{E_1 = \mathrm{Min}\,\{\mathcal{F}(|\psi\rangle)\}_{|\psi\rangle\in\mathcal{H}^{(1)}} = \mathcal{F}(|E_1\rangle)}$$

Proof: $|\psi\rangle = \sum_{i\geq 1} \alpha_i |E_i\rangle \;\Rightarrow\; \mathcal{F}(|\psi\rangle) = \sum_{i\geq 1} |\alpha_i|^2 E_i \geq E_1 = \mathcal{F}(|E_1\rangle)$

... et cetera for **higher states**

▶ Ritz variational method

Choose a suitable (for the given $\hat{H}$) subset of test vectors $|\psi(\boldsymbol{a})\rangle$ controlled by continuous real parameters $\boldsymbol{a} \equiv \{a_1, a_2, \ldots a_n\}$ forming a domain $\mathcal{D}_{\boldsymbol{a}} \subset \mathbb{R}^n$.

Functional $\mathcal{F}(|\psi\rangle) \;\longmapsto\;$ function $\boxed{\mathcal{F}(\boldsymbol{a}) \equiv \mathcal{F}(|\psi(\boldsymbol{a})\rangle) = \frac{\langle\psi(\boldsymbol{a})|\hat{H}|\psi(\boldsymbol{a})\rangle}{\langle\psi(\boldsymbol{a})|\psi(\mathbf{a})\rangle}}$ on $\mathcal{D}_{\boldsymbol{a}}$

The search for an approximate ground state, and eventually also for approximate excited states, is performed within this set of vectors:

Ground state: $\mathrm{Min}\{\mathcal{F}(\boldsymbol{a})\}_{\boldsymbol{a}\in\mathcal{D}_{\boldsymbol{a}}} \equiv \mathcal{F}(\boldsymbol{a}_0) = \tilde{E}_0 \gtrsim E_0$ is an estimate of the g.s. energy and $|\psi(\boldsymbol{a}_0)\rangle \equiv |\tilde{\psi}_0\rangle \approx |E_0\rangle$ is an estimate of the g.s. eigenvector.

Excited states: If the set of test vectors is sufficiently rich, we can select a subdomain $\mathcal{D}^{(1)}_{\boldsymbol{a}} \subset \mathcal{D}_{\boldsymbol{a}}$ such that $\langle\psi(\boldsymbol{a})|\psi(\boldsymbol{a}_0)\rangle = 0 \;\forall \boldsymbol{a} \in \mathcal{D}^{(1)}_{\boldsymbol{a}}$. Then $\mathrm{Min}\{\mathcal{F}(\boldsymbol{a})\}_{\boldsymbol{a}\in\mathcal{D}^{(1)}_{\boldsymbol{a}}} \equiv \mathcal{F}(\boldsymbol{a}_1) = \tilde{E}_1 \gtrsim E_1$ is an estimate of the 1st excitation energy and $|\psi(\boldsymbol{a}_1)\rangle \equiv |\tilde{\psi}_1\rangle \approx |E_1\rangle$ is an estimate of the 1st e.s. eigenvector. For higher states we can proceed analogously (if the set of test functions is really rich).

◄ Historical remark
1909: W. Ritz publishes a method for solving variational problems
1926: E. Schrödinger uses variational arguments in derivation of stationary Sch. eq.
1930's: P. Dirac, J. Frenkel *et al.* formulate dynamical variational principle of QM

■ Stationary perturbation method

The stationary perturbation method is very useful if the actual Hamiltonian $\hat{H}$ is just a small modification of a simpler Hamiltonian $\hat{H}_0$, whose eigensolutions are known. The difference between both Hamiltonians represents a perturbation which is quantified by a dimensionless parameter λ. If expressing the eigensolutions of $\hat{H}$ as power series in λ, one may believe that high-power terms will naturally die out. A closely related dynamical technique is a principal tool of the present theories of fundamental interactions.

$$\hat{H} = \overbrace{\hat{H}_0}^{\text{unperturbed part}} + \overbrace{\lambda \hat{H}'}^{\text{perturbation}}$$

► Formulation of the problem

We look for eigensolutions of a Hamiltonian given by with the perturbation $\lambda \hat{H}'$ much smaller than $\hat{H}_0$.
Here we assume that both Hamiltonians $\hat{H}_0$ and $\hat{H}'$ are comparable in size (their matrix elements in the relevant energy domain are of the same average size), while the dimensionless parameter $\boxed{\lambda \ll 1}$ sets the smallness of the perturbation. In contrast, some textbooks prefer to consider the size of $\hat{H}'$ much smaller than $\hat{H}_0$ and treat λ just as an auxiliary parameter, whose only role is to indicate the power of $\hat{H}'$ in the relevant equations, and set its value to 1 in the final expressions. Both approaches are equivalent.

For each level $i = 0, 1, 2...$ we know the unperturbed energy E_{0i}. The unperturbed eigenvector $|\psi_{0i}\rangle$ is unique if the level is nondegenerate. In the degenerate case the unperturbed eigenvector is ambiguous within the degeneracy subspace $\mathcal{H}_{0i} \equiv \text{Span}\,\{|\psi_{0i;1}\rangle, |\psi_{0i;2}\rangle, \ldots |\psi_{0i;d_i}\rangle\}$. It will turn out that the perturbation selects an appropriate basis in this subspace.

We assume $[\hat{H}_0, \hat{H}'] \neq 0$, so the perturbation has a nontrivial effect. The task is to expresses the eigensolutions as **power-law series** in λ, so that the size of contributions can be assumed to decrease with increasing power:

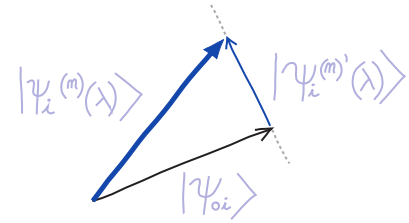
$$\begin{aligned} E_i(\lambda) &= \lambda^0 E_{0i} + \underbrace{\lambda^1 E_{1i} + \lambda^2 E_{2i} + \lambda^3 E_{3i} + \cdots}_{E'_i(\lambda)} \\ |\psi_i(\lambda)\rangle &= \lambda^0 |\psi_{0i}\rangle + \underbrace{\lambda^1 |\psi_{1i}\rangle + \lambda^2 |\psi_{2i}\rangle + \lambda^3 |\psi_{3i}\rangle + \cdots}_{|\psi'_i(\lambda)\rangle} \end{aligned}$$

unnormalized vector

In the nondegenerate case, $|\psi_i(\lambda)\rangle$ represents the expansion of the only eigenvector. In the degenerate case, $|\psi_i(\lambda)\rangle$ expands a *selected vector* from the unperturbed degeneracy subspace $\mathcal{H}_{0i}$. These issues will be clarified below.

Orthogonality condition for the eigenvector correction: $\boxed{\langle\psi_{0i}|\psi_i'(\lambda)\rangle = 0}$

This is a natural requirement since the changes in the direction of the unperturbed vector $|\psi_{0i}\rangle$ can be expressed by normalization. (In some textbooks, the ortogonality is not assumed, but the results are equivalent.)



The term with $\lambda^n \equiv$ the $\boldsymbol{n^{\text{th}}}$**order correction**
The sum of corrections up to $\lambda^n \equiv$ the **total correction in the** $\boldsymbol{n^{\text{th}}}$**order**
The sum of *all* terms up to $\lambda^n \equiv$ the **solution in the** $\boldsymbol{n^{\text{th}}}$ **order**

$$E_i^{(n)}(\lambda) = E_{0i} + \overbrace{\sum_{n'=1}^{n} \lambda^{n'} E_{n'i}}^{E_i^{(n)\prime}(\lambda)} \qquad |\psi_i^{(n)}(\lambda)\rangle = |\psi_{0i}\rangle + \overbrace{\sum_{n'=1}^{n} \lambda^{n'} |\psi_{n'i}\rangle}^{|\psi_i^{(n)\prime}(\lambda)\rangle}$$

Since $\lambda \ll 1$, we may hope in fast convergence, so that some $n = n_{\text{up}}$ gives a sufficient precision:
$$\begin{cases} E_i(\lambda) \approx E_i^{(n_{\text{up}})}(\lambda) \\ |\psi_i(\lambda)\rangle \approx |\psi_i^{(n_{\text{up}})}(\lambda)\rangle \end{cases}$$

Normalization in n^{th}order:
$$|\psi_i^{(n)}(\lambda)\rangle = \overbrace{\frac{1}{\sqrt{1+\langle\psi_i^{(n)\prime}(\lambda)|\psi_i^{(n)\prime}(\lambda)\rangle}}}^{\mathcal{N}^{(n)}(\lambda)} \left[|\psi_{0i}\rangle + |\psi_i^{(n)\prime}(\lambda)\rangle\right]$$

The n^{th}order correction to eigenvectors given as an **expansion in unperturbed eigenbasis**:
$$\boxed{|\psi_{ni}\rangle = \sum_{k\neq i} a_{nik} |\psi_{0k}\rangle}$$
$a_{nii} = 0$ following from the orthogonality condition

▶ Equations for corrections of increasing order

Schrödinger equation:
$$\left[\hat{H}_0 + \lambda \hat{H}'\right]\left(|\psi_{0i}\rangle + \lambda|\psi_{1i}\rangle + \lambda^2|\psi_{2i}\rangle + \lambda^3|\psi_{3i}\rangle + \cdots\right)$$
$$= \left[E_{0i} + \lambda E_{1i} + \lambda^2 E_{2i} + \lambda^3 E_{3i} + \cdots\right]\left(|\psi_{0i}\rangle + \lambda|\psi_{1i}\rangle + \lambda^2|\psi_{2i}\rangle + \lambda^3|\psi_{3i}\rangle + \cdots\right)$$

Comparison of different orders $\propto \lambda^n$:

$$\begin{aligned}
\hat{H}_0|\psi_{0i}\rangle &= E_{0i}|\psi_{0i}\rangle && n=0 \\
\hat{H}_0|\psi_{1i}\rangle + \hat{H}'|\psi_{0i}\rangle &= E_{0i}|\psi_{1i}\rangle + E_{1i}|\psi_{0i}\rangle && n=1 \\
\hat{H}_0|\psi_{2i}\rangle + \hat{H}'|\psi_{1i}\rangle &= E_{0i}|\psi_{2i}\rangle + E_{1i}|\psi_{1i}\rangle + E_{2i}|\psi_{0i}\rangle && n=2 \\
&\cdots \quad \cdots \\
\hat{H}_0|\psi_{ni}\rangle + \hat{H}'|\psi_{(n-1)i}\rangle &= \sum_{n'=0}^{n} E_{n'i}|\psi_{(n-n')i}\rangle && \text{general } n
\end{aligned}$$

▶ Nondegenerate case

The nondegenerate case is easier than the degenerate one, so we start with it. In this case, the solutions in the 0^{th}order are determined from the $n=0$ equation above, which singles out the vector $|\psi_{0i}\rangle$ equal to the unique eigenvector of $\hat{H}_0$.

1st order correction to energy:

Multiply the $n=1$ equation by $\langle\psi_{0i}|$

$$\Rightarrow \quad \underbrace{\langle\psi_{0i}|\hat{H}_0|\psi_{1i}\rangle}_{E_{0i}\langle\psi_{0i}|\psi_{1i}\rangle} + \langle\psi_{0i}|\hat{H}'|\psi_{0i}\rangle = E_{0i}\langle\psi_{0i}|\psi_{1i}\rangle + E_{1i}\overbrace{\langle\psi_{0i}|\psi_{0i}\rangle}^{1}$$

$$\Rightarrow \quad \boxed{E_{1i} = \langle\psi_{0i}|\hat{H}'|\psi_{0i}\rangle}$$

1st order correction to eigenvector:

The $n=1$ equation $\Rightarrow$ $$\left[\hat{H}_0 - E_{0i}\right] \underbrace{\left(\sum_{k\neq i} a_{1ik}|\psi_{0k}\rangle\right)}_{|\psi_{1i}\rangle} = \left[\langle\psi_{0i}|\hat{H}'|\psi_{0i}\rangle - \hat{H}'\right]|\psi_{0i}\rangle$$

Multiply by $\langle\psi_{0j}|$ for $j \neq i$

$$\Rightarrow \quad \sum_{k\neq i}(E_{0j} - E_{0i})\, a_{1ik}\overbrace{\langle\psi_{0j}|\psi_{0k}\rangle}^{\delta_{jk}} = \langle\psi_{0i}|\hat{H}'|\psi_{0i}\rangle\overbrace{\langle\psi_{0j}|\psi_{0i}\rangle}^{0} - \langle\psi_{0j}|\hat{H}'|\psi_{0i}\rangle$$

$$\Rightarrow \quad a_{1ij} = -\frac{\langle\psi_{0j}|\hat{H}'|\psi_{0i}\rangle}{E_{0j}-E_{0i}} \quad \Rightarrow \quad \boxed{|\psi_{1i}\rangle = \sum_{j\neq i}\frac{\langle\psi_{0j}|\hat{H}'|\psi_{0i}\rangle}{E_{0i}-E_{0j}}|\psi_{0j}\rangle}$$

Multiplication by $\langle\psi_{0i}|$ yields just identity
$0 = 0 \Rightarrow a_{1ii}$ undetermined $\Rightarrow$ consistent with the above setting $a_{1ii}=0$

2nd order correction to energy:

Multiply the $n=2$ equation by $\langle\psi_{0i}|$

$$\Rightarrow \quad E_{0i}\langle\psi_{0i}|\psi_{2i}\rangle + \langle\psi_{0i}|\hat{H}'|\psi_{1i}\rangle = E_{0i}\langle\psi_{0i}|\psi_{2i}\rangle + E_{1i}\overbrace{\langle\psi_{0i}|\psi_{1i}\rangle}^{0} + E_{2i}\overbrace{\langle\psi_{0i}|\psi_{0i}\rangle}^{1}$$

$$\Rightarrow \quad E_{2i} = \langle\psi_{0i}|\hat{H}'|\psi_{1i}\rangle \quad \Rightarrow \quad \boxed{E_{2i} = \sum_{j\neq i}\frac{|\langle\psi_{0j}|\hat{H}'|\psi_{0i}\rangle|^2}{E_{0i}-E_{0j}}}$$

General-order correction to energy:

Multiply the general-n equation by $\langle\psi_{0i}|$

$$\Rightarrow \quad E_{0i}\underbrace{\langle\psi_{0i}|\psi_{ni}\rangle}_{0} + \langle\psi_{0i}|\hat{H}'|\psi_{(n-1)i}\rangle = \sum_{n'=0}^{n} E_{n'i}\overbrace{\langle\psi_{0i}|\psi_{(n-n')i}\rangle}^{\delta_{nn'}}$$

$$\Rightarrow \quad \boxed{E_{ni} = \langle\psi_{0i}|\hat{H}'|\psi_{(n-1)i}\rangle}$$

We see that the n^{th}order correction to energy are determined from $(n-1)^{\text{th}}$order correction to the eigenvector.

General-order correction to eigenvector:

$$\left[\hat{H}_0 - E_{0i}\right]\underbrace{\left(\sum_{k\neq i} a_{nik}|\psi_{0k}\rangle\right)}_{|\psi_{ni}\rangle} + \hat{H}'\underbrace{\left(\sum_{k\neq i} a_{(n-1)ik}|\psi_{0k}\rangle\right)}_{|\psi_{(n-1)i}\rangle} = \sum_{n'=1}^{n} E_{n'i}\underbrace{\left(\sum_{k\neq i} a_{(n-n')ik}|\psi_{0k}\rangle\right)}_{|\psi_{(n-n')i}\rangle}$$

Multiply the above general-n equation by $\langle\psi_{0j}|$ for $j \neq i$

$$\Rightarrow \quad [E_{0j} - E_{0i}]\, a_{nij} + \sum_{k\neq i}\langle\psi_{0j}|\hat{H}'|\psi_{0k}\rangle a_{(n-1)ik} = \sum_{n'=1}^{n-1} E_{n'i}a_{(n-n')ij}$$

$$\Rightarrow \qquad \boxed{a_{nij} = \frac{1}{E_{0j} - E_{0i}} \left[\sum_{n'=1}^{n-1} E_{n'i} a_{(n-n')ij} - \sum_{k \neq i} \langle \psi_{0j} | \hat{H}' | \psi_{0k} \rangle a_{(n-1)ik} \right]}$$

We see that the n^{th}order correction to the eigenvector is determined from the corrections to energy & eigenvector of all lower orders $1, 2, \ldots, (n-1)$

If $a_{n'ii} = 0 \; \forall n' \leq (n-1)$, the multiplication by $\langle \psi_{ni}|$ yields just identity $0 = 0$ $\Rightarrow a_{nii}$ undetermined $\Rightarrow$ consistent with the above setting $a_{nii} = 0$

We note that the above-derived corrections contain denominators with differences of the unperturbed energies. These imply that if levels of the unperturbed system come close together, the size of corrections quickly increases. In other words, a generic perturbation gets more efficient in dense parts of the spectrum than in sparse ones.

▶ Degenerate case

What about if the level E_{0i} becomes exactly degenerate? Then the derivation presented above fails and must be redone from the scratch.

The d_i-dimensional degeneracy subspace $\boxed{\mathcal{H}_{0i} = \text{Span}\,\{|\psi_{0i;1}\rangle, |\psi_{0i;2}\rangle, ..., |\psi_{0i;d_i}\rangle\}}$ has a randomly selected basis of vectors satisfying $\langle \psi_{0i;k} | \psi_{0i;l} \rangle = \delta_{kl}$.

The $n = 0$ equation does not determine a unique vector $|\psi_{0i}\rangle \in \mathcal{H}_{0i}$ which would fix the 0^{th}order solution as the starting point for the whole procedure.

We satisfy the $n=0$ equation using $\boxed{|\psi_{0i}\rangle = \sum_{k=1}^{d_i} \alpha_k |\psi_{0i;k}\rangle}$ with $\left\{ \begin{smallmatrix} \alpha_k \equiv \text{unknown} \\ \text{coefficients} \end{smallmatrix} \right\}$ and apply the $n=1$ equation:

$$\hat{H}_0 |\psi_{1i}\rangle + \sum_{k=1}^{d_i} \alpha_k \hat{H}' |\psi_{0i;k}\rangle = E_{0i} |\psi_{1i}\rangle + E_{1i} \sum_{k=1}^{d_i} \alpha_k |\psi_{0i;k}\rangle$$

Multiply by $\langle \psi_{0i;l}|$:

$$E_{0i} \langle \psi_{0i;l} | \psi_{1i} \rangle + \sum_{k=1}^{d_i} \alpha_k \langle \psi_{0i;l} | \hat{H}' | \psi_{0i;k} \rangle = E_{0i} \langle \psi_{0i;l} | \psi_{1i} \rangle + E_{1i} \sum_{k=1}^{d_i} \alpha_k \overbrace{\langle \psi_{0i;l} | \psi_{0i;k} \rangle}^{\delta_{kl}} \quad \Rightarrow$$

$$\boxed{\sum_{k=1}^{d_i} \underbrace{\langle \psi_{0i;l} | \hat{H}' | \psi_{0i;k} \rangle}_{H'_{lk}} \alpha_k = E_{1i} \alpha_l} \quad \Leftrightarrow \quad \boxed{\begin{pmatrix} H'_{11} & H'_{12} & \ldots \\ H'_{21} & H'_{22} & \ldots \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix} = E_{1i} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix}}$$

This represents the **diagonalization of the perturbation matrix** in the degeneracy subspace. We stress that the degeneracy subspace is *not* in general invariant under $\hat{H}'$ (since $[\hat{H}_0, \hat{H}'] \neq 0$), but the above formula implicitly *projects* the action of $\hat{H}'$ to the degeneracy subspace prior the diagonalization.

0^{th}order eigenstates & 1^{st}order energies:

We have d_i energy solutions of polynomial eq. $\quad \text{Det} \begin{pmatrix} H'_{11} - E_{1i} & H'_{12} & \ldots \\ H'_{21} & H'_{22} - E_{1i} & \ldots \\ \vdots & & \ddots \end{pmatrix} = 0$

$\boxed{E_{1i} = E_{1i;k}} \quad k = 1, 2, \ldots d_i$

$\Rightarrow$ The **degeneracy is lifted** in the 1st order correction.

Determination of the corresponding eigenvectors:

$$\begin{pmatrix} H'_{11} & H'_{12} & \dots \\ H'_{21} & H'_{22} & \dots \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} \alpha_{1;k} \\ \alpha_{2;k} \\ \vdots \end{pmatrix} = E_{1i;k} \begin{pmatrix} \alpha_{1;k} \\ \alpha_{2;k} \\ \vdots \end{pmatrix}$$

This equation yields the eigenvector associated with the correction $E_{1i;k}$

$\Rightarrow \boxed{|\psi_{0i}\rangle \mapsto |\tilde{\psi}_{0i;k}\rangle}$

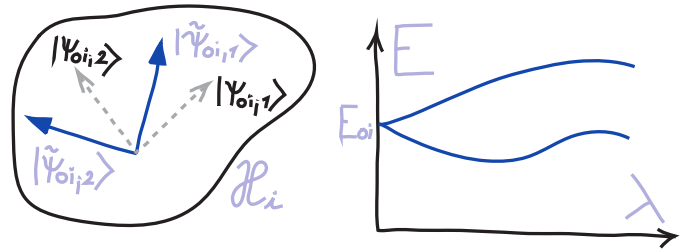
$\Rightarrow$ The perturbation **selects the proper basis** of $\mathcal{H}_{0i}$ in the 0th order.

Eigenfunction in 0th order:

$$|\tilde{\psi}_{0i;k}\rangle = \sum_{l=1}^{d_i} \alpha_{l;k} |\psi_{0i;l}\rangle$$

Energy up to 1st order:

$$\Leftrightarrow \quad E^{(1)}_{i;k}(\lambda) = E_{0i} + \lambda\, E_{1i;k} \qquad k = 1, 2, \dots d_i$$



Special case $d = 2$:

$$\begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = E_{1i} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \quad \Rightarrow \quad \text{Det} \begin{pmatrix} H'_{11}-E_{1i} & H'_{12} \\ H'_{21} & H'_{22}-E_{1i} \end{pmatrix} = 0$$

$$\Rightarrow \text{2 solutions:} \quad E_{1i\pm} = \frac{H'_{11}+H'_{22}}{2} \pm \overbrace{\sqrt{\left(\frac{H'_{11}-H'_{22}}{2}\right)^2 + H'_{12}H'_{21}}}^{D}$$

$$\begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix} \begin{pmatrix} \alpha_{1\pm} \\ \alpha_{2\pm} \end{pmatrix} = E_{1i\pm} \begin{pmatrix} \alpha_{1\pm} \\ \alpha_{2\pm} \end{pmatrix}$$

Lowest-order eigenfunctions & energies:

$$\begin{cases} |\tilde{\psi}_{0i\pm}\rangle = \alpha_{1\pm}|\psi_{0i;1}\rangle + \alpha_{2\pm}|\psi_{0i;2}\rangle \\ E^{(1)}_{i\pm}(\lambda) = E_{0i} + \lambda E_{1i\pm} \end{cases}$$

Higher-order corrections:

Diagonalize the perturbation $\hat{H}'$ in the degeneracy subspace of every level

$\Rightarrow$ orthonormal basis $\left\{\left\{|\tilde{\psi}_{0i;k}\rangle\right\}_{k=1}^{d_i}\right\}_i \quad \Rightarrow \quad \langle\tilde{\psi}_{0i;l}|\hat{H}'|\tilde{\psi}_{0i;k}\rangle = 0$ for $l \neq k$

$\Rightarrow$ the procedure used in non-degenerate case can be reiterated without problems with zero energy denominators. So we obtain:

$$\begin{aligned} E_{i;k}(\lambda) &= E_{0i} + \lambda\langle\tilde{\psi}_{0i;k}|\hat{H}'|\tilde{\psi}_{0i;k}\rangle + \lambda^2 \sum_{j(\neq i)} \sum_{l=1}^{d_j} \frac{|\langle\tilde{\psi}_{0j;l}|\hat{H}'|\tilde{\psi}_{0i;k}\rangle|^2}{E_{0i}-E_{0j}} + \mathcal{O}(\lambda^3) \\ |\psi_{i;k}(\lambda)\rangle &= |\tilde{\psi}_{0i;k}\rangle + \lambda \sum_{j(\neq i)} \sum_{l=1}^{d_j} \frac{\langle\tilde{\psi}_{0j;l}|\hat{H}'|\tilde{\psi}_{0i;k}\rangle}{E_{0i}-E_{0j}} |\tilde{\psi}_{0j;l}\rangle + \mathcal{O}(\lambda^2) \end{aligned}$$

◀ Historical remark

1860's: Ch.-E. Delaunay performs a perturbation analysis of three-body problem

1894: Lord Rayleigh studies harmonic vibrations in presence of small inhomogenities

1926: E. Schrödinger introduces the stationary perturbation theory to QM

■ Application in atomic physics

The primary domain of application of the perturbation theory in the old-day quantum theory was atomic physics. Already the plain hydrogen Hamiltonian needs to be corrected for some subtle internal effects beyond the Coulomb attraction, as well as for effects caused by external electric or magnetic fields.

▶ Alternative eigensolutions of the hydrogen atom

Plain hydrogen Hamiltonian: $\boxed{\hat{H}_0 = -\frac{\hbar^2}{2M}\Delta - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}}$ spectrum $E_n = -\overbrace{\frac{e^2}{4\pi\epsilon_0}\frac{1}{a_\mathrm{B}}}^{\alpha^2 Mc^2}\frac{1}{2n^2}$ $(n=1,2,3\dots)$

Remind (see Sec. 2b) the fine-structure constant $\alpha = \frac{e^2}{4\pi\epsilon_0\lambda\!\!\!^{-}_\mathrm{C}}\frac{1}{Mc^2} = \frac{e^2}{4\pi\epsilon_0\hbar c} \doteq \frac{1}{137}$ and the Bohr radius $a_\mathrm{B} = \frac{\lambda\!\!\!^{-}_\mathrm{C}}{\alpha} = \frac{4\pi\epsilon_0\hbar^2}{Me^2} \doteq 0.53\cdot 10^{-10}\,\mathrm{m}$ (with $\lambda\!\!\!^{-}_\mathrm{C} \equiv \frac{\hbar}{Mc}$).

The eigenvectors are usually expressed as $|\psi_{nlm_l m_s}\rangle$ in the basis of observables $\hat{H}, \hat{L}^2, \hat{L}_z, \hat{S}_z$, but we can also express them as $|\psi_{nljm_j}\rangle$ in the basis of observables $\hat{H}, \hat{L}^2, \hat{J}^2, \hat{J}_z$, using the total (orbital+spin) angular momentum $\vec{\hat{J}}$:

Uncoupled eigenstates: $[\hat{L}_i, \hat{H}_0] = 0 = [\hat{S}_i, \hat{H}_0] \quad\Rightarrow\quad [\underbrace{\hat{L}_i + \hat{S}_i}_{\hat{J}_i}, \hat{H}_0] = 0 \quad i=1,2,3$

$$\boxed{|\psi_{nlm_l m_s}\rangle} \equiv \overbrace{R_{nl}(r)Y_{lm_l}(\vartheta,\varphi)}^{\psi_{nlm_l}(\vec{r})} \overbrace{|\tfrac{1}{2}, m_s\rangle}^{|\uparrow\rangle \text{ or } |\downarrow\rangle}$$

Nomenclature: $nl_{m_s} \equiv \underbrace{1s_{\uparrow\downarrow}}_{E_1}, \underbrace{2s_{\uparrow\downarrow}, 2p_{\uparrow\downarrow}}_{E_2}, \underbrace{3s_{\uparrow\downarrow}, 3p_{\uparrow\downarrow}, 3d_{\uparrow\downarrow}}_{E_3}, \underbrace{4s_{\uparrow\downarrow}, 4p_{\uparrow\downarrow}, 4d_{\uparrow\downarrow}, 4f_{\uparrow\downarrow}}_{E_4} \dots$

Coupled eigenstates:

$$\boxed{|\Psi_{nljm_j}\rangle} = \underbrace{C^{jm_j}_{l(m_j-\frac{1}{2})\frac{1}{2}(+\frac{1}{2})}}_{\pm\sqrt{\frac{l\pm m_j+\frac{1}{2}}{2l+1}}} \underbrace{\psi_{nl(m_j-\frac{1}{2})}(\vec{r})}_{R_{nl}Y_{l(m_j-\frac{1}{2})}} \underbrace{|\uparrow\rangle}_{\binom{1}{0}} + \underbrace{C^{jm_j}_{l(m_j+\frac{1}{2})\frac{1}{2}(-\frac{1}{2})}}_{\sqrt{\frac{l\mp m_j+\frac{1}{2}}{2l+1}}} \underbrace{\psi_{nl(m_j+\frac{1}{2})}(\vec{r})}_{R_{nl}Y_{l(m_j+\frac{1}{2})}} \underbrace{|\downarrow\rangle}_{\binom{0}{1}}$$

$\boxed{j = l \pm \frac{1}{2}}$

$$= R_{nl}(r) \underbrace{\frac{1}{\sqrt{2l+1}} \begin{pmatrix} \pm\sqrt{l\pm m_j+\frac{1}{2}}\; Y_{l(m_j-\frac{1}{2})}(\vartheta,\varphi) \\ \sqrt{l\mp m_j+\frac{1}{2}}\; Y_{l(m_j+\frac{1}{2})}(\vartheta,\varphi) \end{pmatrix}}_{\mathcal{Y}_{ljm_j}(\vartheta,\varphi)} \quad \textbf{spinor spherical functions}$$

Nomenclature: $nl_j \equiv \underbrace{1s_{\frac{1}{2}}}_{E_1}, \underbrace{2s_{\frac{1}{2}}, 2p_{\frac{1}{2}}, 2p_{\frac{3}{2}}}_{E_2}, \underbrace{3s_{\frac{1}{2}}, 3p_{\frac{1}{2}}, 3p_{\frac{3}{2}}, 3d_{\frac{3}{2}}, 3d_{\frac{5}{2}}}_{E_3}, \dots$

▶ Stark effect

Hydrogen atom in a homogeneous external **electric field** of intensity $\vec{\mathcal{E}}_\lambda \equiv \lambda\mathcal{E}_1\vec{n}_z$ (we introduce a dimensionless factor λ to scale the intensity):

$\hat{H} = \hat{H}_0 + \lambda\hat{H}'$ with $\boxed{\hat{H}' = e\mathcal{E}_1 z} \equiv \hat{T}^1_0$ component of a spherical vector

Unperturbed hydrogen solutions expressed in the uncoupled basis $|\psi_{nlm_l m_s}\rangle$

Selection rules for matrix elements:

(a) $\langle\psi_{nlm_l m_s}|\hat{H}'|\psi_{nlm_l m_s}\rangle = 0 \quad\Leftarrow\quad$ parity conservation $(\int \overbrace{|\psi_{nlm_l}(\vec{r})|^2}^{\text{even}}\, z\, d\vec{r} = 0)$

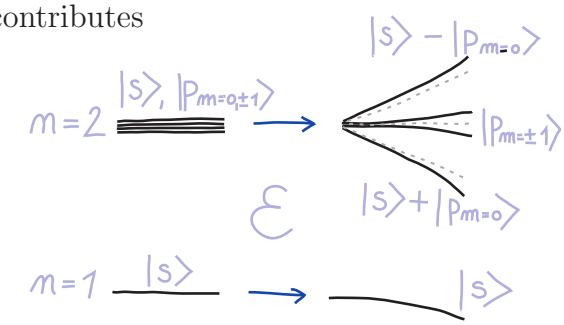
(b) $\langle\psi_{n'l'm'_l m'_s}|\hat{H}'|\psi_{nlm_l m_s}\rangle = 0$ for $m'_l \neq m_l$ or $m'_s \neq m_s$ or $|l-l'|>1 \quad\Leftarrow$ Wigner−Eckart theorem

We disregard spin quantum number m_s as the interaction does not affect it

Ground-state: the 1st order term vanishes (reasoning: any state with a good parity shows no electric dipole moment ⇒ no linear effect of an electric field)

Correction up to **2nd order**: $E_1^{(2)} = E_1 + (e\mathcal{E}_\lambda)^2 \sum_{n=2}^{\infty} \sum_{l=0}^{n-1} \sum_{m_l=-l}^{+l} \frac{|\langle\psi_{nlm_l}|z|\psi_{100}\rangle|^2}{E_1 - E_n} < E_1$

Excited-states: the **1st order** term contributes (reasoning: "accidental" degeneracy in the H atom involves states with different parity ⇒ a superposition of such states, as obtained in the degenerate-case perturb. expression, can yield electric dipole moment $\neq 0$)



Example: $n = 2$ shell with $l = 0, 1$

We proceed according to the degenerate-case perturbation theory. According to the above selection rules, the only nonzero matrix element within the degeneracy subspace is the following one (its calculation is not presented here):

$$\langle\psi_{210}|\hat{H}'|\psi_{200}\rangle = \langle\psi_{200}|\hat{H}'|\psi_{210}\rangle = -3a_\mathrm{B}e\mathcal{E}_1$$

$$-3a_\mathrm{B}e\mathcal{E}_1 \begin{pmatrix} 0&0&1&0\\ 0&0&0&0\\ 1&0&0&0\\ 0&0&0&0 \end{pmatrix} \begin{pmatrix} \alpha_{200}\\ \alpha_{21(-1)}\\ \alpha_{210}\\ \alpha_{21(+1)} \end{pmatrix} = \Delta E \begin{pmatrix} \alpha_{200}\\ \alpha_{21(-1)}\\ \alpha_{210}\\ \alpha_{21(+1)} \end{pmatrix} \quad \Rightarrow$$

$\lvert\psi_{0;k}\rangle$		$E_2^{(1)}$
$\frac{1}{\sqrt{2}}(\lvert\psi_{200}\rangle+\lvert\psi_{210}\rangle)$	⇒	$E_2 - 3a_\mathrm{B}e\mathcal{E}_\lambda$
$\frac{1}{\sqrt{2}}(\lvert\psi_{200}\rangle-\lvert\psi_{210}\rangle)$	⇒	$E_2 + 3a_\mathrm{B}e\mathcal{E}_\lambda$
$\lvert\psi_{21(-1)}\rangle$	⇒	E_2
$\lvert\psi_{21(+1)}\rangle$	⇒	E_2

The states with eigenvalues $\Delta E \neq 0$ show the linear Stark effect, those with $\Delta E = 0$ show the quadratic Stark effect.

▶ Zeeman effect

Hydrogen atom in a homogeneous external **magnetic field** of induction $\vec{B}_\lambda \equiv \lambda B_1 \vec{n}_z$ (where we again use a dimensionless field scaling factor λ):

$$\hat{H} = \hat{H}_0 + \lambda\hat{H}' \quad \text{with} \quad \boxed{\hat{H}' = -\tfrac{e}{2M}B_1(\hat{L}_z + 2\hat{S}_z)} = -\tfrac{e}{2M}B_1(\hat{J}_z + \hat{S}_z)$$

Here we used $\hat{H}' = -(\hat{\vec{\mu}}_l + \hat{\vec{\mu}}_s)\cdot\vec{B}$ with the orbital and spin magnetic moments expressed via gyromagnetic ratios $g_l = 1$ and $g_s = 2$ (Sec. 2b).

The perturbation is **diagonalized in the uncoupled basis**:

$$\langle\psi_{nlm_lm_s}|\hat{H}'|\psi_{nlm_lm_s}\rangle = -\underbrace{\tfrac{e\hbar}{2M}}_{\mu_\mathrm{B}\ \text{(Bohr magneton)}} B_1(m_l + 2m_s)$$

This is the exact solution, no perturbation theory is needed.

The 1st order perturbation formula can be used to express the energy corrections in the **coupled basis**: $\langle\Psi_{nljm_j}|\hat{H}'|\Psi_{nljm_j}\rangle =$ (using $\hat{L}_z + 2\hat{S}_z = \hat{J}_z + \hat{S}_z$)

$$-\mu_\mathrm{B}B_1\left[m_j + \tfrac{1}{2}(C^{jm_j}_{l(m_j-\frac{1}{2})\frac{1}{2}(+\frac{1}{2})})^2 - \tfrac{1}{2}(C^{jm_j}_{l(m_j+\frac{1}{2})\frac{1}{2}(-\frac{1}{2})})^2\right] = \begin{cases} -\mu_\mathrm{B}B_1\frac{2l+2}{2l+1}m_j & \text{for } j = l+\frac{1}{2} \\ -\mu_\mathrm{B}B_1\frac{2l}{2l+1}m_j & \text{for } j = l-\frac{1}{2} \end{cases}$$

▶ Spin-orbital coupling

Correction caused by an interaction of the spin **magnetic moment** of electron with the magnetic field generated by its orbital motion. In the electron's rest frame, this can be seen as an interaction of its magnetic moment with the magnetic field produced by a "moving" nucleus (then a relativistic effect, so-called Thomas precession, must be taken into account). The crucial operator term that appears in the perturbation Hamiltonian is $(\hat{\vec{L}}\cdot\hat{\vec{S}})$, which is why this correction is called the spin-orbital interaction. To evaluate the action of this operator, we use the identity $\hat{\vec{J}}^2 = \big(\hat{\vec{L}}+\hat{\vec{S}}\big)^2 = \hat{\vec{L}}^2+\hat{\vec{S}}^2+2\hat{\vec{L}}\cdot\hat{\vec{S}}$, which leads to an expression diagonal in the coupled basis $|\psi_{nljm_j}\rangle$. The resulting perturbation term for the hydrogen Hamiltonian reads as follows:

$$\hat{H}' = \tfrac{e^2}{4\pi\epsilon_0}\tfrac{1}{2M^2c^2}\tfrac{1}{r^3}(\hat{\vec{L}}\cdot\hat{\vec{S}}) = \tfrac{1}{4}\alpha^4Mc^2\big(\tfrac{a_\mathrm{B}}{r}\big)^3\tfrac{1}{\hbar^2}\left(\hat{\vec{J}}^2-\hat{\vec{L}}^{\,2}-\hat{\vec{S}}^{\,2}\right)$$

1st order effect in the **coupled basis**:

$$\langle\psi_{nljm_j}|\hat{H}'|\psi_{nljm_j}\rangle = \tfrac{1}{4}\alpha^4Mc^2\left[j(j{+}1)-l(l{+}1)-\tfrac{3}{4}\right]\overbrace{\langle\psi_{nljm_j}|\big(\tfrac{a_\mathrm{B}}{r}\big)^3|\psi_{nljm_j}\rangle}^{a_\mathrm{B}^3\int_0^\infty \frac{1}{r^3}|R_{nl}(r)|^2r^2dr\equiv\langle(\frac{r}{a_\mathrm{B}})^{-3}\rangle_{nl}}$$

$$= \begin{cases} +\tfrac{1}{4}\alpha^4Mc^2\langle(\tfrac{r}{a_\mathrm{B}})^{-3}\rangle_{nl}\,l & \text{for } j=l{+}\tfrac{1}{2} \\ -\tfrac{1}{4}\alpha^4Mc^2\langle(\tfrac{r}{a_\mathrm{B}})^{-3}\rangle_{nl}\,(l{+}1) & \text{for } j=l{-}\tfrac{1}{2}\end{cases}$$

Assuming $\langle(\frac{r}{a_\mathrm{B}})^k\rangle_{nl}\sim 1$, we see that the relative corrections with respect to the unperturbed energies are of the order $\frac{\Delta E_{nl}}{E_n}\sim\alpha^2\sim 10^{-4}$.

▶ Relativistic correction

The correction due to the spin-orbital coupling is of the same order of magnitude as another correction of a completely different nature, namely the correction caused by relativistic deviations from the familiar kinetic energy formula $\frac{p^2}{2M}$.

Rel. **kinetic energy**: $T = \underbrace{\sqrt{(Mc^2)^2+(pc)^2}}_{Mc^2\sqrt{1+(\frac{p}{Mc})^2}} - Mc^2 \approx \underbrace{\tfrac{p^2}{2M} - \tfrac{1}{2Mc^2}\left(\tfrac{p^2}{2M}\right)^2}_{\sqrt{1+\delta}=1+\frac{\delta}{2}-\frac{\delta^2}{8}+\ldots} + \ldots$

The effect of this correction can be treated within the non-relativistic QM, adding to $\hat{H}_0$ a perturbation term:

$$\hat{H}' = -\tfrac{1}{2Mc^2}\left(\tfrac{\hat{p}^2}{2M}\right)^2 = -\tfrac{1}{2Mc^2}(\hat{H}_0-\hat{V})^2$$

1st order effect in the **coupled basis**:

$$\langle\psi_{nljm_j}|\hat{H}'|\psi_{nljm_j}\rangle = -\tfrac{1}{2Mc^2}\left[E_n^2 - 2E_n\overbrace{\langle\psi_{nljm_j}|\hat{V}|\psi_{nljm_j}\rangle}^{\alpha^2Mc^2\langle(\frac{r}{a_\mathrm{B}})^{-1}\rangle_{nl}} + \overbrace{\langle\psi_{nljm_j}|\hat{V}^2|\psi_{nljm_j}\rangle}^{(\alpha^2Mc^2)^2\langle(\frac{r}{a_\mathrm{B}})^{-2}\rangle_{nl}}\right]$$

Using an estimate $\langle(\frac{r}{a_\mathrm{B}})^k\rangle_{nl}\sim 1$, we obtain relative corrections $\frac{\Delta E_{nl}}{E_n}\sim\alpha^2\sim 10^{-4}$.

▶ Fine structure of hydrogen levels

After the precise evaluation of all radial integrals, the spin-orbital coupling and the relativistic correction together yield a formula describing the fine structure

of hydrogen levels: $\boxed{\Delta E_{\rm FS} \approx -\alpha^4 Mc^2 \frac{1}{4n^4}\left(\frac{2n}{j+\frac{1}{2}} - \frac{3}{2}\right)}$ We see that this formula partly lifts the accidental degeneracy of unperturbed hydrogen levels in quantum number l (see Sec. 4b). Note that the Zeeman splitting for magnetic field strengths $B \in (1, 10)$ T would be of the same order of magnitude.

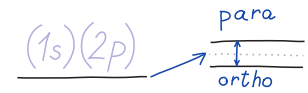
▶ Helium atom

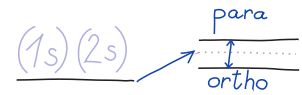
We know (Sec. 2b) that the non-relativistic description of multi-electron atoms has to include the mutual electric repulsion of electrons (besides single-particle terms of individual electrons expressing their kinetic energy and potential energy in the attractive Coulomb field of the nucleus). This in general requires to use many-body techniques such as the mean-field method. Here we present a simple treatment of the 2-electron Hamiltonian of helium in terms of the perturbation theory. The Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'$ (we set $\lambda = 1$) is defined by:
$\hat{H}_0 = -\frac{\hbar^2}{2M}(\Delta_1 + \Delta_2) - \frac{2e^2}{4\pi\epsilon_0}\left(\frac{1}{|\vec{x}_1|} + \frac{1}{|\vec{x}_2|}\right) \qquad \hat{H}' = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{x}_1 - \vec{x}_2|}$
The calculation can be performed in the coupled spin basis of both electrons:
$|S, M_S\rangle = \begin{cases} |0,0\rangle & \textbf{singlet} \text{ (antisymmetric under exchange)} \\ |1,M_S\rangle & \textbf{triplet} \text{ (symmetric under exchange)} \end{cases}$
As the total 2-electron wavefunction must be antisymmetric under the exchange (fermions), the orbital part associated with spin singlet/triplet is symmetric/antisymmetric:

$$\Psi_{0\pm}(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}\big[\overbrace{\psi_{n_1 l_1 m_1}(\vec{x}_1)}^{\psi_1(\vec{x}_1)}\overbrace{\psi_{n_2 l_2 m_2}(\vec{x}_2)}^{\psi_2(\vec{x}_2)} \pm \overbrace{\psi_{n_2 l_2 m_2}(\vec{x}_1)}^{\psi_2(\vec{x}_1)}\overbrace{\psi_{n_1 l_1 m_1}(\vec{x}_2)}^{\psi_1(\vec{x}_2)}\big]$$

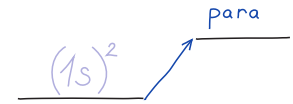
Define $E^{\rm A}_{12} = \begin{cases} \frac{e^2}{4\pi\epsilon_0}\int \psi_1^*(\vec{x}_1)\psi_2^*(\vec{x}_2)\frac{1}{|\vec{x}_1-\vec{x}_2|}\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\ d\vec{x}_1 d\vec{x}_2 \\ \frac{e^2}{4\pi\epsilon_0}\int \psi_2^*(\vec{x}_1)\psi_1^*(\vec{x}_2)\frac{1}{|\vec{x}_1-\vec{x}_2|}\psi_2(\vec{x}_1)\psi_1(\vec{x}_2)\ d\vec{x}_1 d\vec{x}_2 \end{cases}$

and $E^{\rm B}_{12} = \begin{cases} \frac{e^2}{4\pi\epsilon_0}\int \psi_1^*(\vec{x}_1)\psi_2^*(\vec{x}_2)\frac{1}{|\vec{x}_1-\vec{x}_2|}\psi_2(\vec{x}_1)\psi_1(\vec{x}_2)\ d\vec{x}_1 d\vec{x}_2 \\ \frac{e^2}{4\pi\epsilon_0}\int \psi_2^*(\vec{x}_1)\psi_1^*(\vec{x}_2)\frac{1}{|\vec{x}_1-\vec{x}_2|}\psi_1(\vec{x}_1)\psi_2(\vec{x}_2)\ d\vec{x}_1 d\vec{x}_2 \end{cases}$





1st order energy correction:
Singlet & triplet spin states are degenerate, but $\hat{H}'$ is diagonal in these states ⇒ the nondegenerate case expression is applicable:



$\langle\Psi_{0\pm}|\hat{H}'|\Psi_{0\pm}\rangle = \frac{1}{2}(E^{\rm A}_{12} + E^{\rm A}_{12} \pm E^{\rm B}_{12} \pm E^{\rm B}_{12}) = E^{\rm A}_{12} \pm E^{\rm B}_{12}$

For spin $\left\{\begin{matrix}\text{singlet} \\ \text{triplet}\end{matrix}\right\}$ states the energies up to 1st order are: $E_i^{(1)} = E_{0i} + \begin{cases} E^{\rm A}_{12} + E^{\rm B}_{12} \\ E^{\rm A}_{12} - E^{\rm B}_{12} \end{cases}$

We stress that the correction is in fact not small (potential energy of the electron-electron interaction is comparable to that of the proton-electron interaction), so higher-order expressions would be needed for a qualitative description. Nevertheless, the above calculation shows the most essential effect.

The splitting of singlet & triplet states is a direct witness of the indistinguishability principle in action! The corresponding subsets of the helium spectrum (connected only by weak electromagnetic transitions) form two seemingly distinct helium species, called **parahelium** & **orthohelium**.

◄ Historical remark

1892: F. Paschen & C. Runge discover the splitting of He spectrum
1897: P. Zeeman discovers the splitting of atomic lines in magnetic field
1913: J. Stark & A. Lo Surdo discover the effect of electric field on atomic levels
1916: A. Sommerfeld introduces the fine-structure constant and calculates the relativistic splitting of hydrogen levels within the old QM
1925: so-called anomalous Zeeman effect contributes to the discovery of spin
1925-6: L. Thomas presents relativistic calculation of atomic spin-orbital interaction
1926: W. Heisenberg explains the split He spectrum via electron exchange symmetry

■ Application to level dynamics

So far it was assumed that the parameter λ, weighting the perturbation term in the Hamiltonian, has a fixed (small) value. However, one may think of Hamiltonians $\hat{H}(\lambda)$ for which $\lambda \in \mathbb{R}$ is a control parameter that can vary in a large domain. The energy spectrum $E_i(\lambda)$ and the set of eigenvectors $|\psi_i(\lambda)\rangle$ change with running λ and one may use the perturbation theory to write down a set of differential equations governing these changes (sometimes referred to as "level dynamics") in terms of local properties of the spectrum at given λ. The most interesting situations are encountered if the variation of λ leads to a qualitative change of the nature of the evolving eigenstates.

► Hamiltonian with a linear parametric dependence

We assume a linear dependence: $\boxed{\hat{H}(\lambda) = \hat{H}_0 + \lambda\,\hat{H}'}$ $\quad \lambda \in (-\infty, +\infty)$

Perturbative treatment at any λ: $\hat{H}(\lambda+\delta\lambda) = \underbrace{\hat{H}_0 + \lambda\,\hat{H}'}_{\hat{H}(\lambda)} + (\delta\lambda)\,\hat{H}'$

Level dynamics:

evolving energy levels $\boxed{E_i(\lambda) \quad \longleftrightarrow \quad x_i(t)}$ "particle trajectories" in 1D

► Local "dynamical" equations obtained from the perturbation theory

$\frac{d}{d\lambda}E_i(\lambda) = \langle\psi_i(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle \quad \Rightarrow \boxed{\dot{E}_i = H'_{ii}}$ velocity

$\frac{d^2}{d\lambda^2}E_i(\lambda) = 2\sum_{j(\neq i)} \frac{|\langle\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle|^2}{E_i(\lambda)-E_j(\lambda)} \Rightarrow \boxed{\ddot{E}_i = 2\sum_{j(\neq i)} \frac{|H'_{ji}|^2}{E_i-E_j}}$ acceleration

The "force" on the right-hand side of the last equation consists of terms $\propto \frac{1}{E_i-E_j}$, which are analogous to the Coulomb repulsion force $|\vec{F}| \propto \frac{1}{|\vec{x}_i-\vec{x}_j|}$ on particle i

interacting with another charged particle j in a 2D world. However, mind that in the present case, the numerator in the force expression cannot be factorized to individual "charges": $|H'_{ji}|^2 \neq q_j q_i$.

$$\tfrac{d}{d\lambda}\langle\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle = \langle\tfrac{d}{d\lambda}\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle + \langle\psi_j(\lambda)|\hat{H}'|\tfrac{d}{d\lambda}\psi_i(\lambda)\rangle =$$
$$\sum_{k(\neq j)} \tfrac{\langle\psi_j(\lambda)|\hat{H}'|\psi_k(\lambda)\rangle}{E_j(\lambda)-E_k(\lambda)}\langle\psi_k(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle + \sum_{k(\neq i)}\langle\psi_j(\lambda)|\hat{H}'|\psi_k(\lambda)\rangle\tfrac{\langle\psi_k(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle}{E_i(\lambda)-E_k(\lambda)}$$

$$\Rightarrow \quad \boxed{\dot{H}'_{ji} = \sum_{k(\neq j)} \tfrac{H'_{jk}H'_{ki}}{E_j-E_k} + \sum_{k(\neq i)} \tfrac{H'_{jk}H'_{ki}}{E_i-E_k}} \quad \text{evolution of matrix elements } H'_{ji}$$

For given $E_i(0)$ & $H'_{ji}(0)$ $(\forall\, i,j)$ the above system of differential equations allows one can calculate $E_i(\lambda)$ & $H'_{ji}(\lambda)$ for any λ. There exist many **"integrals of motion"** (in the sense $\lambda \equiv t$), in fact so many of them that the system is integrable. For instance:

$$P = \mathrm{Tr}\hat{H}' = \sum_i H'_{ii} = \sum_i \dot{E}_i = \text{const}$$
$$W = \tfrac{1}{2}\mathrm{Tr}(\hat{H}')^2 = \tfrac{1}{2}\sum_{i,j} H'_{ij}H'_{ji} = \tfrac{1}{2}\sum_i \dot{E}_i^2 + \tfrac{1}{2}\sum_{i\neq j}|H'_{ij}|^2 = \text{const}$$

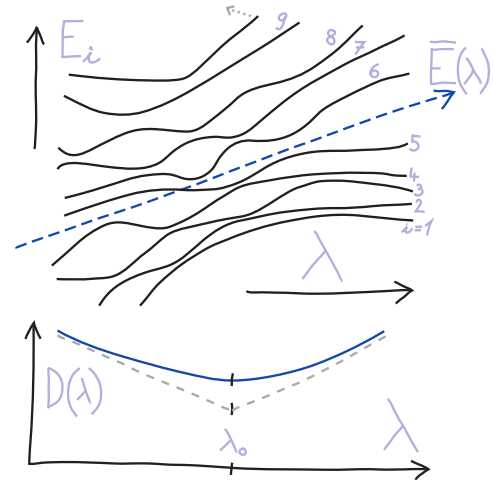
▶ Global properties of spectrum
for finite dimension d

The "center of mass" of the spectrum evolves linearly with λ:

$$\bar{E}(\lambda) \equiv \tfrac{1}{n}\sum_i E_i(\lambda) = \tfrac{1}{n}\mathrm{Tr}\hat{H}(\lambda)$$
$$= \left[\tfrac{1}{n}\mathrm{Tr}\hat{H}_0\right] + \lambda\left[\tfrac{1}{n}\hat{H}'\right]$$

The variance (squared spread) of the spectrum evolves quadratically with λ:

$$D(\lambda) \equiv \sqrt{\tfrac{1}{n}\sum_i [E_i(\lambda)-\bar{E}(\lambda)]^2}$$
$$= \sqrt{\tfrac{1}{n}\sum_i E_i(\lambda)^2 - \bar{E}^2(\lambda)} =$$



$$\sqrt{\left[\tfrac{1}{n}\mathrm{Tr}\hat{H}_0^2 - \tfrac{1}{n^2}\mathrm{Tr}^2\hat{H}_0\right] + \lambda\left[\tfrac{2}{n}\mathrm{Tr}(\hat{H}_0\hat{H}') - \tfrac{2}{n^2}\mathrm{Tr}\hat{H}_0\mathrm{Tr}\hat{H}'\right] + \lambda^2\left[\tfrac{1}{n}\mathrm{Tr}(\hat{H}')^2 - \tfrac{1}{n^2}\mathrm{Tr}^2\hat{H}'\right]}$$

The spectrum is maximally compressed [reaches a minimal spread $D(\lambda)$] at a certain value $\lambda = \lambda_0$, while for $\lambda \to \pm\infty$ the spectrum freely expands: $D(\lambda) \propto \lambda$.

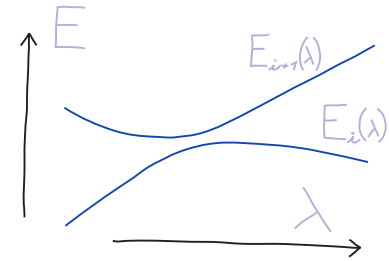
▶ No-crossing rule

The equation for $\ddot{E}_i$, which contains the repulsive 2D Coulomb "force", prevents the levels of the spectrum to cross each other. Consider a crossing of two levels at $\lambda = \lambda_\times$. Near the crossing, the dynamics of the two levels is well approximated by the corresponding 2-level Hamiltonian, which in general yields:

$$\hat{h}(\lambda)=\begin{pmatrix} e_1(\lambda) & v(\lambda) \\ v(\lambda)^* & e_2(\lambda)\end{pmatrix} \Rightarrow \text{energies } E_{\frac{1}{2}}(\lambda)=\tfrac{e_1(\lambda)+e_2(\lambda)}{2}\mp\sqrt{\left[\tfrac{e_1(\lambda)-e_2(\lambda)}{2}\right]^2+|v(\lambda)|^2}$$

To get $E_1(\lambda_\times)=E_2(\lambda_\times)$, one needs to simultaneously satisfy 2 real equations: $e_1(\lambda_\times)=e_2(\lambda_\times)$ and $|v(\lambda_\times)|=0$. This is not generically achievable with just a single real variable parameter λ, except of some accidental rare cases.

Instead of real crossings there exist numerous so-called **avoided crossings** of energy levels (close encounters with subsequent split-ups). At such places, the corresponding eigenfunctions change very rapidly, as can be seen from the overlap formula ($\lambda\to\lambda+\delta\lambda$ survival probability):



$$\mathfrak{p}_i(\lambda,\delta\lambda)\equiv|\langle\psi_i(\lambda+\delta\lambda)|\psi_i(\lambda)\rangle|^2=1-\delta\ell_i^2(\lambda)\approx 1-(\delta\lambda)^2\sum_{j(\neq i)}\tfrac{|\langle\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle|^2}{[E_i(\lambda)-E_j(\lambda)]^2}$$

Here, $\delta\ell_i^2(\lambda)=g_i^{\lambda\lambda}(\lambda)\,(\delta\lambda)^2$ can be interpreted as an infinitesimal squared **distance** between parameter points λ and $\lambda+\delta\lambda$ with respect to the variation of the i^{th}level eigenfunction. Then $g_i^{\lambda\lambda}$ is identified with the i^{th}level **quantum metric tensor** (generalization to matrices $g_i^{\lambda\mu}$ in higher-dimensional parameter spaces is obvious). We see that near the avoided crossing $g_i^{\lambda\lambda}(\lambda)$ is large, so the distance $\ell_i(\lambda_0,\lambda)=\int_{\lambda_0}^{\lambda}\sqrt{g_i^{\lambda\lambda}(\lambda')}d\lambda'$ from λ_0 to λ grows quickly when λ goes through the avoided crossing.

Proof of the overlap formula: $|\langle\psi_i(\lambda+\delta\lambda)|\psi_i(\lambda)\rangle|^2=$

$$\langle\psi_i(\lambda+\delta\lambda)\overbrace{|\psi_i(\lambda)\rangle\langle\psi_i(\lambda)|}^{\hat{I}-\sum_{j(\neq i)}|\psi_j(\lambda)\rangle\langle\psi_j(\lambda)|}\psi_i(\lambda+\delta\lambda)\rangle=1-\sum_{j(\neq i)}\overbrace{|\langle\psi_j(\lambda)|\psi_i(\lambda+\delta\lambda)\rangle|^2}^{(\delta\lambda)^2\frac{|\langle\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle|^2}{[E_i(\lambda)-E_j(\lambda)]^2}}$$

On the other hand, **real crossings** are abundant if matrix elements H'_{ji} between some subsets of levels vanish identically. This typically happens because of some **symmetries** of the system. For example, the rotational symmetry yields $H'_{ji}=0$ for levels i,j with total angular momentum quantum numbers $j_i\neq j_j$:

$$0=\langle\psi_j(\lambda)|\underbrace{[\hat{H}',\hat{J}^2]}_{0}|\psi_i(\lambda)\rangle=\hbar^2\underbrace{[j_i(j_i+1)-j_j(j_j+1)]}_{\neq 0}\underbrace{\langle\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle}_{\Rightarrow\ =0}$$

We stress that the crossing of levels with different symmetry quantum numbers has no effect on the corresponding eigenvectors.

For a given pair of levels i and $i+1$, the *avoided crossings* (minimal spacing $\Delta=E_{i+1}-E_i$) appear at individual points along a single parameter axis λ, and generally on some $(n$–$1)$-dimensional subsets of n-dimensional parameter spaces $\boldsymbol{\lambda}\equiv(\lambda_1,...,\lambda_n)$, in particular along some curves in $n=2$ spaces. In contrast, the *real degeneracies* of levels with the same symmetry quantum numbers form

$(n-2)$-dimensional subsets in n-dimensional parameter spaces, so in particular they appear as isolated points (so-called **diabolic points**) in $n=2$ spaces.

▶ Quantum phase transitions

In some systems, an increasing size parameter N (typically a number of particles or other elementary constituents) induces lowering of matrix elements

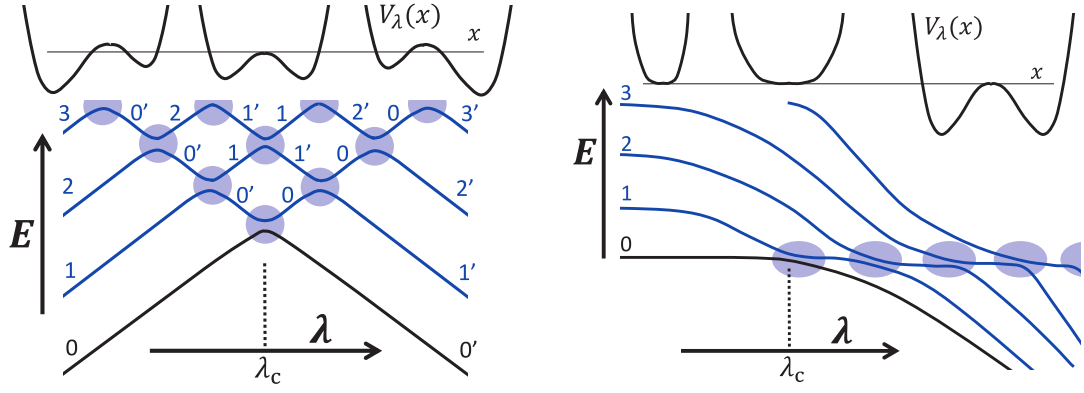
$$H'_{ji}(\lambda) \equiv \langle\psi_j(\lambda)|\hat{H}'|\psi_i(\lambda)\rangle = [E_j(\lambda)-E_i(\lambda)]\langle\dot{\psi}_j(\lambda)|\psi_i(\lambda)\rangle$$

This is due to the asymptotic behavior $\langle\dot{\psi}_j(\lambda)|\psi_i(\lambda)\rangle \overset{N\to\infty}{\longrightarrow} 0$ resulting from a dominantly power-law scaling of scalar products with N (this would be exact for states factorized in individual constituents). As a consequence, the avoided crossings become **gapless** in the limit $N\to\infty$.

Assume that $E_1(\lambda_c)-E_0(\lambda_c) \overset{N\to\infty}{\longrightarrow} 0$. The point λ_c of asymptotically unavoided crossing of the **ground & first-excited states** is the **critical point** of the (ground-state) quantum phase transition. From the degenerate perturbation theory at $\lambda=\lambda_c$ we obtain generic eigensolutions for small $\delta\lambda=\lambda-\lambda_c$:

$$E_0(\lambda)\approx E_0(\lambda_c))+\begin{cases}\delta\lambda\, E_{10+} & \text{for } \delta\lambda<0\\ \delta\lambda\, E_{10-} & \text{for } \delta\lambda>0\end{cases} \qquad E_1(\lambda)\approx E_0(\lambda_c))+\begin{cases}\delta\lambda\, E_{10-} & \text{for } \delta\lambda<0\\ \delta\lambda\, E_{10+} & \text{for } \delta\lambda>0\end{cases}$$

where $E_{10+}>E_{10-}$ are eigenvalues of $\hat{H}'$ in the degeneracy subspace. The levels and the corresponding eigenvectors swap at $\lambda=\lambda_c \Rightarrow$ the first derivative of energy $\frac{d}{d\lambda}E_0(\lambda)$ and the eigenvector $|\psi_0(\lambda)\rangle$ are discontinuous. This situation is referred to as the **discontinuous** (first order) quantum phase transition. It is commonly pictured via a Hamiltonian with two potential wells, one increasing and one decreasing in energy: the critical point is where both wells become degenerate. Such systems also typically show multiple crossings of excited states, in which the structures of the corresponding wavefunctions swap.



Another type of ground-state criticality, a **continuous** quantum phase transition, arises when the matrix element $H'_{10}(\lambda)$ increases with $\lambda\to\lambda_c$ and the level energies are affected so that $E_0(\lambda)$ does not develop a discontinuity but a softer kind of nonanalyticity that occurs in some higher derivatives $\frac{d^k}{d\lambda^k}E_0(\lambda_c)$. Also

the eigenvector $|\psi_0(\lambda)\rangle$ changes continuously, with nonanalyticity affecting only some derivatives. This is often pictured via a single-well Hamiltonian evolving in such a way that the minimum becomes locally flat (quartic) at $\lambda = \lambda_c$ and bifurcates into two quadratic minima (and one maximum in between). Again, the accompanying crossings of excited states often come in some typical patterns.

◀ Historical remark

1929: J. von Neumann & E. Wigner formulate the no-crossing rule
1932: L. Landau & C. Zener calculate transition rate for a 2-level avoided crossing
1970's-present: investigation of quantum phase transitions in specific systems
1980: J.P. Provost & G. Vallee introduce the quantum metric tensor
1980's: P. Pechukas & T. Yukawa elaborate the Coulomb analogy for level dynamics

11. NONSTATIONARY APPROXIMATION METHODS

The goal of this section is to introduce some techniques for approximate solutions of quantum dynamical problems. We start with the most commonly used method — the nonstationary perturbation theory — and then briefly outline some computational approaches to externally driven systems, which attract growing attention due to their potential role in quantum simulations and related applications.

■ Nostationary perturbation method

The basic approximation method for nonstationary problems is conceptually close to the stationary perturbation method. It assumes the total Hamiltonian being split to the principal stationary part $\hat{H}_0$ and a small perturbation $\lambda\hat{H}'(t)$, which may (but does not have to) be time-dependent. The task is to estimate the probabilities per time unit for transitions between various eigenstates of the main Hamiltonian induced by the perturbation. Here we focus mainly on the general formulation of the method. We will see that its application to realistic problems, particularly to decay and scattering processes, may be technically involved because of a rather difficult structure of the corresponding Hilbert spaces (associated with typically composite participating objects) and intricate mixtures of discrete & continuous energy spectra.

▶ General setup

Total Hamiltonian assumed in the form $\boxed{\hat{H}(t) = \hat{H}_0 + \lambda\hat{H}'(t)}$ where:

$$\left.\begin{array}{lcl} \hat{H}_0 & \equiv & \text{free stationary Hamiltonian} \\ \hat{H}'(t) & \equiv & \text{generally time dependent perturbation} \\ \lambda & \equiv & \text{dimensionless parameter} \end{array}\right\} \quad \begin{array}{l} \text{matrix elements of } \hat{H}_0 \\ \text{and } \hat{H}'(t) \text{ are of about} \\ \text{the same size, } \lambda \ll 1 \end{array}$$

The task is to evaluate probabilities of transitions between eigenstates of $\hat{H}_0$ as a function of time in the form of a power-law series in λ

▶ Typology of applications

Example I: stimulated transition $\boxed{A \leftrightarrow A^*}$

The Hamiltonian $\hat{H}_0$ describes a bound quantum system with a discrete energy spectrum $\{E_{0i}\}_i$, while the perturbation $\lambda\hat{H}'(t)$ represents a non-stationary external field inducing transitions between the unperturbed eigenstates $\{|E_{0i}\rangle\}_i$. These states may be taken as a basis of the Hilbert space $\mathcal{H}$ of the problem.

Example II: spontaneous decay $\boxed{A^* \to A + \gamma}$

The Hamiltonian $\hat{H}_0 = \hat{H}_\mathrm{a} + \hat{H}_\gamma$ describes a bound system (e.g., an atom or atomic nucleus) with discrete energy spectrum $\{E_{0i}\}_i$ and the free electromagnetic field (photons) with continuous energy spectrum $E_\gamma \in [0, +\infty)$. The time-independent perturbation $\lambda\hat{H}'$ represents the interaction of the system with the electromagnetic field. The initial state is $|\psi_{0i}\rangle \equiv |E_{0i}\rangle_\mathrm{a} \otimes |0\rangle_\gamma$ (an excited state of the system and the electromagnetic vacuum). The final states are of the form $|\psi_{0j}\rangle \equiv |E_{0j}\rangle_\mathrm{a} \otimes |\vec{k}\nu\rangle_\gamma$ (the system's ground or lower excited state, $j < i$, and a single-photon state with a given wave vector $\vec{k}$ and polarization ν). The Hilbert space $\mathcal{H} = \mathcal{H}_\mathrm{a} \otimes \mathcal{H}_\gamma$ can decomposed into two relevant parts: the space of initial states $\mathcal{H}_\mathrm{ini} \equiv \mathcal{H}_\mathrm{a} \otimes \mathcal{H}_\gamma^{(0)}$ and the space of final states $\mathcal{H}_\mathrm{fin} \equiv \mathcal{H}_\mathrm{a} \otimes \mathcal{H}_\gamma^{(1)}$, where $\mathcal{H}_\gamma^{(N_\gamma)}$ is the photon Fock space segment with N_γ photons.

Example III: scattering $\boxed{a + A \to B + b}$

The free Hamiltonian $\hat{H}_0$ with continuous energy spectrum represents non-interacting particles a, A, B, b that will participate in the process and the stationary perturbation term $\lambda\hat{H}'$ describes all their interactions. We stress that at least some of the participating particles are in general composite and write states in the corresponding Hilbert spaces as $|\vec{p}\rangle|\phi\rangle_{a,b}$ or $|\vec{p}\rangle|\Phi\rangle_{A,B}$, where $\vec{p}$ stands for an overall momentum and ϕ or Φ for a relevant internal state of the given particle. The initial state (in the center-of-mass system, where the sum of linear momenta is equal to zero) reads as $|\psi_{0i}\rangle \equiv |\vec{p}_i\rangle|\phi_i\rangle_a \otimes |-\vec{p}_i\rangle|\Phi_i\rangle_A$, the final state as $|\psi_{0j}\rangle \equiv |\vec{p}_j\rangle|\Phi_j\rangle_B \otimes |-\vec{p}_j\rangle|\phi_j\rangle_b$, where the indices i and j are used to label the initial and final states. The relevant initial and final Hilbert spaces are $\mathcal{H}_\mathrm{ini} \equiv \mathcal{H}_a \otimes \mathcal{H}_A$ and $\mathcal{H}_\mathrm{fin} \equiv \mathcal{H}_B \otimes \mathcal{H}_b$.

▶ Dyson series for transition amplitudes

It is favorable to move to the **Dirac interaction picture** of the time evolution, identifying the free Hamiltonian with $\hat{H}_0$. This immediately yields the desired power-law series in the perturbation.

$$\begin{aligned}
&\text{Operators:} \quad \hat{A}_\mathrm{D}(t) = \hat{U}_0^\dagger(t)\,\hat{A}_\mathrm{S}\,\overbrace{\hat{U}_0(t)}^{e^{-i\frac{\hat{H}_0 t}{\hbar}}} \quad \Rightarrow \quad \begin{cases} \hat{H}_{0\mathrm{D}} = \hat{H}_{0\mathrm{S}} \equiv \hat{H}_0 \\ \hat{H}'_\mathrm{D}(t) = \hat{U}_0^\dagger(t)\hat{H}'(t)\hat{U}_0(t) \end{cases} \\
&\text{Vectors:} \qquad |\psi(t)\rangle_\mathrm{D} = \hat{U}_0^\dagger(t)|\psi(t)\rangle_\mathrm{S} \quad \Rightarrow \quad i\hbar\tfrac{d}{dt}|\psi(t)\rangle_\mathrm{D} = \hat{H}'_\mathrm{D}(t)|\psi(t)\rangle_\mathrm{D}
\end{aligned}$$

Dyson series for evolution operator:

$$\hat{U}_{\rm D}(t,t_0) = \hat{I} + \left(-\tfrac{i}{\hbar}\lambda\right)^1 \int_{t_0}^{t} \hat{H}'_{\rm D}(t_1)\,dt_1 + \left(-\tfrac{i}{\hbar}\lambda\right)^2 \int_{t_0}^{t}\int_{t_0}^{t_2} \hat{H}'_{\rm D}(t_2)\hat{H}'_{\rm D}(t_1)\,dt_1 dt_2 + \ldots$$
$$+ \left(-\tfrac{i}{\hbar}\lambda\right)^n \int_{t_0}^{t}\int_{t_0}^{t_n}\cdots\int_{t_0}^{t_2} \hat{H}'_{\rm D}(t_n)\hat{H}'_{\rm D}(t_{n-1})\cdots\hat{H}'_{\rm D}(t_1)\; dt_1 \ldots dt_{n-1}dt_n + \ldots$$

This series can be rewritten to yield amplitudes of transitions between individual eigenstates of $\hat{H}_0$ within the time interval $[t_0,t]$:

wavefunction	$\lvert\psi_{0i}\rangle \longrightarrow \lvert\psi_{0j}\rangle$
unperturbed energy	$E_{0i} \longrightarrow E_{0j}$
transition frequency	$\omega_{ji} = \frac{E_{0j}-E_{0i}}{\hbar}$

$$\mathfrak{a}_{ji}(t,t_0) \equiv \langle\psi_{0j}|\hat{U}_{\rm D}(t,t_0)|\psi_{0i}\rangle = \delta_{ij} + \left(-\tfrac{i}{\hbar}\lambda\right)^1 \int_{t_0}^{t} \underbrace{\langle\psi_{0j}|\hat{H}'_{\rm D}(t_1)|\psi_{0i}\rangle}_{H'_{ji}(t_1)e^{i\omega_{ji}t_1}}\,dt_1 +$$
$$+ \left(-\tfrac{i}{\hbar}\lambda\right)^2 \int_{t_0}^{t}\int_{t_0}^{t_2} \sum_k \overbrace{\langle\psi_{0j}|\hat{H}'_{\rm D}(t_2)|\psi_{0k}\rangle}^{H'_{ji}(t_1)e^{i\omega_{jk}t_2}} \overbrace{\langle\psi_{0k}|\hat{H}'_{\rm D}(t_1)|\psi_{0i}\rangle}^{H'_{ji}(t_1)e^{i\omega_{ki}t_1}}\,dt_1 dt_2 + \ldots$$
$$+ \left(-\tfrac{i}{\hbar}\lambda\right)^n \int_{t_0}^{t}\int_{t_0}^{t_n}\cdots\int_{t_0}^{t_2} \sum_{k_{n-1}}\sum_{k_{n-2}}\cdots\sum_{k_1} \overbrace{\langle\psi_{0j}|\hat{H}'_{\rm D}(t_n)|\psi_{0k_{n-1}}\rangle}^{H'_{jk_{n-1}}(t_n)e^{i\omega_{jk_{n-1}}t_n}} \overbrace{\langle\psi_{0k_{n-1}}|\hat{H}'_{\rm D}(t_{n-1})|\psi_{0k_{n-2}}\rangle}^{H'_{k_{n-1}k_{n-2}}(t_{n-1})e^{i\omega_{k_{n-1}k_{n-2}}t_{n-1}}} \cdots$$
$$\cdots \underbrace{\langle\psi_{0k_1}|\hat{H}'_{\rm D}(t_1)|\psi_{0i}\rangle}_{H'_{k_1i}(t_1)e^{i\omega_{k_1i}t_1}}\,dt_1\cdots dt_{n-1}dt_n + \ldots\ldots$$

This leads to the following **perturbation series**:

$$\mathfrak{a}_{ji}(t,t_0) = \sum_{n=0}^{\infty} \mathfrak{a}_{nji}(t,t_0) \quad = \quad \delta_{ij} \qquad [n=0]$$
$$[n=1] \qquad + \left(-\tfrac{i}{\hbar}\lambda\right)^1 \int_{t_0}^{t} H'_{ji}(t_1)e^{i\omega_{ji}t_1}dt_1$$
$$[n=2] \qquad + \left(-\tfrac{i}{\hbar}\lambda\right)^2 \int_{t_0}^{t}\int_{t_0}^{t_2} \sum_k H'_{jk}(t_2)e^{i\omega_{jk}t_2}H'_{ki}(t_1)e^{i\omega_{ki}t_1}dt_1dt_2 \quad + \quad \ldots$$
$$[\text{gen. } n] \qquad + \left(-\tfrac{i}{\hbar}\lambda\right)^n \int_{t_0}^{t}\int_{t_0}^{t_n}\cdots\int_{t_0}^{t_2} \sum_{k_{n-1}}\sum_{k_{n-2}}\cdots\sum_{k_1} H'_{jk_{n-1}}(t_n)e^{i\omega_{jk_{n-1}}t_n}$$
$$\cdots H'_{k_{n-1}k_{n-2}}(t_{n-1})e^{i\omega_{k_{n-1}k_{n-2}}t_{n-1}}\cdots H'_{k_1i}(t_1)e^{i\omega_{k_1i}t_1}dt_1\cdot\cdot dt_{n-1}dt_n$$
$$+ \ldots\ldots$$

▶ S-matrix

The dependence of $\mathfrak{a}_{ji}(t,t_0)$ on times t_0 & t can be removed by considering an *asymptotic time limit* with respect to a certain short time scale (see below). The resulting so-called scattering matrix (S-matrix) includes asymptotic-time amplitudes of the $i \to j$ transitions:

$$\mathfrak{a}_{ji}(t,t_0) \longmapsto S_{ji} \equiv \begin{cases} \lim\limits_{t\to\infty} \mathfrak{a}_{ji}(+t,0) & (\text{with } t_0 = 0) \quad \text{(a)} \\ \lim\limits_{t\to\infty} \mathfrak{a}_{ji}(+t,-t) & (\text{with } t_0 = -\infty) \quad \text{(b)} \end{cases}$$

Case (a) applied if the interaction is "homogeneous" in time (decay processes)
Case (b) applied if interaction $\hat{H}'_{\rm D}(t)$ can be "centered" at $t=0$ (scattering)

▶ Limiting time scales

The nonstationary perturbation method describes quantum processes on the time scale somewhere in between two limiting scales: $T_< \ll \Delta t \ll T_>$.

Upper time scale: Fast convergence of the above series is expected if the time difference $(t-t_0)$ is much smaller than a characteristic time scale of the *exact state evolution*. The scale $T_>$ is therefore given by the total energy width of the evolving state in the eigenbasis of the full Hamiltonian.

$$t-t_0 \ll T_> \sim \frac{\hbar}{\sqrt{\langle\langle E^2\rangle\rangle_{\psi(t)}}}$$

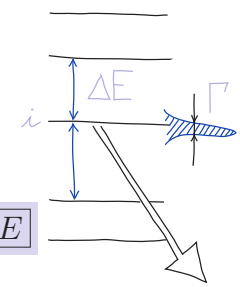
Example: for a decay process, the upper scale $T_>$ is associated with the mean lifetime $\tau=\frac{\hbar}{\Gamma}$ (with $\Gamma\equiv$ width of the Breit-Wigner peak) of the decaying state.

Note: for a time-dependent perturbation, $T_>$ should be evaluated from a maximal energy width acquired during the evolution: $T_> \sim \text{Min}\left\{\hbar/\sqrt{\langle\langle E^2\rangle\rangle_{\psi(t')}}\right\}_{t'\in[t_0,t]}$

Lower time scale : The "asymptotic-time" S-matrix is defined for time differences $(t-t_0)$ much longer than a short time scale associated with the system's *internal or single-particle dynamics*. For systems with discrete spectra, this scale is determined by the average density of unperturbed energy levels around the initial state.

$$\hbar\,\varrho_0(E_{0i}) \approx \frac{2\hbar}{E_{0(i+1)}-E_{0(i-1)}} \sim T_< \ll t-t_0$$

Examples: For decay processes of composite objects, $T_<$ represents a characteristic period of motions of internal particles. For scattering of particles with a short-range interaction, $T_<$ is given by the time spent by the colliding particles within the interaction distance.



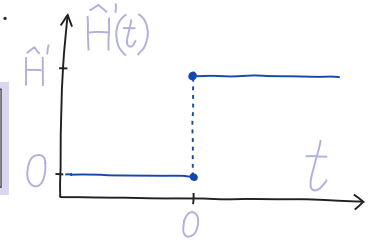
Consequence: For a discrete spectrum, the time window $(T_<, T_>)$ for application of the nonstationary perturbation method exists *iff* the total energy width of the initial state is much less than the spacing of unperturbed levels: $\Gamma \ll \Delta E$

▶ Step perturbation

Consider first the case in which the perturbation is switched on abruptly, in a step-like fashion, at time $t=0$. This is, in fact, the same as if we describe the $t>0$ effects of a **stationary perturbation** $\hat{H}'$ on a system, which was prepared at $t=0$ in the initial eigenstate $|\psi_{0i}\rangle$ of $\hat{H}_0$.

Perturbation Hamiltonian

$$\left[\hat{H}'(t)=\hat{H}',\ t_0=0\right] \text{ or } \left[\hat{H}'(t)=\begin{cases} 0 & t<0, \\ \hat{H}' & t\geq 0, \end{cases} \quad t_0\leq 0\right]$$



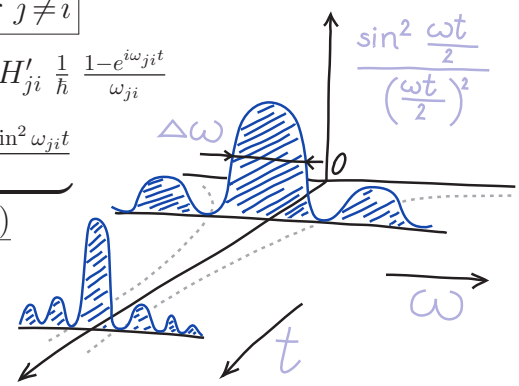
Transition amplitude & probability up to 1st order contribution

We consider transitions $\boxed{|\psi_{0i}\rangle \to |\psi_{0j}\rangle \text{ for } j \neq i}$

$$\mathfrak{a}_{ji}^{(1)}(t) = \mathfrak{a}_{1ji}(t) = -\tfrac{i}{\hbar}\lambda H'_{ji} \int_0^t e^{i\omega_{ji}t_1} dt_1 = \lambda H'_{ji}\ \tfrac{1}{\hbar}\ \tfrac{1-e^{i\omega_{ji}t}}{\omega_{ji}}$$

$$\mathfrak{p}_{ji}^{(1)}(t) = |\mathfrak{a}_{ji}^{(1)}(t)|^2 = \tfrac{1}{\hbar^2}|\lambda H'_{ji}|^2 \underbrace{\frac{(1-\cos\omega_{ji}t)^2+\sin^2\omega_{ji}t}{\omega_{ji}^2}}_{\frac{4\sin^2\left(\frac{\omega_{ji}}{2}t\right)}{\omega_{ji}^2}}$$

$$= \boxed{\tfrac{1}{\hbar^2}|\lambda H'_{ji}|^2\ \frac{\sin^2\left(\frac{\omega_{ji}}{2}t\right)}{\left(\frac{\omega_{ji}}{2}t\right)^2}\ t^2}$$



The right way of treating this expression:

(a) Consider **long time** $t \gg \frac{\hbar}{\Gamma}$ (see above) $\Rightarrow$ $\boxed{t \to \infty}$ $\Rightarrow$ $\boxed{\frac{\sin^2\left(\frac{\omega_{ji}}{2}t\right)}{\left(\frac{\omega_{ji}}{2}t\right)^2}\ t \approx 2\pi\,\delta(\omega_{ji})}$

$$\frac{\sin^2(\alpha x)}{\alpha x^2} = \begin{cases} \alpha \text{ for } x=0, \\ 0 \text{ for } x=\frac{\pi}{\alpha}, \frac{2\pi}{\alpha}, \cdots, \end{cases} \qquad \int_{-\infty}^{+\infty} \frac{\sin^2(\alpha x)}{\alpha x^2} dx = \pi \qquad \Rightarrow \qquad \lim_{\alpha\to\infty} \frac{\sin^2(\alpha x)}{\alpha x^2} = \pi\delta(x)$$

$$\Rightarrow \mathfrak{p}_{ji}^{(1)}(t) \approx \tfrac{2\pi}{\hbar}\,|\lambda H'_{ji}|^2\,\delta(E_{0j}-E_{0i})\,t$$

(b) Instead of transition probability calculate the **transition rate**

$$\boxed{\boxed{\mathcal{R}_{ji}(t) \equiv \tfrac{d}{dt}\mathfrak{p}_{ji}(t)}} \quad \Rightarrow \quad \mathcal{R}_{ji}^{(1)} = \tfrac{2\pi}{\hbar}|\lambda H'_{ji}|^2\delta(E_{0j}-E_{0i})$$

(c) **Sum over all final states** at energy $E_f{=}E_{0i}$ making use of averaging with respect to an ϵ-smoothened density of final states $\varrho_f(E_f)_\epsilon \equiv \sum_j \underbrace{\delta_\epsilon(E_f-E_{0j})}_{\overset{\text{e.g.}}{=}\ \frac{1}{\pi}\frac{\epsilon}{\epsilon^2+(E_f-E_{0j})^2}}$

Remark: The density of *final states* at energy E_{0i} differs in general from the density of *initial states* at the same energy. This is so because initial and final states are often treated as vectors in different Hilbert spaces. Consider the the decay $A^* \to A + \gamma$ of an excited system A^* (example II above): Here $\mathcal{H}_{\text{ini}} \equiv \mathcal{H}_{\text{a}} \otimes \mathcal{H}_\gamma^{(0)}$ (the space of states with no photon is equivalent to $\mathcal{H}_{\text{a}}$ alone) and $\mathcal{H}_{\text{fin}} \equiv \mathcal{H}_{\text{a}} \otimes \mathcal{H}_\gamma^{(1)}$ (the space of system-field states with a single photon). Therefore, the density of *final* states at energy $E_f \equiv E_{0j} + E_\gamma = E_{0i}$ is calculated in the larger space $\mathcal{H}_{\text{fin}}$.

The summation over final states leads to the following general expression:

$$\boxed{\mathcal{R}_{ji}(t) \mapsto \mathcal{R}_{fi}(t)} = \underbrace{\tfrac{2\pi}{\hbar}\sum_j |\lambda H'_{ji}|^2 \underbrace{\delta(E_{0j}-E_{0i})}_{\mapsto\ \delta_\epsilon(E_{0i}-E_{0j})}}_{\approx\langle|\lambda H'_{ji}|^2\rangle_f \sum_j \delta_\epsilon(E_{0i}-E_{0j})} = \underbrace{\tfrac{2\pi}{\hbar}\langle|\lambda H'_{ji}|^2\rangle_f}_{\substack{\text{average with} \\ \text{respect to } \varrho_f(E_f)_\epsilon}} \underbrace{\varrho_f(E_f{=}E_{0i})_\epsilon}_{\overset{\epsilon\to 0}{\longrightarrow}\ \varrho_f(E_{0i})}$$

▶ Fermi golden rule

The above derivation is summarized in a very useful and famous formula, whose validity turns out to be much wider than in the presently studied case:

$$\boxed{\mathcal{R}^{(1)}_{fi} = \frac{2\pi}{\hbar}\left\langle |\lambda H'_{ji}|^2 \right\rangle_f \varrho_f(E_{0i})}$$ where $\begin{cases} \langle|\lambda H'_{ji}|^2\rangle_f \equiv \text{squared matrix element averaged over available final states} \\ \varrho_f(E_{0i}) \equiv \text{density of final states at final energy } E_f = E_{0i} \end{cases}$

▶ 2nd order correction

$$\mathfrak{a}_{2ji}(t) = \left(-\tfrac{i}{\hbar}\lambda\right)^2 \sum_k H'_{jk}H'_{ki} \underbrace{\int_0^t\int_0^{t_2} e^{i\omega_{jk}t_2}e^{i\omega_{ki}t_1}dt_1dt_2}_{\omega_{ki}+\omega_{jk}=\omega_{ji} \;\Rightarrow\; -\left[\frac{e^{i\omega_{ji}t}-1}{\omega_{ki}\omega_{ji}} - \frac{e^{i\omega_{jk}t}-1}{\omega_{jk}\omega_{ki}}\right]} = \lambda^2 \sum_k H'_{jk}H'_{ki}\left[\frac{e^{\frac{i}{\hbar}(E_{0j}-E_{0i})t}-1}{(E_{0k}-E_{0i})(E_{0j}-E_{0i})} - \frac{e^{\frac{i}{\hbar}(E_{0j}-E_{0k})t}-1}{(E_{0j}-E_{0k})(E_{0k}-E_{0i})}\right]$$

Assuming $E_{0j} \neq E_{0k} \neq E_{0i}$ (so $H'_{jk}H'_{ki} \approx 0$ for equal energies) we may neglect the second time-dependent term (otherwise special treatment needed). The first term yields the same dependence on $(E_{0j} - E_{0i})$ as the 1st-order correction:

$$\boxed{\mathcal{R}^{(2)}_{fi} = \frac{2\pi}{\hbar}\left\langle \left|\lambda H'_{ji} + \lambda^2 \sum_k \frac{H'_{jk}H'_{ki}}{E_{0i}-E_{0k}}\right|^2 \right\rangle_f \varrho_f(E_{0i})}$$ "direct" + "virtual" transitions

◀ Historical remark

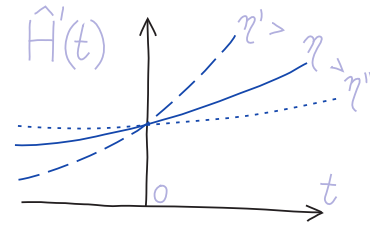
1927-30: Paul Dirac derives the 1st & 2nd order perturbative expressions and applies the theory to calculations of electromagnetic transition rates in atoms & nuclei
1950: Enrico Fermi coins the name "golden rule" for the general 1st order expression

▶ Exponential perturbation

Another perturbation type, for which the Dyson series can be evaluated explicitly, is the one with an exponential time dependence. In this case, we move the initial time $t_0 \to -\infty$ and look at the effect of a slowly rising term $\hat{H}'(t)$.

Perturbation Hamiltonian

$$\boxed{\hat{H}'(t) = e^{\eta t}\hat{H}'} \quad \eta \geq 0$$



Initial state $|\psi_{0i}\rangle$ prepared at $t_0 \to -\infty$
Final state $|\psi_{0j}\rangle$ with $j \neq i$ measured at any t

Transition rate up to 1st order contribution

Transition amplitude: $\mathfrak{a}^{(1)}_{ji}(t) = -\frac{i}{\hbar}\lambda H'_{ji}\int_{-\infty}^{t} e^{(\eta+i\omega_{ji})t_1}dt_1 = -\frac{i}{\hbar}\lambda H'_{ji}\frac{e^{(\eta+i\omega_{ji})t}}{\eta+i\omega_{ji}}$

Transition probability: $\mathfrak{p}^{(1)}_{ji}(t) = |\mathfrak{a}^{(1)}_{ji}(t)|^2 = \frac{1}{\hbar^2}|\lambda H'_{ji}|^2\frac{e^{2\eta t}}{\eta^2+\omega_{ji}^2}$

Transition rate:

$$\frac{d}{dt}\mathfrak{p}^{(1)}_{ji}(t) = \boxed{\mathcal{R}^{(1)}_{ji}(t) = \tfrac{2\pi}{\hbar^2}|\lambda H'_{ji}|^2 \underbrace{\tfrac{1}{\pi}\frac{\eta}{\eta^2+\omega_{ji}^2}}_{\hbar\Omega_{\rm BW}(E_{0j}-E_{0i})} e^{2\eta t}}$$

$\Omega_{\rm BW}(E) \equiv$ **Breit-Wigner** energy distribution (Sec. 5a) with the width $\boxed{\Gamma = 2\hbar\eta}$

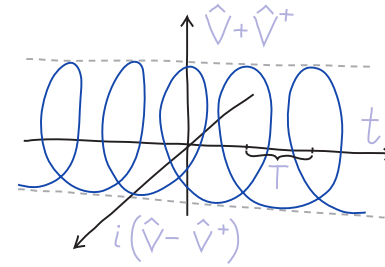
Adiabatic limit $(\eta, \Gamma \to 0)$

$\lim_{\Gamma\to 0} \Omega_{\rm BW}(E_{0j}-E_{0i}) = \delta(E_{0j}-E_{0i}) \quad \Rightarrow \quad \lim_{\eta\to 0} \mathcal{R}^{(1)}_{ji} = \frac{2\pi}{\hbar}|\lambda H'_{ji}|^2 \delta(E_{0j}-E_{0i})$

This is consistent with the previous result on constant $\hat{H}' \Rightarrow$ golden rule

▸ Harmonic perturbation

Expressions similar to those derived above apply also to harmonic perturbations with period $T=\frac{2\pi}{\omega}$. In this case, however, the perturbation induces transitions up and down to final energies $E_i+\hbar\omega$ or $E_i-\hbar\omega$.



Perturbation Hamiltonian

$$\boxed{\hat{H}'(t) = \hat{V}e^{+i\omega t}+\hat{V}^\dagger e^{-i\omega t}} = \begin{cases} (\hat{V}+\hat{V}^\dagger)\cos(\omega t) \\ +i(\hat{V}-\hat{V}^\dagger)\sin(\omega t) \end{cases}$$

Initial state $|\psi_{0i}\rangle$ at $t_0 = 0$

Up/down transition rates to 1st order

Transition amplitude to $|\psi_{0j}\rangle (j \neq i)$:

$$\mathfrak{a}^{(1)}_{ji}(t) = -\frac{i\lambda}{\hbar}\left[V_{ji}\int_0^t e^{i(\omega_{ji}+\omega)t_1}dt_1 + V^*_{ij}\int_0^t e^{i(\omega_{ji}-\omega)t_1}dt_1\right]$$
$$= \frac{\lambda}{\hbar}\left[V_{ji}\frac{1-e^{i(\omega_{ji}+\omega)t}}{\omega_{ji}+\omega} + V^*_{ij}\frac{1-e^{i(\omega_{ji}-\omega)t}}{\omega_{ji}-\omega}\right]$$

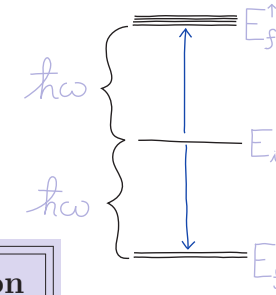
Transition probability:

$$\mathfrak{p}^{(1)}_{ji}(t) = \frac{\lambda^2}{\hbar^2}\left[|V_{ji}|^2 \frac{\sin^2\left(\frac{\omega_{ji}+\omega}{2}t\right)}{\left(\frac{\omega_{ji}+\omega}{2}t\right)^2}t^2 + |V_{ij}|^2 \frac{\sin^2\left(\frac{\omega_{ji}-\omega}{2}t\right)}{\left(\frac{\omega_{ji}-\omega}{2}t\right)^2}t^2 + 2\mathrm{Re}\Big(V_{ji}V_{ij}\overbrace{-2e^{i\omega t}\frac{\cos\omega_{ji}t-\cos\omega t}{\omega_{ji}^2-\omega^2}}\frac{1-e^{i(\omega_{ji}+\omega)t}}{\omega_{ji}+\omega}\frac{1-e^{-i(\omega_{ji}-\omega)t}}{\omega_{ji}-\omega}\Big)\right]$$

The first 2 terms yield: $2\pi t\,\delta(\omega_{ji}+\omega)$ & $2\pi t\,\delta(\omega_{ji}-\omega)$

The last term for $\omega_{ji} = \pm\omega \underbrace{+\epsilon}_{\to 0}$ is negligible relative to the previous terms:

$$\propto -\frac{\cos\omega_{ji}t-\cos\omega t}{\omega_{ji}^2-\omega^2} = -\frac{\cos(\pm\omega+\epsilon)t-\cos\omega t}{(\pm\omega+\epsilon)^2-\omega^2} \xrightarrow{\epsilon\to 0} t\,\frac{\sin\omega t}{2\omega} \sim 0$$



Transition rates

$$\boxed{\mathcal{R}^{(1)}_{fi} = \begin{cases} \frac{2\pi}{\hbar}\left\langle|\lambda V_{ji}|^2\right\rangle_f \varrho_f(E_{0i}-\hbar\omega) & \textbf{stimulated emission} \\ \frac{2\pi}{\hbar}\left\langle|\lambda V_{ij}|^2\right\rangle_f \varrho_f(E_{0i}+\hbar\omega) & \textbf{absorption} \end{cases}}$$

◂ Historical remark

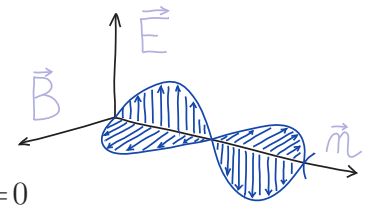
1916: A. Einstein theoretically discovers stimulated emission and discusses the detailed balance between absorption and emission processes
1950's: Application of these ideas in the construction of laser

■ Application to stimulated electromagnetic transitions

The above results of the perturbation theory for a periodic field can be directly applied to atoms or nuclei interacting with external classical electromagnetic

waves of appropriate wavelengths. We outline these issues here, leaving the discussion of the spontaneous emissions of electromagnetic quanta to Sec. 14 (where the quantization of electromagnetic field will be outlined).

▶ Planar electromagnetic wave



Vector potential: $\vec{k}$

$\vec{A}(\vec{x},t) = A_0\,\vec{\varepsilon}\cos\big(\overbrace{\tfrac{\omega}{c}\vec{n}}\cdot\vec{x}-\omega t\big)$

with $|\vec{n}|=1=|\vec{\varepsilon}|$ and $\boxed{\vec{\varepsilon}\cdot\vec{n}=0}$ following from the Coulomb gauge condition $\vec{\nabla}\cdot\hat{\vec{A}}(\hat{\vec{x}},t)=0$

$\Rightarrow$ el. & mg. field intensities: $\begin{pmatrix}\vec{E}(\vec{x},t)\\ \vec{B}(\vec{x},t)\end{pmatrix} = -A_0\begin{pmatrix}\omega\,\vec{\varepsilon}\ \sin(\vec{k}\cdot\vec{x}-\omega t)\\ \frac{\omega}{c}\,[\vec{n}\times\vec{\varepsilon}]\ \sin(\vec{k}\cdot\vec{x}-\omega t)\end{pmatrix}$

$\Rightarrow$ averaged energy density: $\langle w\rangle = \frac{1}{2}[\epsilon_0\langle\vec{E}^2(\vec{x},t)\rangle+\mu_0^{-1}\langle\vec{B}^2(\vec{x},t)\rangle] = \frac{1}{2}\epsilon_0 A_0^2\omega^2$

$\Rightarrow$ averaged energy flow: $\langle P\rangle = \langle w\rangle c = \frac{1}{2}\epsilon_0 A_0^2\omega^2 c$

▶ Hamiltonian of particles in the external elmg. wave field

Ensemble of N charged interacting particles in a classical elmg. field:

$$\hat{H}(t) = \sum_{k=1}^{N}\tfrac{1}{2M_k}\Big[\hat{\vec{p}}_k - q_k\vec{A}(\hat{\vec{x}}_k,t)\Big]^2 + \sum_{k=1}^{N}V(\hat{\vec{x}}_k,t) + \sum_{k=1}^{N}\sum_{l=k+1}^{N}W(\hat{\vec{x}}_k,\hat{\vec{x}}_l)$$

with $V(\vec{x},t)$ & $\vec{A}(\vec{x},t)$ standing for the scalar & vector potentials of the external field, and $W(\vec{x},\vec{x}')$ for the potential of a mutual interaction (of any nature) of the particles. Neglecting $q_k^2\vec{A}(\hat{\vec{x}}_k,t)^2$, setting the scalar potential $V=0$ (elmg. field far from its sources) and assuming the Coulomb gauge $\vec{\nabla}\cdot\vec{A}(\hat{\vec{x}},t)=0$:

$$\hat{H}(t) \approx \underbrace{\sum_{k=1}^{N}\tfrac{1}{2M_k}\hat{\vec{p}}_k^{\,2} + \sum_{k=1}^{N}\sum_{l=k+1}^{N}W(\hat{\vec{x}}_k,\hat{\vec{x}}_l)}_{\hat{H}_0} \underbrace{-\sum_{k=1}^{N}\tfrac{q_k}{M_k}\Big[\vec{A}(\hat{\vec{x}}_k,t)\cdot\hat{\vec{p}}_k\Big]}_{-\int\vec{A}(\vec{x},t)\cdot\vec{j}_{\rm el}(\vec{x})\,d\vec{x}\ \equiv\ \hat{H}'(t)}$$

For the above planar elmg. wave we thus get the harmonic perturbation:

$$\hat{H}'(t) = -\tfrac{A_0}{2}\sum_{k=1}^{N}\tfrac{q_k}{M_k}\Big[\underbrace{e^{-i\frac{\omega}{c}\vec{n}\cdot\hat{\vec{x}}_k}(\vec{\varepsilon}\cdot\hat{\vec{p}}_k)}_{\propto\hat{V}\ \leftrightarrow\ \text{stimul. emission}}\ e^{+i\omega t} + \underbrace{e^{+i\frac{\omega}{c}\vec{n}\cdot\hat{\vec{x}}_k}(\vec{\varepsilon}\cdot\hat{\vec{p}}_k)}_{\propto\hat{V}^\dagger\ \leftrightarrow\ \text{absorption}}e^{-i\omega t}\Big]$$

emission: $\hbar\omega = E_{0i}-E_{0j}$ **absorption**: $\hbar\omega = E_{0j}-E_{0i}$

So the external elmg. wave interacting with the particle system of energy E_{0i} induces stimulated emission and/or absorption, depending on whether the wave frequency ω matches some of the internal frequencies ω_{ij} or ω_{ji}.

▶ Absorption cross section

In the following, we focus on the absorption processes (the procedure for stimulated emission is analogous). We define the absorption cross section, which can

be seen as an *area* on the plane perpendicular to the incident wave propagation direction. The elmg. energy passing through this area is being continuously transferred to the system: $\boxed{\sigma_{ji}^{\rm abs} = \dfrac{\text{energy absorbed in unit time}}{\text{incoming energy flow}} = \dfrac{\hbar\omega\ \mathcal{R}_{ji}}{\frac{1}{2}\epsilon_0 A_0^2 \omega^2 c}}$

Perturbation theory prediction ($1^{\rm st}$order):
$\sigma_{ji}^{\rm abs} \approx \frac{\pi}{\epsilon_0 \omega c} \left| \left\langle \psi_{0j} \left| \sum_{k=1}^{N} \frac{q_k}{M_k} e^{+i\frac{\omega}{c}\vec{n}\cdot\hat{\vec{x}}_k} (\vec{\varepsilon}\cdot\hat{\vec{p}}_k) \right| \psi_{0i} \right\rangle \right|^2 \delta(E_{0i}+\hbar\omega - E_{0j})$

▶ Electric dipole approximation

Assume that the atom/nucleus size $\boxed{R \ll \lambda}$ radiation wavelength

$\Rightarrow \quad e^{+i\frac{\omega}{c}\vec{n}\cdot\hat{\vec{x}}_k} = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(i\,\frac{\omega}{c}\,\vec{n}\cdot\hat{\vec{x}}_k \right)^n \approx 1$ (only the $n=0$ term considered)

$\left\langle \psi_{0j} \left| \sum_{k=1}^{N} \frac{q_k}{M_k}\, e^{+i\frac{\omega}{c}\vec{n}\cdot\hat{\vec{x}}_k} (\vec{\varepsilon}\cdot\hat{\vec{p}}_k) \right| \psi_{0i} \right\rangle \approx \left\langle \psi_{0j} \left| \vec{\varepsilon}\cdot \sum_{k=1}^{N} \frac{q_k}{M_k} \hat{\vec{p}}_k \right| \psi_{0i} \right\rangle = \ldots$

Trick: $\hat{\vec{p}}_k = -\frac{i}{\hbar} M_k [\hat{\vec{x}}_k, \hat{H}_0] \Rightarrow \qquad \cdots = \frac{i}{\hbar} \underbrace{(E_{0j} - E_{0i})}_{\hbar\omega} \left\langle \psi_{0j} \left| \vec{\varepsilon}\cdot \underbrace{\sum_{k=1}^{N} q_k \hat{\vec{x}}_k}_{\hat{\vec{D}}} \right| \psi_{0i} \right\rangle$

where we introduced the operator of **electric dipole moment**:

$\Rightarrow \quad \sigma_{ji}^{\rm abs} \approx \frac{\pi\omega}{\epsilon_0 c} \left| \langle \psi_{0j} | \vec{\varepsilon}\cdot\hat{\vec{D}} | \psi_{0i} \rangle \right|^2 \delta(E_{0i}+\hbar\omega - E_{0j})$

For $\vec{\varepsilon} = \vec{n}_x$: $\boxed{\sigma_{ji}^{\rm abs}\, d\omega \approx \frac{\pi\omega}{\epsilon_0 \hbar c} \left| \langle \psi_{0j} | \hat{D}_x | \psi_{0i} \rangle \right|^2} \neq 0$ *iff* $\boxed{|j_i - 1| \le j_j \le (j_i + 1)}$

The above condition for the initial- & final-state spin quantum numbers j_i & j_j follows from the Wigner-Eckart theorem applied to the $\lambda = 1$ tensor operator $\hat{\vec{D}}$ (see Sec. 4b).

▶ Beyond electric dipole approximation

We look at the $\boldsymbol{n=1}$ **term** in the expansion of $\boxed{\langle \psi_{0j} | \sum_{k=1}^{N} \frac{q_k}{M_k} e^{+i\frac{\omega}{c}\vec{n}\cdot\hat{\vec{x}}_k} (\vec{\varepsilon}\cdot\hat{\vec{p}}_k) | \psi_{0i} \rangle}$

It contains matrix elements of quantity $(\vec{n}\cdot\hat{\vec{x}}_k)(\vec{\varepsilon}\cdot\hat{\vec{p}}_k) = (\vec{\varepsilon}\cdot\hat{\vec{p}}_k)(\vec{n}\cdot\hat{\vec{x}}_k) + i\hbar \underbrace{(\vec{\varepsilon}\cdot\vec{n})}_{0}$
$= \frac{1}{2}(\hat{F}_{k+} + \hat{F}_{k-})$, where we define $\hat{F}_{k\pm} = (\vec{\varepsilon}\cdot\hat{\vec{p}}_k)(\vec{n}\cdot\hat{\vec{x}}_k) \pm (\vec{\varepsilon}\cdot\hat{\vec{x}}_k)(\vec{n}\cdot\hat{\vec{p}}_k)$.

(a) Electric quadrupole term arises from the component $\hat{F}_{k+}$ treated using the same trick as above: $i\frac{\omega}{c}\langle\psi_{0j}| \sum_{k=1}^{N} \frac{q_k}{2M_k} [(\vec{\varepsilon}\cdot \underbrace{\hat{\vec{p}}_k}_{-\frac{i}{\hbar}M_k[\hat{\vec{x}}_k,\hat{H}_0]})(\vec{n}\cdot\hat{\vec{x}}_k) + (\vec{\varepsilon}\cdot\hat{\vec{x}}_k)(\vec{n}\cdot \underbrace{\hat{\vec{p}}_k}_{-\frac{i}{\hbar}M_k[\hat{\vec{x}}_k,\hat{H}_0]})] |\psi_{0i}\rangle$
$= \frac{\omega}{2\hbar c}(E_{0j} - E_{0i}) \langle\psi_{0j}| \sum_{k=1}^{N} q_k (\vec{n}\cdot\hat{\vec{x}}_k)(\vec{\varepsilon}\cdot\hat{\vec{x}}_k) |\psi_{0i}\rangle = \frac{\omega^2}{2c} \sum_{l,m=1}^{3} n_l \varepsilon_m \langle\psi_{0j}| \hat{Q}_{lm} |\psi_{0i}\rangle$ where
$\hat{Q}_{lm} = \sum_{k=1}^{N} q_k (\hat{x}_{kl}\hat{x}_{km} - \frac{1}{3}\delta_{lm}\hat{x}_{kl}^2)$ (with the last term, which ensures $\sum_{l=1}^{3} \hat{Q}_{ll} = 0$, being added without any harm because of $\vec{\varepsilon}\cdot\vec{n} = 0$) are Cartesian components of the

$\lambda=2$ electric quadrupole tensor. Thus the angular-momentum selection rules for electric quadrupole transitions are: $|j_i-2| \le j_j \le (j_i+2)$

(b) Magnetic dipole term arises from the component $\hat{F}_{k-}$: Using the identity $(\vec{\varepsilon}\cdot\hat{\vec{p}}_k)(\vec{n}\cdot\hat{\vec{x}}_k)-(\vec{\varepsilon}\cdot\hat{\vec{x}}_k)(\vec{n}\cdot\hat{\vec{p}}_k)=[\vec{n}\times\vec{\varepsilon}]\cdot\underbrace{[\hat{\vec{x}}_k\times\hat{\vec{p}}_k]}_{\hat{\vec{L}}_k}$ we get: $i\frac{\omega}{c}\langle\psi_{0j}|\sum_{k=1}^{N}\frac{q_k}{2M_k}\hat{F}_{k-}|\psi_{0i}\rangle$ $= i\frac{\omega}{c}[\vec{n}\times\vec{\varepsilon}]\cdot\langle\psi_{0j}|\sum_{k=1}^{N}\overbrace{\frac{q_k}{2M_k}\hat{\vec{L}}_k}^{\hat{\vec{\mu}}_k}|\psi_{0i}\rangle = i\frac{\omega}{c}[\vec{n}\times\vec{\varepsilon}]\cdot\langle\psi_{0j}|\hat{\vec{\mu}}|\psi_{0i}\rangle$, with $\hat{\vec{\mu}}$ denoting the orbital magnetic dipole moment. For particles with spin the spin magnetic moment needs to be added. Since the magnetic dipole moment is a $\lambda=1$ tensor, the selection rules for magnetic dipole transitions are: $|j_i-1| \le j_j \le (j_i+1)$

► Multipole expansion

To systematically evaluate transitions of higher multiopolarities λ, it is convenient to expand the incoming planar wave into the spherical waves. This is not quite trivial as one needs to correctly treat the wave polarization, which on the quantum level results from the **photon spin** (s=1).

Plane wave expansion into spherical harmonics & Bessel functions (cf. Sec. 13):

$$e^{i\vec{k}\cdot\vec{x}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} i^l\; j_l(kr)\; Y^*_{lm}\Big(\frac{\vec{k}}{k}\Big)\, Y_{lm}\big(\frac{\vec{x}}{x}\big)$$

To include the polarization, we introduce circular & linear polarization bases in a general coordinate system $\left\{\begin{smallmatrix}\vec{e}_{\pm}=\mp\frac{1}{\sqrt{2}}(\vec{e}_x\pm i\vec{e}_y)\\ \vec{e}_0=\vec{e}_z\end{smallmatrix}\right\}$ so that an arbitrary linear polarization vector can be written as: $\vec{\varepsilon}=\sqrt{\frac{4\pi}{3}}\sum_{\nu=0,\pm1} Y^*_{1\nu}(\vec{\varepsilon})\;\vec{e}_\nu$ (note that the circular polarization vector $\vec{e}_0$ is present because the evaluation is performed in an arbitrary coordinate system unrelated to the wave vector $\vec{k}$).

Introduce a "vector spherical function" with total angular momentum (multipolarity) λ:

$$\vec{\mathcal{Y}}_{l\lambda\mu}\big(\tfrac{\vec{x}}{x}\big)=\sum_{\nu,m} C^{\lambda\mu}_{1\nu lm}\vec{e}_\nu Y_{lm}\big(\tfrac{\vec{x}}{x}\big) \;\Leftrightarrow\; \vec{e}_\nu Y_{lm}\big(\tfrac{\vec{x}}{x}\big)=\sum_{\lambda,\mu} C^{\lambda\mu}_{1\nu lm}\vec{\mathcal{Y}}_{l\lambda\mu}\big(\tfrac{\vec{x}}{x}\big)$$

$$\boxed{\vec{\varepsilon}\,e^{i\vec{k}\cdot\vec{x}} = \tfrac{(4\pi)^{\frac{3}{2}}}{3}\sum_{\lambda,\mu}\sum_{l,m}\sum_{\nu} i^l\, C^{\lambda\mu}_{1\nu lm}\; Y^*_{1\nu}(\vec{\varepsilon})\; Y^*_{lm}\Big(\frac{\vec{k}}{k}\Big)\underbrace{j_l(kr)\;\vec{\mathcal{Y}}_{l\lambda\mu}\big(\tfrac{\vec{x}}{x}\big)}_{\text{spatial dependence}}}$$

For each multipolarity λ one can separate terms with both parities, **electric** component Eλ with parity $(-1)^\lambda$ and **magnetic** component Mλ with parity $(-1)^{\lambda+1}$, and construct expressions for the rates of the corresponding transitions. The previously treated terms are identified with E1 (electric dipole), E2 (electric quadrupole) and M1 (magnetic dipole) transitions.

◄ Historical remark

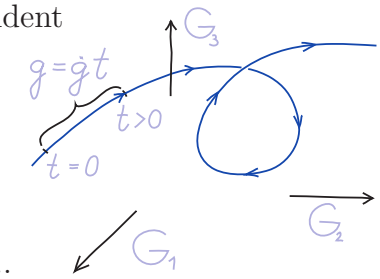
1900's-10's: Multipole expansion of elmg. field elaborated within the classical theory
1940's-50's: Multipole expansion applied in QM (M.E. Rose *et al.*)

■ Driven systems

We will now briefly deal with problems combining parameter-dependent and time-dependent descriptions. The aim will be to analyze the dynamics of systems whose Hamiltonian parameters are driven, i.e., varied with a given, externally controlled time dependence. This can be achieved with the aid of some approximation techniques based on suitable perturbative expansions.

▸ "Forward" driven system

Consider Hamiltonian $\hat{H}(\vec{G})$ depending on a set of parameters $\vec{G} \equiv (G_1, G_2, \dots)$ and define a curve $\vec{G}(g)$ in the parameter space described by variable $g \in \mathbb{R}$. We denote $\hat{H}\big(\vec{G}(g)\big) \equiv \hat{H}(g)$ and the corresponding eigenvalues and eigenvectors as $E_i(g)$ and $|\psi_i(g)\rangle$. Now consider motion $g(t) = \dot{g}t$ along the curve, assuming (without any loss of generality) $\dot{g} = \text{constant}$. The actual "speed" in the parameter space $\dot{\vec{G}}(t) = \dot{g}\,\frac{d\vec{G}}{dg}\big|_{g=g(t)}$ depends on the selected parametrization $\vec{G}(g)$ and generally varies. So we switch to a time-dependent problem: $\boxed{\hat{H}(\vec{G}) \longrightarrow \hat{H}\big(\vec{G}(g(t))\big) \equiv \hat{H}(\dot{g}t)}$



The speed $\dot{g}$ is assumed to be "small" and the task is to approximate the evolution induced by the Hamiltonian $\hat{H}(\dot{g}t)$ on the level of precision which is consistent with a selected power $\dot{g}^0, \dot{g}^1, \dot{g}^2 \dots$

▸ Equations for instantaneous eigenvectors

Stationary Schr. eq.: $\hat{H}(g)|\psi_i(g)\rangle = E_i(g)|\psi_i(g)\rangle$

$\Rightarrow \quad \frac{d\hat{H}(g)}{dg}|\psi_i(g)\rangle + \hat{H}(g)|\frac{d\psi_i}{dg}(g)\rangle = \frac{dE_i(g)}{dg}|\psi_i(g)\rangle + E_i(g)|\frac{d\psi_i}{dg}(g)\rangle$

Multiply by $\langle\psi_j(g)|$ for $j \neq i$:

$\langle\psi_j|\frac{d\hat{H}}{dg}|\psi_i\rangle + E_j\langle\psi_j|\frac{d\psi_i}{dg}\rangle = \frac{dE_i}{dg}\overbrace{\langle\psi_j|\psi_i\rangle}^{0} + E_i\langle\psi_j|\frac{d\psi_i}{dg}\rangle$

$$\Rightarrow \quad \boxed{\langle\psi_j(g)|\frac{d\psi_i}{dg}(g)\rangle = \frac{\langle\psi_j(g)|\frac{d\hat{H}}{dg}(g)|\psi_i(g)\rangle}{E_i(g) - E_j(g)}} \qquad \text{for } j \neq i$$

For $j = i$ we use: $\frac{d}{dg}\langle\psi_i|\psi_i\rangle = \langle\frac{d\psi_i}{dg}|\psi_i\rangle + \langle\psi_i|\frac{d\psi_i}{dg}\rangle = 2\,\mathrm{Re}\langle\psi_i|\frac{d\psi_i}{dg}\rangle = 0$

$$\Rightarrow \quad \boxed{\langle\psi_i(g)|\frac{d\psi_i}{dg}(g)\rangle = i\phi_i(g)} \qquad \text{with } \phi_i(g) \in \mathbb{R}$$

With substitutions $g \to \dot{g}t$ and $\frac{d}{dg} \to \frac{1}{\dot{g}}\frac{d}{dt}$ the above formulas become t-dependent

▸ Time evolution by the driven Hamiltonian

Expansion in the instantaneous eigenbasis: $\boxed{|\psi(t)\rangle = \sum_j \alpha_j(t)|\psi_j(\dot{g}t)\rangle}$

Nonstationary Schr. eq.: $i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}(\dot{g}t)|\Psi(t)\rangle$

$$\Rightarrow i\hbar\sum_j \big(\dot\alpha_j(t)|\psi_j(\dot g t)\rangle+\alpha_j(t)\tfrac{d}{dt}|\psi_j(\dot g t)\rangle\big)=\sum_j \alpha_j(t)E_j(\dot g t)|\psi_j(\dot g t)\rangle$$

Multiply by $\langle\psi_i(\dot g t)|$: $\quad i\hbar\dot\alpha_i(t)+i\hbar\sum_j \alpha_j(t)\ \underbrace{\langle\psi_i(\dot g t)|\tfrac{d}{dt}\psi_j(\dot g t)\rangle}\ =\alpha_i(t)E_i(\dot g t)$

Here we use the previously derived result and obtain a system of coupled differential equations for $\alpha_i(t)$:

$\dot g\frac{\langle\psi_j(g)|\frac{d\hat H}{dg}(g)|\psi_i(g)\rangle}{E_i(g)-E_j(g)}$	$i\dot g\phi_i(g)$
for $i\neq j$	for $i=j$

$$\frac{d\alpha_i}{dt}(t)=\big[-\tfrac{i}{\hbar}E_i(\dot g t)+i\dot g\phi_i(\dot g t)\big]\,\alpha_i(t)+\dot g\sum_{j(\neq i)}\frac{\langle\psi_j(\dot g t)|\frac{d\hat H}{dg}(\dot g t)|\psi_i(\dot g t)\rangle}{E_i(\dot g t)-E_j(\dot g t)}\alpha_j(t)\qquad \begin{matrix}\frac{d}{dt}=\dot g\frac{d}{dg}\\ \dot g t=g\end{matrix}$$

▶ Adiabatic approximation

Let the initial state is one of the $g=0$ eigenstates: $\boxed{|\psi(t=0)\rangle\equiv|\psi_i(g=0)\rangle}$

$\Rightarrow \alpha_j(0)=\delta_{ij}$. We further assume that $\boxed{\dot g \text{ is very small} \to 0}$ (adiabatic limit).

The offdiagonal terms of the above set of differential eqns. yield contributions $\propto \dot g^p$ with $p\geq 1$ to the solutions $\alpha_j(t)$
$\Rightarrow$ they can be neglected in the 0^{th}order (so called adiabatic) approximation.
So the 0^{th}order solution reads as follows:

$$\alpha_j(t)=\delta_{ij}\,\underbrace{e^{-\frac{i}{\hbar}\int_0^t E_i(\dot g t')dt'}}_{\text{dynamical phase}}\ \underbrace{e^{i\int_0^g \phi_i(g')dg'}}_{\text{geometrical factor}}$$

The non-adiabatic $p\geq 1$ terms $\propto \dot g^1, \dot g^2...$ can be also systematically constructed within the so-called adiabatic perturbation theory (not discussed here).

▶ Adiabatic state preparation

We see that the adiabatic approximation yields $|\alpha_j(t)|^2=\delta_{ij}$, so in the true $\dot g\to 0$ limit the driven system remains all the time in the instantaneous eigenstate $|\psi_i(g)\rangle$ following from the initial eigenstate $|\psi_i(0)\rangle$. This result is known as the **adiabatic theorem**. However, for $\dot g$ small but $\neq 0$ this remains a good approximation *iff* the levels do not come too close to each other (see the energy denominator in the neglected term of the above equation).

The adiabatic theorem is used in various protocols of quantum computation & quantum state preparation. An N-qubit system is prepared in the ground state $|\psi_0(\vec G)\rangle$ of a parameter-dependent Hamiltonian $\hat H(\vec G)$ at an initial parameter point $\vec G=\vec G(0)$, where the ground state is *fully separable* (e.g., spins at low temperature in strong external magnetic field). An adiabatic parameter change $\vec G(t)$ in time interval $t\in[0,\tau]$ then drives the system into a *highly entangled* ground state of the Hamiltonian at the final parameter point $\vec G(\tau)$ (corresponding, e.g., to mutually interacting spins with vanishing external field). Note that $|\psi_0(\vec G(\tau))\rangle$ cannot typically be prepared directly by cooling down the system at

point $\vec{G}(\tau)$ becuase of a too complicated structure of the corresponding thermodynamic potentials. The entangled state $|\psi_0(\vec{G}(\tau))\rangle$ can be used as a resource for various quantum information applications, including quantum computation. The crucial question, which decides about the practical applicability of the procedure, concerns the *scaling* of the time τ, which still ensures adiabaticity of the driving, with the increasing number N of qubits.

► **Berry phase**

We saw that the adiabatic evolution generates two types of phase factors:

(a) dynamical phase $\boxed{\varphi_i^{\rm dyn}(t) = -\frac{1}{\hbar}\int_0^t E_i\big(g(t')\big)dt'}$ derived from the standard evolution of energy eigenstates

(b) geometrical phase (Berry's phase) $\boxed{\varphi_i^{\rm geo}(t) = \int_0^{g(t)} \phi_i(g')dg'}$ depending only on the geometrical path in the parameter space $\vec{G}$.

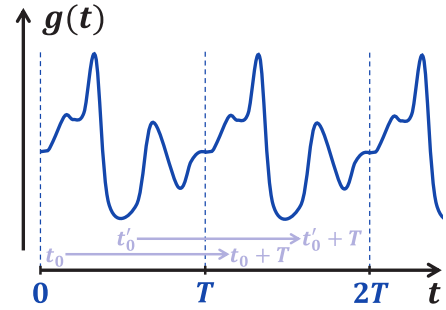
$g(t)=\dot{g}t \;\Rightarrow\; \varphi_i^{\rm dyn}(t) \propto \dot{g}^{-1} \overset{\dot{g}\to 0}{\to} \infty$, but $\varphi_i^{\rm geo}(t)$ is finite

In fact, the phases of Hamiltonian eigenvectors in the space of $\vec{G}$ can be chosen arbitrarily, having no physical meaning: physics is *invariant under local gauge (phase) transformations* of eigenvectors $|\psi_i(\vec{G})\rangle$. However, the geometrical phase can yield a nonzero value $\boxed{\varphi_i^{\rm geo}[\wp] = \oint_\wp \phi_i(g')dg'}$ even for the adiabatic drive along a **closed path** $\wp$ returning back to the initial point. Such phase changes are gauge-independent and have measurable implications.

► **Periodically driven systems**

Consider a driven Hamiltonian $\hat{H}\big(\vec{G}(g(t))\big)$ with a periodic dependence $g(t)=g(t+T)$, where $T=\frac{2\pi}{\omega}$. Any periodic Hamiltonian $\hat{H}(t)=\hat{H}(t+T)$ can be written as

$$\boxed{\hat{H}(t) = \hat{H}_0 + \sum_{\substack{k=-\infty\\k\neq 0}}^{+\infty} \hat{V}_k e^{ik\omega t}} \quad \text{with } \hat{V}_{-k}=\hat{V}_{+k}^\dagger$$



In particular, there exist the following two special types of periodic driving:

(a) **harmonic** ($\hat{V}_k=0$ if $|k|\geq 2$): $\hat{H}(t)=\hat{H}_0+(\hat{V}_1+\hat{V}_1^\dagger)\cos\omega t + i(\hat{V}_1-\hat{V}_1^\dagger)\sin\omega t$

(b) **kicked** ($\hat{V}_k=\hat{V}\neq 0$ if $k\neq 0$): $\hat{H}(t)=\hat{H}_0-\hat{V}+\hat{V}T\sum_{l=-\infty}^{+\infty}\delta(t-lT)$

The evolution operator over 1 period $\boxed{\hat{U}(t_0+T,t_0)\equiv\hat{F}(t_0)}$ ≡ Floquet operator

$$\hat{F}(t_0') = \hat{U}(t_0'+T,t_0') = \underbrace{\hat{U}(t_0'+T,t_0+T)}_{\hat{U}(t_0',t_0)}\hat{F}(t_0)\hat{U}(t_0,t_0') = \hat{U}^{-1}(t_0,t_0')\hat{F}(t_0)\hat{U}(t_0,t_0')$$

Floquet states $|\phi_i(t_0)\rangle$ and the corresponding **quasienergies** $\mathcal{E}_i$ are solutions of the eigenproblem: $\boxed{\hat{F}(t_0)|\phi_i(t_0)\rangle = e^{-\frac{i}{\hbar}\mathcal{E}_i T}|\phi_i(t_0)\rangle}$ where the values $\mathcal{E}_i$ do not

depend on t_0 and $|\phi_i(t_0')\rangle = \hat{U}(t_0,t_0')|\phi_i(t_0)\rangle$.

Any initial state can be expanded as $|\psi(t_0)\rangle = \sum_i \overbrace{\langle\phi_i(t_0)|\psi(t_0)\rangle}^{\alpha_i} |\phi_i(t_0)\rangle$ and its evolution from t_0 to $t = t_0 + nT + \Delta t$ with integer n and $\Delta t \in [0,t)$ reads as $|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle = \sum_i \alpha_i e^{-\frac{i}{\hbar}n\mathcal{E}_i T}|\phi_i(t_0+\Delta t)\rangle$. So the general evolution is solved via the full set of Floquet eigensolutions within 1 period.

The unitary operator $\hat{F}(t_0)$ can be expressed as an exponential of a selfadjoint operator $\hat{H}_{\rm F}(t_0)$, called the effective (Floquet) Hamiltonian: $\boxed{\hat{F}(t_0) = e^{-\frac{i}{\hbar}\hat{H}_{\rm F}(t_0)T}}$

It can be expressed as series in powers of the period: $\boxed{\hat{H}_{\rm F}(t_0) = \sum_{n=0}^{\infty} \hat{h}_n(t_0) T^n}$

Example: **periodically switched Hamiltonian**

$\boxed{\hat{H}(t) = g(t)\hat{H}_1 + [1-g(t)]\hat{H}_2}$ with $g(t) = \begin{cases} 1 \text{ for } t \bmod T \in [0, fT), \\ 0 \text{ for } t \bmod T \in [fT, T), \end{cases}$ $f \in (0,1)$

$\hat{F}(0) = e^{-\frac{i}{\hbar}\hat{H}_2(1-f)T} e^{-\frac{i}{\hbar}\hat{H}_1 fT} = e^{-\frac{i}{\hbar}\hat{H}_{\rm F}(0)T}$ expressed by the BCH formula (Sec. 4a):

$e^{\hat{X}}e^{\hat{Y}} = e^{\hat{X}+\hat{Y}+\frac{1}{2}[\hat{X},\hat{Y}]+\frac{1}{12}([\hat{X},[\hat{X},\hat{Y}]]+[\hat{Y},[\hat{Y},\hat{X}]])+\cdots}$ $\Rightarrow$ $\hat{H}_{\rm F}(0) =$

$$\underbrace{f\hat{H}_1 + (1-f)\hat{H}_2}_{\hat{h}_0(0)} + \underbrace{\frac{f(1-f)}{2\hbar} i[\hat{H}_1, \hat{H}_2]}_{\hat{h}_1(0)} T - \underbrace{\frac{f(1-f)}{12\hbar^2}\big[f\hat{H}_1 - (1-f)\hat{H}_2, [\hat{H}_1, \hat{H}_2]\big]}_{\hat{h}_2(0)} T^2 + \cdots$$

Periodic drivings of various types can be used in **quantum simulations** of systems with the corresponding Hamiltonians $\hat{H} = \hat{H}_{\rm F}(t_0)$. If T is much smaller than the time scale of the internal dynamics, the series for $\hat{H}_{\rm F}(t_0)$ can be truncated. For instance, a very fast switching between $\hat{H}_1$ & $\hat{H}_2$ in the last example effectively simulates the Hamiltonian $\hat{H} = f\hat{H}_1 + (1-f)\hat{H}_2 = \hat{h}_0(0)$.

◀ Historical remark

1884: G. Floquet develops formalism for solutions of periodic differential equations
1928: Max Born & Vladimir Fock formulate the quantum adiabatic theorem
1984: Michael Berry presents the theory of geometrical phase (later linked to an earlier work of S. Pancharatnam from 1956)
1980's-present: perturbative approaches to forward & periodically driven systems
1990's-present: use of periodically driven external fields for trapping particles in quantum experiments and simulating complex quantum Hamiltonians
2000-present: development of adiabatic protocols for quantum computation

12. SCATTERING: ITERATIVE APPROACHES

Description of the processes induced by scattering of particles belongs to the most important application domains of quantum theory. Knowing the the initial state and the interaction Hamiltonian between all particles involved in the scattering process, can we predict all outcomes and their probabilities? And inversely: knowing the outcomes & probabilities for various initial states, can we determine the form of the interaction Hamiltonian? This may resemble a task to analyze an internal structure

of a watch by detecting tiny parts shot out when the thing is smashed on an anvil. In the quantum world, this is often the only research method available.

The scattering theory is a rather wide area, of which we are going to taste only a little bit. Here is a general typology of scattering processes:

(1) $a + A \to A + a$	**elastic scattering** (total kinetic energy conserved)
(2) $a + A \to A^* + a^*$	**inelastic scattering** (intrinsic excitations of particles involved, total kinetic energy not conserved)
(3) $a + A \to B + b + b' + \ldots$	more **complex reaction** (reconfiguration of the interacting particles, appearance of new objects)

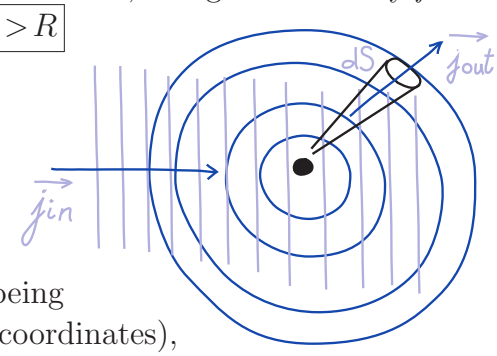
Scattering theory is closely related to the nonstationary perturbation theory. Indeed, the solution of the scattering problem can be searched in the form of a power series in the particle interaction strength. This approach will be elaborated in the present section. We will start with an intuitive stationary description of elastic scattering and then proceed to a rather powerful formalism which will allow us to transform general nonstationary scattering problems into equivalent stationary problems that support iterative solutions.

■ Elementary description of elastic scattering

In a large part of this and the following sections we will deal with elastic scattering — the simplest scattering process which does not change the nature or internal structure of the scattered objects. We first focus on an elementary description of this process, based on solving the *stationary* Schrödinger equation with an appropriate asymptotic form of the wavefunction.

▸ Scattering by a fixed potential

Consider a spinless projectile (a particle with the scalar wavefunction) moving in a fixed potential field. This corresponds to elastic scattering of the projectile on an *infinite-mass* scattering center (target particle). We further assume that the target–projectile interaction has a limited reach, being described by *finite-range potential* satisfying $\boxed{V(\vec{x}) \approx 0 \text{ for } |\vec{x}| > R}$



The projectile's initial state coincides with one of the momentum eigenstates. Choosing the initial momentum $\vec{p} = p\vec{n}_z$, we start with the incoming plane wave $\psi(\vec{x}) \propto e^{ikz}$ with $k = \frac{p}{\hbar}$. To determine the probability distribution for the projectile being scattered to various angles ϑ, φ (spherical coordinates), we apply the method of probability currents outlined in Sec. 5a: We solve the stationary Schrödinger equation $\left[-\frac{\hbar^2}{2M}\Delta + V(\vec{x})\right]\psi(\vec{x}) = E\psi(\vec{x})$ with energy

$E = \frac{(\hbar k)^2}{2M}$ equal to the initial kinetic energy (this energy has to belong to the **continuous spectrum** of the full Hamiltonian so that it corresponds to *unbound states*) and with the following **asymptotic form** of the wavefunction:

$$\psi_k(\vec{x}) \overset{|\vec{x}|\gg R}{\sim} \underbrace{e^{ikz}}_{\substack{\text{incoming}\\ \text{plane wave}}} + \underbrace{f_k(\vartheta,\varphi)\,\frac{e^{ikr}}{r}}_{\substack{\text{outgoing}\\ \text{spherical wave}}}$$

The function $f_k(\vartheta,\varphi)$, which is called the **scattering amplitude**, modulates the amplitude of the outgoing spherical wave in various directions. This function contains all relevant information on the scattering of the incoming particle with momentum $\vec{p} = \hbar k \vec{n}_z$ to various angles (ϑ,φ).

▶ Differential cross section

Probabilities of scattering to various final states are usually quantified by the corresponding **cross sections**. In general, the production **rate** $\mathcal{R}_\mathrm{X}$ of a given final state X (the number of X events per unit time) is given by $\boxed{\mathcal{R}_\mathrm{X} = N j_\mathrm{in} \sigma_\mathrm{X}}$ where N is the number scattering centers, j_in is the flux of incoming particles and σ_X is the cross section of the process X (it can be seen as an area perpendicular to the incoming flux such that the passage of the incoming particle through this area leads to the process X). If X depends on a continuous variable x, we can introduce a differential cross section defined by $\boxed{\frac{d}{dx}\mathcal{R}_{\mathrm{X}(x)} = N j_\mathrm{in} \frac{d\sigma_{\mathrm{X}(x)}}{dx}}$ The integral cross section is given by $\sigma_\mathrm{X} = \int dx \frac{d\sigma_{\mathrm{X}(x)}}{dx}$.

In the present case $N = 1$ and the outgoing state X depends on two spherical angles (ϑ,φ), so it is convenient to differentiate σ_X with respect to the space angle element $d\Omega = \sin\vartheta\, d\vartheta d\varphi$. The rate of the scattering events to the direction around (ϑ,φ) measured by a detector of front area S placed at distance r from the target would be $\mathcal{R}_{(\vartheta,\varphi)} = N j_\mathrm{in} \frac{S}{r^2} \frac{d\sigma}{d\Omega}(\vartheta,\varphi)$. The differential cross section $\frac{d\sigma}{d\Omega}(\vartheta,\varphi)$ can be determined from the above ansatz wavefunction:

Incoming flux: $\vec{j}_\mathrm{in} = \frac{\hbar k}{M}\vec{n}_z$

Outgoing flux in direction (ϑ,φ) & distance r: $\vec{j}_\mathrm{out}(r,\vartheta,\varphi) = \frac{|f_k(\vartheta,\varphi)|^2}{r^2}\frac{\hbar k}{M}\vec{n}_r$

$$\Rightarrow \quad d\sigma(\vartheta,\varphi) = \frac{\text{outgoing flux to space angle } d\Omega \text{ around } (\vartheta,\varphi)}{\text{incoming flux}} = \frac{|\vec{j}_\mathrm{out}(r,\vartheta,\varphi)|\overbrace{r^2 d\Omega}^{dS}}{|\vec{j}_\mathrm{in}|} = |f_k(\vartheta,\varphi)|^2 d\Omega$$

$$\Rightarrow \quad \text{differential cross section for elastic scattering:} \quad \boxed{\left(\tfrac{d\sigma}{d\Omega}\right)_k(\vartheta,\varphi) = |f_k(\vartheta,\varphi)|^2}$$

▶ Transformation to the center-of-mass coordinates

We need to adapt the above-outlined procedure to the cases when the target particle is not fixed in space (does not have infinite mass). Elastic scattering of two *finite-mass* particles represents a genuine **two-body problem**. The familiar way of solving this problem proceeds via separating the relative target-projectile degree of freedom from that related the system's center of mass:

2 particles with masses $\binom{M_1}{M_2}$. Position & momentum operators $\binom{\hat{\vec{x}}_1}{\hat{\vec{x}}_2}$ & $\binom{\hat{\vec{p}}_1}{\hat{\vec{p}}_2}$
Transformation to new coordinates & momenta:

$$\boxed{\begin{aligned}\hat{\vec{x}}_\mathrm{c} &= \tfrac{M_1}{M_1+M_2}\hat{\vec{x}}_1 + \tfrac{M_2}{M_1+M_2}\hat{\vec{x}}_2\\ \hat{\vec{x}}_\mathrm{r} &= \hat{\vec{x}}_1 - \hat{\vec{x}}_2\end{aligned}} \Leftrightarrow \boxed{\begin{aligned}\hat{\vec{p}}_\mathrm{c} &= \hat{\vec{p}}_1 + \hat{\vec{p}}_2\\ \hat{\vec{p}}_\mathrm{r} &= \tfrac{M_2}{M_1+M_2}\hat{\vec{p}}_1 - \tfrac{M_1}{M_1+M_2}\hat{\vec{p}}_2\end{aligned}}$$ **center of mass**
relative

Commutators: $[\hat{x}_{\mathrm{c}i}, \hat{p}_{\mathrm{c}j}] = [\hat{x}_{\mathrm{r}i}, \hat{p}_{\mathrm{r}j}] = i\hbar\delta_{ij}, \quad [\hat{x}_{\mathrm{c}i}, \hat{p}_{\mathrm{r}j}] = [\hat{x}_{\mathrm{r}i}, \hat{p}_{\mathrm{c}j}] = 0$
$\Rightarrow$ corresponding Poisson brackets $\Rightarrow$ the transformation is **canonical**

Transformation of the Hamiltonian:
Kinetic energy of both particles: $\hat{T} = \frac{\hat{\vec{p}}_1^{\,2}}{2M_1} + \frac{\hat{\vec{p}}_2^{\,2}}{2M_2} = \frac{\hat{\vec{p}}_\mathrm{c}^{\,2}}{2(M_1+M_2)} + \frac{\hat{\vec{p}}_\mathrm{r}^{\,2}}{2\frac{M_1M_2}{M_1+M_2}}$

Define **reduced mass**: $\boxed{\mathcal{M} = \dfrac{M_1M_2}{M_1+M_2}}$

Potential depending on $\underbrace{\vec{x}_1 - \vec{x}_2}_{\vec{x}_\mathrm{r}} \Rightarrow$ Hamiltonian $\hat{H} = \overbrace{\frac{\hat{\vec{p}}_\mathrm{c}^{\,2}}{2M_\mathrm{tot}}}^{\hat{H}_\mathrm{c}} + \overbrace{\frac{\hat{\vec{p}}_\mathrm{r}^{\,2}}{2\mathcal{M}} + V(\hat{\vec{x}}_\mathrm{r})}^{\hat{H}_\mathrm{r}}$

This represents the separation of center-of-mass and relative motions. Solution of the Schrödinger eq. with $\hat{H}_\mathrm{c}$ is a plane wave in center-of-mass coordinates. We need to solve the equation with $\hat{H}_\mathrm{r}$ in relative coordinates. This represents just the $\boxed{M \mapsto \mathcal{M}}$ change with respect to the fixed-potential problem.

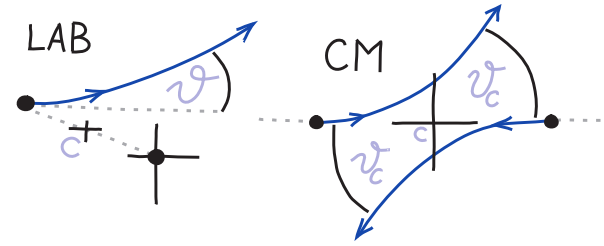
▶ Transformation of scattering angles & cross section

Once the two-body problem is solved in the the center-of-mass (CM) system (as described above), one has to return back to the laboratory (LAB) system, in which the scattering angles and cross sections are measured.

Notation: particle 1 ≡ projectile, particle 2 ≡ target
$\vec{v}_1, \vec{v}_2,\ \vec{p}_1, \vec{p}_2,\ \vartheta, \varphi$ ≡ velocities & momenta & scattering angles in LAB
$\vec{v}_{\mathrm{C}1}, \vec{v}_{\mathrm{C}2},\ \vec{p}_{\mathrm{C}1}, \vec{p}_{\mathrm{C}2},\ \vartheta_\mathrm{C}, \varphi_\mathrm{C}$ ≡ velocities & momenta & scattering angles in CM

Center-of-mass speed in LAB:

$$\boxed{\vec{u} = \tfrac{M_1}{M_1+M_2}\vec{v}_1 + \tfrac{M_2}{M_1+M_2}\vec{v}_2}$$
$= \text{constant}$ (along z)



$\vec{p}_{\mathrm{C}1} = M_1(\vec{v}_1 - \vec{u}) = \mathcal{M}(\vec{v}_1 - \vec{v}_2) \equiv +\vec{p}_\mathrm{C} = \vec{p}_\mathrm{r} \qquad \vec{p}_{\mathrm{C}2} = M_2(\vec{v}_2 - \vec{u}) = \mathcal{M}(\vec{v}_2 - \vec{v}_1) = -\vec{p}_\mathrm{C} = -\vec{p}_\mathrm{r}$

It is obvious that $\boxed{\varphi = \varphi_\mathrm{C}}$ and we can set $\varphi = 0$

$\Rightarrow \quad p_1 \sin\vartheta = p_\mathrm{C} \sin\vartheta_\mathrm{C} \qquad p_1 \cos\vartheta - M_1 u = p_\mathrm{C} \cos\vartheta_\mathrm{C}$

$\Rightarrow \quad \boxed{\tan\vartheta = \frac{p_\mathrm{C}\sin\vartheta_\mathrm{C}}{p_\mathrm{C}\cos\vartheta_\mathrm{C} + M_1 u}} \qquad \boxed{\tan\vartheta_\mathrm{C} = \frac{p_1\sin\vartheta}{p_1\cos\vartheta - M_1 u}}$ transformation $\vartheta \leftrightarrow \vartheta_\mathrm{C}$

Outgoing fluxes in both LAB & CM systems must be *the same*:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\rm L} d\Omega_{\rm L} \stackrel{!}{=} \left(\frac{d\sigma}{d\Omega}\right)_{\rm C} d\Omega_{\rm C} \quad \Rightarrow \quad \left(\frac{d\sigma}{d\Omega}\right)_{\rm L} = \left(\frac{d\sigma}{d\Omega}\right)_{\rm C} \frac{d\Omega_{\rm C}}{d\Omega_{\rm L}}$$

$$d\Omega_{\rm L} = \sin\vartheta d\vartheta d\varphi$$
$$d\Omega_{\rm C} = \sin\vartheta_{\rm C} d\vartheta_{\rm C} d\varphi_{\rm C}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\rm L}(\vartheta,\varphi) = \left(\frac{d\sigma}{d\Omega}\right)_{\rm C}(\vartheta_{\rm C},\varphi_{\rm C}) \underbrace{\frac{\sin\vartheta_{\rm C}}{\sin\vartheta}\frac{d\vartheta_{\rm C}}{d\vartheta}}_{\frac{p_1}{p_1-M_1u}\frac{d}{d\vartheta}\arctan\frac{p_1\sin\vartheta}{p_1\cos\vartheta-M_1u}}$$

relation between LAB & CM differential cross sections

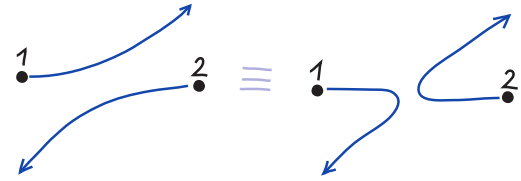
From now on we will work in CM, *skipping the indices* "C" and "R".

▶ Scattering of indistinguishable particles

Quantum indistinguishability of identical particles has a substantial effect on the cross section of elastic scattering. Depending on whether the scattered particles are identical bosons or fermions, the asymptotic wavefunction in CM $\psi(\vec{x}) \propto e^{ikz} + f_k(\vartheta,\varphi)\frac{e^{ikr}}{r}$ must be symmetrized or antisymmetrized with respect to the particle exchange.

Exchange of particles in CM:

$$\vec{x} \mapsto -\vec{x} \;\Rightarrow\; \begin{cases} r \mapsto r \\ \vartheta \mapsto \pi-\vartheta \\ \varphi \mapsto \pi+\varphi \end{cases}$$



Symmetrized wavefunction (for example ${}^4_2\mathrm{He} + {}^4_2\mathrm{He}$ scattering):

$$\psi(\vec{x}) \propto \left[e^{ikz} + e^{-ikz}\right] + \left[f_k(\vartheta,\varphi) + f_k(\pi-\vartheta,\pi+\varphi)\right]\frac{e^{ikr}}{r}$$

Cross section:

$$\left(\frac{d\sigma}{d\Omega}\right)^{+}_{k} = \tfrac{1}{2}\left\{|f_k(\vartheta,\varphi)|^2 + |f_k(\pi-\vartheta,\pi+\varphi)|^2 + 2\mathrm{Re}[f_k(\vartheta,\varphi)f_k^*(\pi-\vartheta,\pi+\varphi)]\right\}$$

where $\frac{1}{2}$ comes from the normalization of the incoming flux.

The same expression applies for 2 fermions in antisymmetric spin state (for example $e + e$ in spin singlet).

Antisymmetrized wavefunction (for example $e + e$ in spin triplet):

$$\psi(\vec{x}) \propto \left[e^{ikz} - e^{-ikz}\right] + \left[f_k(\vartheta,\varphi) - f_k(\pi-\vartheta,\pi+\varphi)\right]\frac{e^{ikr}}{r}$$

Cross section:

$$\left(\frac{d\sigma}{d\Omega}\right)^{-}_{k} = \tfrac{1}{2}\left\{|f_k(\vartheta,\varphi)|^2 + |f_k(\pi-\vartheta,\pi+\varphi)|^2 - 2\mathrm{Re}[f_k(\vartheta,\varphi)f_k^*(\pi-\vartheta,\pi+\varphi)]\right\}$$

Example: **unpolarized $e + e$ scattering**

Probabilities for finding spin singlet & triplet states are $\frac{1}{4}$ & $\frac{3}{4}$ $\Rightarrow$

$$\left(\frac{d\sigma}{d\Omega}\right)_{k} = \tfrac{1}{4}\left(\frac{d\sigma}{d\Omega}\right)^{+}_{k} + \tfrac{3}{4}\left(\frac{d\sigma}{d\Omega}\right)^{-}_{k} =$$
$$= \tfrac{1}{2}\left\{|f_k(\vartheta,\varphi)|^2 + |f_k(\pi-\vartheta,\pi+\varphi)|^2 - \mathrm{Re}[f_k(\vartheta,\varphi)f_k^*(\pi-\vartheta,\pi+\varphi)]\right\}$$

◀ Historical remark

1926: M. Born applies QM to scattering processes (probabilistic interpretation)
1930: N. Mott describes the effects of indistinguishability in Coulomb scattering

■ General formalism: Lippmann-Schwinger equation

We now turn to a rigorous theory of scattering processes. It is based on the so-called Lippmann-Schwinger equation, which transforms general quantum scattering problems — genuinely time dependent — to a stationary form, and moreover allows for a perturbative expansion of its solutions.

▸ Full & free Hamiltonians and their evolution & Green operators

The full Hamiltonian of the system is supposed to have the form $\boxed{\hat{H}=\hat{H}_0+\hat{V}}$ where $\hat{H}_0$ represents the free Hamiltonian of the particles involved in the scattering process and $\hat{V}$ is their mutual interaction.

$\hat{U}_0(t)=e^{-\frac{i}{\hbar}\hat{H}_0 t}$	$\hat{G}_0^{\pm}(E)=\frac{1}{E-\hat{H}_0\pm i\epsilon}$	**free** evolution & Green operators
$\hat{U}(t)=e^{-\frac{i}{\hbar}\hat{H}t}$	$\hat{G}^{\pm}(E)=\frac{1}{E-\hat{H}\pm i\epsilon}$	**full** evolution & Green operators

Here, the energy representation of retarded and advanced Green operators are obtained as follows:

$$\hat{G}^{+}(E)=\big(-\tfrac{i}{\hbar}\big)\lim_{\epsilon\to 0+}\int_{-\infty}^{+\infty}\overbrace{\Theta(t')e^{-\frac{i}{\hbar}\hat{H}t}}^{\hat{G}^{+}(t,0)}e^{+\frac{i}{\hbar}(E+i\epsilon)t'}dt'=\big(-\tfrac{i}{\hbar}\big)\lim_{\epsilon\to 0+}\Big[\frac{e^{-\frac{i}{\hbar}(\hat{H}-E-i\epsilon)t}}{-\frac{i}{\hbar}(\hat{H}-E-i\epsilon)}\Big]_0^{\infty}$$
$$=\big(-\tfrac{i}{\hbar}\big)\big[0-\lim_{\epsilon\to 0+}\tfrac{1}{-\frac{i}{\hbar}(\hat{H}-E-i\epsilon)}\big]=\lim_{\epsilon\to 0+}\tfrac{1}{E-\hat{H}+i\epsilon}\equiv\tfrac{1}{E-\hat{H}+i\epsilon}$$

$$\hat{G}^{-}(E)=\big(-\tfrac{i}{\hbar}\big)\lim_{\epsilon\to 0+}\int_{-\infty}^{+\infty}\overbrace{-\Theta(-t')e^{-\frac{i}{\hbar}\hat{H}t}}^{\hat{G}^{-}(t,0)}e^{+\frac{i}{\hbar}(E-i\epsilon)t'}dt'=\big(+\tfrac{i}{\hbar}\big)\lim_{\epsilon\to 0+}\Big[\frac{e^{-\frac{i}{\hbar}(\hat{H}-E+i\epsilon)t}}{-\frac{i}{\hbar}(\hat{H}-E+i\epsilon)}\Big]_{-\infty}^{0}$$
$$=\big(+\tfrac{i}{\hbar}\big)\big[\lim_{\epsilon\to 0+}\tfrac{1}{-\frac{i}{\hbar}(\hat{H}-E+i\epsilon)}-0\big]=\lim_{\epsilon\to 0+}\tfrac{1}{E-\hat{H}-i\epsilon}\equiv\tfrac{1}{E-\hat{H}-i\epsilon}$$

Note that the fraction $\frac{1}{\hat{O}}=\hat{O}^{-1}$ means inversion. The infinitesimal quantity $\epsilon>0$ is used to make the above integrals converging. Due to the $\pm i\epsilon$ term, the expressions for $\hat{G}^{\pm}(E)$ do not diverge at states $|\Psi\rangle$ satisfying $\hat{H}|\Psi\rangle=E|\Psi\rangle$. At last we prepare for later use the following identities:

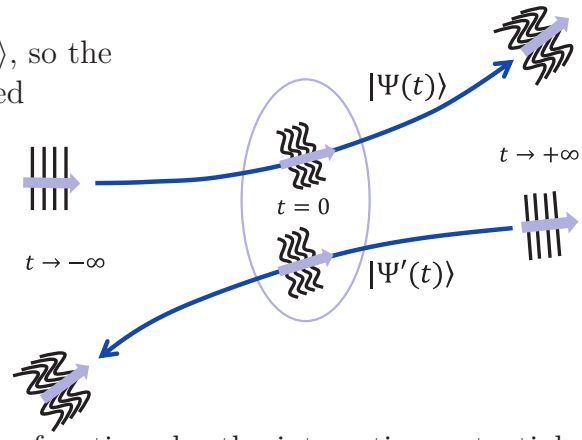
$$\hat{U}(+t)\hat{U}_0(-t)=\hat{I}+\int_0^t\overbrace{\tfrac{d}{dt'}\big[\hat{U}(+t')\hat{U}_0(-t')\big]}^{\hat{U}(t')\left(-\frac{i}{\hbar}\hat{H}\right)\hat{U}_0(-t')+\hat{U}(t')\left(+\frac{i}{\hbar}\hat{H}_0\right)\hat{U}_0(-t')}dt'=\hat{I}-\tfrac{i}{\hbar}\int_0^t\hat{U}(+t')\hat{V}\hat{U}_0(-t')dt'$$

$$\hat{U}(-t)\hat{U}_0(+t)=\hat{I}+\int_0^t\underbrace{\tfrac{d}{dt'}\big[\hat{U}(-t')\hat{U}_0(+t')\big]}_{\hat{U}(-t')\left(+\frac{i}{\hbar}\hat{H}\right)\hat{U}_0(t')+\hat{U}(-t')\left(-\frac{i}{\hbar}\hat{H}_0\right)\hat{U}_0(t')}dt'=\hat{I}+\tfrac{i}{\hbar}\int_0^t\hat{U}(-t')\hat{V}\hat{U}_0(+t')dt'$$

▸ Transformation to $t=0$

We consider a scattering process in which the initial state $|\Psi(-\infty)\rangle$ of the particles involved is prepared at time $t\to-\infty$ and evolves to a final state $|\Psi(+\infty)\rangle$ at $t\to+\infty$. A quantum measurement of scattering products may identify the final state with a plethora of other states $|\Psi'(+\infty)\rangle$. The task is to determine the amplitudes $\langle\Psi'(+\infty)|\Psi(+\infty)\rangle$, which characterize the corresponding transitions from $|\Psi(-\infty)\rangle$ to $|\Psi'(+\infty)\rangle$. From unitarity of quantum evolution we

get $\langle\Psi'(+\infty)|\Psi(+\infty)\rangle = \langle\Psi'(t)|\Psi(t)\rangle$, so the transition amplitudes can be obtained from the corresponding evolving states at any finite time t.



We assume that the interaction between the particles takes place only in a limited time domain near $t \approx 0$, so it is quite natural to shift all the evolving states to $t = 0$.

To avoid distortions of the total wavefunctions by the interaction potentials, we perform the shift using the *free* evolution operator:

$$\textbf{incoming state}\quad |\Psi(-\infty)\rangle \longmapsto |\Psi_{\rm in}\rangle = \lim_{t\to\infty} \hat{U}_0(+t)\overbrace{\hat{U}(-t)|\Psi(0)\rangle}^{|\Psi(-t)\rangle}$$

$$\textbf{outgoing state}\quad |\Psi'(+\infty)\rangle \longmapsto |\Psi_{\rm out}\rangle = \lim_{t\to\infty} \hat{U}_0(-t)\underbrace{\hat{U}(+t)|\Psi'(0)\rangle}_{|\Psi'(+t)\rangle}$$

From this and from the above prepared relations we obtain:

$$|\Psi(0)\rangle = \lim_{t\to\infty} \hat{U}(+t)\hat{U}_0(-t)|\Psi_{\rm in}\rangle = \left[\hat{I} - \tfrac{i}{\hbar}\int_0^\infty \hat{U}(+t')\hat{V}\hat{U}_0(-t')dt'\right]|\Psi_{\rm in}\rangle$$

$$|\Psi'(0)\rangle = \lim_{t\to\infty} \hat{U}(-t)\hat{U}_0(+t)|\Psi_{\rm out}\rangle = \left[\hat{I} + \tfrac{i}{\hbar}\int_0^\infty \hat{U}(-t')\hat{V}\hat{U}_0(+t')dt'\right]|\Psi_{\rm out}\rangle$$

▶ Expansion of incoming & outgoing states to "plane waves"

We now use the eigenbasis $\{|\Phi_{En}\rangle\}$ of the free Hamiltonian: $\boxed{\hat{H}_0|\Phi_{En}\rangle = E|\Phi_{En}\rangle}$

In case of a potential scattering, these states would be plane waves, with n denoting a degeneracy index which determines the direction of wave propagation. In the 1D space (e.g., in tunneling problems) the index takes only 2 discrete values $n = \pm 1$, while in 2D & 3D scattering problems it is a continuous quantity expressing a unit vector $\vec{n}$.

The expansion the incoming & outgoing states yields

$$\boxed{|\Psi_{\rm in}\rangle = \int dE \sum_n \alpha_{En}|\Phi_{En}\rangle} \qquad \boxed{|\Psi_{\rm out}\rangle = \int dE \sum_n \alpha'_{En}|\Phi_{En}\rangle}$$

where $\alpha_{En}, \alpha'_{En} \equiv$ coefficients and $\sum_n$ possibly means an integral $\int d\vec{n}$.

From the above-derived expressions we obtain:

$$|\Psi(0)\rangle = \int dE \sum_n \alpha_{En} \overbrace{\left[\hat{I} - \tfrac{i}{\hbar}\int_0^\infty \hat{U}(+t')\hat{V}\hat{U}_0(-t')dt'\right]}^{|\Psi^+_{En}\rangle} |\Phi_{En}\rangle$$

$$|\Psi'(0)\rangle = \int dE \sum_n \alpha'_{En} \underbrace{\left[\hat{I} + \tfrac{i}{\hbar}\int_0^\infty \hat{U}(-t')\hat{V}\hat{U}_0(+t')dt'\right]}_{|\Psi^-_{En}\rangle} |\Phi_{En}\rangle$$

$$\Rightarrow \quad \boxed{\langle\Psi'0)|\Psi(0)\rangle = \iint dE\, dE' \sum_{n,n'} \alpha^*_{E'n'}\alpha_{En}\langle\Psi^-_{E'n'}|\Psi^+_{En}\rangle}$$

▶ Equations for $|\Psi^{\pm}_{En}\rangle$

For the incoming & outgoing states identified with plane waves $|\Phi_{En}\rangle$ & $|\Phi_{E'n'}\rangle$, respectively, the above relation can be diagrammatically expressed in the form:

$$\begin{array}{lcll} \text{incoming state} & & t=0 \text{ state} & \text{outgoing state} \\ |\Psi_{\text{in}}\rangle = |\Phi_{En}\rangle & \longrightarrow & |\Psi^{+}_{En}\rangle & \\ & & |\Psi^{-}_{E'n'}\rangle & \longleftarrow \quad |\Phi_{E'n'}\rangle = |\Psi_{\text{out}}\rangle \end{array} \Rightarrow \begin{cases} \text{amplitude of} \\ |\Phi_{En}\rangle \to |\Phi_{E'n'}\rangle \\ \text{transition} \\ = \langle \Psi^{-}_{E'n'} | \Psi^{+}_{En}\rangle \end{cases}$$

The vectors $|\Psi^{\pm}_{En}\rangle$ can be further evaluated as:

$$\begin{aligned} |\Psi^{+}_{En}\rangle &= \big[\hat{I} - \tfrac{i}{\hbar}\int_0^\infty e^{-\frac{i}{\hbar}\hat{H}t'} e^{+\frac{i}{\hbar}Et'} dt'\big]\hat{V}|\Phi_{En}\rangle \\ &= \big[\hat{I} - \lim_{\epsilon\to 0+} \tfrac{i}{\hbar}\int_0^\infty e^{-\frac{i}{\hbar}(\hat{H}-E-i\epsilon)t'} dt'\big]\hat{V}|\Phi_{En}\rangle \\ &= \big[\hat{I} + \lim_{\epsilon\to 0+} \tfrac{1}{E-\hat{H}+i\epsilon}\hat{V}\big]|\Phi_{En}\rangle \end{aligned} \qquad \begin{aligned} |\Psi^{-}_{En}\rangle &= \big[\hat{I} + \tfrac{i}{\hbar}\int_0^\infty e^{+\frac{i}{\hbar}\hat{H}t'} e^{-\frac{i}{\hbar}Et'} dt'\big]\hat{V}|\Phi_{En}\rangle \\ &= \big[\hat{I} + \lim_{\epsilon\to 0+} \tfrac{i}{\hbar}\int_0^\infty e^{+\frac{i}{\hbar}(\hat{H}-E+i\epsilon)t'} dt'\big]\hat{V}|\Phi_{En}\rangle \\ &= \big[\hat{I} + \lim_{\epsilon\to 0+} \tfrac{1}{E-\hat{H}-i\epsilon}\hat{V}\big]|\Phi_{En}\rangle \end{aligned}$$

Skipping the "lim" symbol (see the definition of the Green operator) we get:

$$|\Psi^{\pm}_{En}\rangle = \left[\hat{I} + \overbrace{\frac{1}{E-\hat{H}\pm i\epsilon}}^{\hat{G}^{\pm}(E)}\hat{V}\right]|\Phi_{En}\rangle$$

Lippmann-Schwinger equation in explicit form (LSE)

In principle, this formula explicitly determines the desired states $|\Psi^{\pm}_{En}\rangle$ for each plane wave $|\Phi_{En}\rangle$. However, to evaluate the full Green operators $\hat{G}^{\pm}(E)$ for a general Hamiltonian $\hat{H}=\hat{H}_0+\hat{V}$ is usually a difficult task. We would like to use the free Green operators $\hat{G}^{\pm}_0(E)$ associated with $\hat{H}_0$ only. Manipulating with the LSE equation $|\Psi^{\pm}_{En}\rangle = \big[\hat{I} + \frac{1}{E-\hat{H}_0-\hat{V}\pm i\epsilon}\hat{V}\big]|\Phi_{En}\rangle$ we obtain:

$$(E-\hat{H}_0-\hat{V}\pm i\epsilon)|\Psi^{\pm}_{En}\rangle = [E-\hat{H}_0-\hat{V}\pm i\epsilon+\hat{V}]|\Phi_{En}\rangle$$
$$(E-\hat{H}_0\pm i\epsilon)|\Psi^{\pm}_{En}\rangle = [E-\hat{H}_0\pm i\epsilon]|\Phi_{En}\rangle + \hat{V}|\Psi^{\pm}_{En}\rangle$$

$$|\Psi^{\pm}_{En}\rangle = |\Phi_{En}\rangle + \overbrace{\frac{1}{E-\hat{H}_0\pm i\epsilon}}^{\hat{G}^{\pm}_0(E)}\hat{V}|\Psi^{\pm}_{En}\rangle$$

Lippmann-Schwinger equation in implicit form (LSI)

This formula indeed makes use of the free Green operators, but the price we pay for this is that the searched solution $|\Psi^{\pm}_{En}\rangle$ occurs also on the right-hand side of the equation, so it is determined only implicitly. Fortunately, as shown below, the solution can be written in an iterative form.

We may consider both the LSE & LSI equations as modified forms of the Schrödinger equation, which are however tailored directly to the scattering problem. Indeed, using $\hat{H}_0|\Phi_{En}\rangle = E|\Phi_{En}\rangle$ in the equation above the LSI yields:

$$(E-\hat{H}_0\pm i\epsilon)|\Psi^{\pm}_{En}\rangle = [E-E\pm i\epsilon]|\Phi_{En}\rangle + \hat{V}|\Psi^{\pm}_{En}\rangle \;\Rightarrow\; (\hat{H}_0+\hat{V})|\Psi^{\pm}_{En}\rangle = E|\Psi^{\pm}_{En}\rangle$$

$\Rightarrow$ $|\Psi^{\pm}_{En}\rangle$ is a solution of the stationary Schrödinger equation with the full Hamiltonian $\hat{H}$ which has the property: $\boxed{|\Psi^{\pm}_{En}\rangle \to |\Phi_{En}\rangle \text{ for } \hat{V} \to 0}$

▶ Iterative solution of the LSI

The LSI can apparently be expanded in an iterative way. If we repeatedly substitute $|\Phi_{En}\rangle + \hat{G}^{\pm}_0(E)\hat{V}|\Psi^{\pm}_{En}\rangle$ for $|\Psi^{\pm}_{En}\rangle$ on the right-hand side, we obtain:

$$\boxed{|\Psi^{\pm}_{En}\rangle = \big[\hat{I} + \hat{G}^{\pm}_0(E)\hat{V} + \hat{G}^{\pm}_0(E)\hat{V}\hat{G}^{\pm}_0(E)\hat{V} + \cdots\cdots\big]|\Phi_{En}\rangle}$$

This is apparently a series in powers of $\hat{V}$, so if the interaction is small compared to the free Hamiltonian, the series can be understood as a perturbative expansion of the solution $|\Psi^{\pm}_{En}\rangle$.

This can be equivalently expressed through the ***T*-operator** defined by: $\boxed{\hat{T}^{\pm}(E)|\Phi_{En}\rangle = \hat{V}|\Psi^{\pm}_{En}\rangle}$

The LSI in terms of this operator reads as: $|\Psi^{\pm}_{En}\rangle = [\hat{I} + \hat{G}^{\pm}_0(E)\hat{T}^{\pm}(E)]|\Phi_{En}\rangle$.
Multiplying this formula by $\hat{V}$ from left we obtain:
$\hat{T}^{\pm}(E)|\Phi_{En}\rangle = [\hat{V} + \hat{V}\hat{G}^{\pm}_0(E)\hat{T}^{\pm}(E)]|\Phi_{En}\rangle \quad \Rightarrow \quad \hat{T}^{\pm}(E) = \hat{V} + \hat{V}\hat{G}^{\pm}_0(E)\hat{T}^{\pm}(E)$

$$\Rightarrow \qquad \boxed{\hat{T}^{\pm}(E) = \hat{V} + \hat{V}\hat{G}^{\pm}_0(E)\hat{V} + \hat{V}\hat{G}^{\pm}_0(E)\hat{V}\hat{G}^{\pm}_0(E)\hat{V} + \cdots\cdots}$$

▶ S-matrix

The scattering matrix $\hat{S}$ (so-called S-matrix, cf. Sec. 11) expresses probability amplitudes of transitions $|\Phi_{En}\rangle \longrightarrow |\Phi_{E'n'}\rangle$ that occur in the scattering process. We already know that this amplitude is equal to $\langle\Psi^{-}_{E'n'}|\Psi^{+}_{En}\rangle$, so we can write:

$$\boxed{\langle\Phi_{E'n'}|\hat{S}|\Phi_{En}\rangle = \langle\Psi^{-}_{E'n'}|\Psi^{+}_{En}\rangle}$$

Using LSE & LSI consecutively on both sides of the scalar product we derive:

$$\langle\underbrace{\Psi^{-}_{E'n'}}_{\text{LSE...}}|\Psi^{+}_{En}\rangle = \langle\Phi_{E'n'}|\hat{I} + \hat{V}\tfrac{1}{E'-\hat{H}+i\epsilon}|\Psi^{+}_{En}\rangle = \langle\Phi_{E'n'}|\underbrace{\Psi^{+}_{En}}_{\text{LSI...}}\rangle + \langle\Phi_{E'n'}|\hat{V}|\Psi^{+}_{En}\rangle\tfrac{1}{E'-E+i\epsilon}$$

$$= \langle\Phi_{E'n'}|\Phi_{En}\rangle + \langle\Phi_{E'n'}|\overbrace{\tfrac{1}{E-\hat{H}_0+i\epsilon}}^{\frac{1}{E-E'+i\epsilon}}\hat{V}|\Psi^{+}_{En}\rangle + \langle\Phi_{E'n'}|\hat{V}|\Psi^{+}_{En}\rangle\tfrac{1}{E'-E+i\epsilon}$$

$$= \underbrace{\langle\Phi_{E'n'}|\Phi_{En}\rangle}_{\delta(E-E')\delta_{nn'}} + \underbrace{\big(\tfrac{1}{E-E'+i\epsilon} + \tfrac{1}{E'-E+i\epsilon}\big)}_{-2i\pi\frac{1}{\pi}\frac{\epsilon}{(E-E')^2+\epsilon^2} \overset{\epsilon\to 0}{\longrightarrow} -2i\pi\delta(E-E')} \langle\Phi_{E'n'}|\hat{V}|\Psi^{+}_{En}\rangle$$

$$\Rightarrow \qquad \boxed{\langle\Phi_{E'n'}|\hat{S}|\Phi_{En}\rangle = \delta(E-E')\delta_{nn'} - 2i\pi\,\delta(E-E')\,\langle\Phi_{E'n'}|\hat{V}|\Psi^{+}_{En}\rangle}$$

From the T-operator expression we finally obtain:

$$\boxed{\begin{aligned}\langle\Phi_{E'n'}|\hat{S}|\Phi_{En}\rangle &= \delta(E-E')\times\\ &\Big[\delta_{nn'} - 2i\pi\,\langle\Phi_{E'n'}|\hat{V} + \hat{V}\hat{G}^{\pm}_0(E)\hat{V} + \hat{V}\hat{G}^{\pm}_0(E)\hat{V}\hat{G}^{\pm}_0(E)\hat{V} + \cdots|\Phi_{En}\rangle\Big]\end{aligned}}$$

◂ Historical remark
1937: J.A. Wheeler introduces the scattering matrix in nuclear processes
1943-4: W. Heisenberg elaborates a general scheme of the S-matrix theory
1950: B.A. Lippmann & J. Schwinger derive the LSE & LSI equations

■ Application to elastic scattering

The above-developed theory based on the Lippmann-Schwinger equation and its iterative solution will now be applied in the simplest setting of the elastic scattering (no change of the target/projectile internal structure). We move back from the S-matrix to the description using the differential cross section.

▸ Evaluation of LSI for elastic scattering by a potential $V(\vec{x})$

The general notation is transformed to the coordinate representation:
$\boxed{|\Psi^{\pm}_{En}\rangle \equiv \psi^{\pm}_{\vec{k}}(\vec{x})}$ and $\boxed{|\Phi_{En}\rangle \equiv \phi_{\vec{k}}(\vec{x})}$ with $\vec{k} \equiv$ the initial wave vector

The LSI$^+$ equation: $\boxed{\psi^{+}_{\vec{k}}(\vec{x}) = \phi_{\vec{k}}(\vec{x}) + \int \langle \vec{x} \,| \tfrac{1}{E-\hat{H}_0+i\hbar\epsilon} |\vec{x}\,'\rangle \langle \vec{x}\,'|\hat{V}|\psi^{+}_{\vec{k}}\rangle \, d\vec{x}\,'}$

(a) $\langle \vec{x}\,'|\hat{V}|\psi^{+}_{\vec{k}}\rangle = V(\vec{x}\,')\,\psi^{+}_{\vec{k}}(\vec{x}\,')$ **local potential**

(b) $\langle \vec{x} \,| \tfrac{1}{E-\hat{H}_0+i\hbar\epsilon} |\vec{x}\,'\rangle = \iint \underbrace{\langle \vec{x}|\vec{p}\,'\rangle}_{\frac{1}{(2\pi\hbar)^{\frac{3}{2}}} e^{+\frac{i}{\hbar}\vec{p}\,'\cdot\vec{x}}} \underbrace{\langle \vec{p}\,'| \tfrac{1}{E-\hat{H}_0+i\hbar\epsilon} |\vec{p}\,''\rangle}_{\frac{1}{E-\frac{1}{2\mathcal{M}}\vec{p}\,'^2+i\hbar\epsilon}\delta(\vec{p}\,'-\vec{p}\,'')} \underbrace{\langle \vec{p}\,''|\vec{x}\,'\rangle}_{\frac{1}{(2\pi\hbar)^{\frac{3}{2}}} e^{-\frac{i}{\hbar}\vec{p}\,''\cdot\vec{x}\,'}} d\vec{p}\,' d\vec{p}\,'' = \dots$

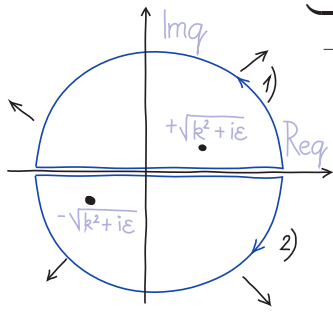
$E \equiv \frac{(\hbar k)^2}{2\mathcal{M}} \quad \frac{2\mathcal{M}\epsilon}{\hbar} \equiv \varepsilon \quad \vec{p}\,' \equiv \hbar\vec{q}$ polar coordinates of $\vec{q}$ with $\vec{n}_z \propto (\vec{x}-\vec{x}\,')$

$$= \frac{1}{(2\pi\hbar)^3}\int \frac{e^{\frac{i}{\hbar}\vec{p}\,'\cdot(\vec{x}-\vec{x}\,')}}{E-\frac{1}{2\mathcal{M}}\vec{p}\,'^2+i\hbar\epsilon}\, d\vec{p}\,' = \frac{2\mathcal{M}}{\hbar^2(2\pi)^3}\int \frac{e^{i\vec{q}\cdot(\vec{x}-\vec{x}\,')}}{k^2-q^2+i\varepsilon}\, d\vec{q} = \frac{2\mathcal{M}}{\hbar^2(2\pi)^3}\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} \frac{e^{iq|\vec{x}-\vec{x}\,'|\cos\vartheta}}{k^2-q^2+i\varepsilon} q^2 \sin\vartheta\, d\varphi\, d\vartheta\, dq$$

$$= \frac{2\mathcal{M}}{(2\pi\hbar)^2}\int_0^{\infty}\left[-\frac{e^{iq|\vec{x}-\vec{x}\,'|\cos\vartheta}}{iq|\vec{x}-\vec{x}\,'|}\right]_{\vartheta=0}^{\vartheta=\pi} \frac{1}{k^2-q^2+i\varepsilon} q^2 dq = -\frac{2\mathcal{M}}{(2\pi\hbar)^2}\frac{1}{i|\vec{x}-\vec{x}\,'|}\int_0^{\infty} \frac{e^{+iq|\vec{x}-\vec{x}\,'|}-e^{-iq|\vec{x}-\vec{x}\,'|}}{q^2-k^2-i\varepsilon}\, q\, dq$$

Poles at $q = \pm\sqrt{k^2+i\varepsilon} \approx \pm\left(k + i\frac{\varepsilon}{2k}\right) \quad \Rightarrow \quad$ use the residuum theorem

$$= -\frac{2\mathcal{M}}{(2\pi\hbar)^2}\frac{1}{i|\vec{x}-\vec{x}\,'|}\frac{1}{2}\left[\underbrace{\int_{-\infty}^{+\infty} \frac{e^{+iq|\vec{x}-\vec{x}\,'|}}{q^2-k^2-i\varepsilon}\, q\, dq}_{\to 2\pi i\ \frac{e^{ik|\vec{x}-\vec{x}\,'|}}{2k}\ k} - \underbrace{\int_{-\infty}^{+\infty} \frac{e^{-iq|\vec{x}-\vec{x}\,'|}}{q^2-k^2-i\varepsilon}\, q\, dq}_{\to -2\pi i\ \frac{e^{ik|\vec{x}-\vec{x}\,'|}}{2k}\ k}\right] \xrightarrow{\varepsilon\to 0} \underbrace{-\frac{2\mathcal{M}}{\hbar^2}\frac{1}{4\pi}\frac{e^{ik|\vec{x}-\vec{x}\,'|}}{|\vec{x}-\vec{x}\,'|}}_{=\langle\vec{x}|\hat{G}_0^{+}(E)|\vec{x}\,'\rangle}$$



The **free Green function** $\langle\vec{x}|\hat{G}_0^{+}(E)|\vec{x}\,'\rangle \equiv G_k^{+}(\vec{x},\vec{x}\,')$ in x-representation satisfies the following equation:
$(\Delta + k^2)G_k^{+}(\vec{x},\vec{x}\,') = \delta(\vec{x}-\vec{x}\,')$

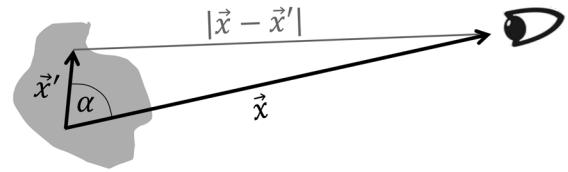
LSI$^+$ in x-representation:

$$\boxed{\psi^{+}_{\vec{k}}(\vec{x}) = \phi_{\vec{k}}(\vec{x}) - \frac{2\mathcal{M}}{\hbar^2}\frac{1}{4\pi}\int \frac{e^{ik|\vec{x}-\vec{x}\,'|}}{|\vec{x}-\vec{x}\,'|} V(\vec{x}\,')\,\psi^{+}_{\vec{k}}(\vec{x}\,')\, d\vec{x}\,'}$$

▶ Asymptotic wavefunction for a finite-range potential

Now we show that for finite-range potentials the solutions $\psi^+_{\vec{k}}(\vec{x})$ of the above LSI$^+$ equation automatically satisfies the asymptotic condition for the elastic scattering, $\psi^+_{\vec{k}}(\vec{x}) \propto e^{i\vec{k}\cdot\vec{x}} + f_{\vec{k}}(\vartheta,\varphi)\frac{e^{ikr}}{r}$, where (ϑ,φ) are spherical angles with respect to $\vec{n}_z = \frac{\vec{k}}{k}$. To this end, assume $V(\vec{x}) \approx 0$ for $|\vec{x}| > R$ and consider $\psi^+_{\vec{k}}(\vec{x})$ for $|\vec{x}| \gg R \gtrsim |\vec{x}\,'|$:

$$
\begin{aligned}
&|\vec{x}-\vec{x}\,'| = \sqrt{r^2+r'^2-2rr'\cos\alpha} \\
&\approx r + \tfrac{d}{dr'}\sqrt{r^2+r'^2-2rr'\cos\alpha}\,\big|_{r'=0} r' \\
&= r - r'\cos\alpha \\
&\Rightarrow \quad \tfrac{e^{ik|\vec{x}-\vec{x}\,'|}}{|\vec{x}-\vec{x}\,'|} \approx e^{-ikr'\cos\alpha}\,\tfrac{e^{ikr}}{r}
\end{aligned}
$$



$\boxed{\vec{k}\,' = k\,\dfrac{\vec{x}}{|\vec{x}|}}$ scattering direction $\Rightarrow$

$$
\psi^+_{\vec{k}}(\vec{x}) = \overbrace{\phi_{\vec{k}}(\vec{x})}^{(2\pi)^{-\frac{3}{2}}\, e^{i\vec{k}\cdot\vec{x}}} + \underbrace{\left[-\tfrac{2\mathcal{M}}{\hbar^2}\tfrac{1}{4\pi}\overbrace{\int e^{-i\vec{k}\,'\cdot\vec{x}\,'} V(\vec{x}\,')\,\psi^+_{\vec{k}}(\vec{x}\,')\,d\vec{x}\,'}^{(2\pi)^{\frac{3}{2}}\,\langle\phi_{\vec{k}'}|\hat{V}|\psi^+_{\vec{k}}\rangle}\right]}_{\text{LSI}^+\text{ equation}} \underbrace{\frac{e^{ikr}}{r}}_{(2\pi)^{-\frac{3}{2}}\, f_{\vec{k}}(\vec{k}\,')}
$$

$\Rightarrow$ explicit expression of the scattering amplitude from the exact solution $\psi^+_{\vec{k}}(\vec{x})$:

$$
\boxed{f_{\vec{k}}(\vartheta,\varphi) \equiv f_{\vec{k}}(\vec{k}\,') = -\tfrac{2\mathcal{M}}{\hbar^2}\sqrt{\tfrac{\pi}{2}}\int e^{-i\vec{k}\,'\cdot\vec{x}\,'} V(\vec{x}\,')\,\psi^+_{\vec{k}}(\vec{x}\,')\,d\vec{x}\,' = -\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\,\langle\phi_{\vec{k}'}|\hat{V}|\psi^+_{\vec{k}}\rangle}
$$

▶ Born series

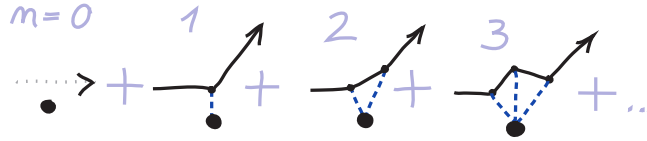
With the aid of the T-operator defined by $\boxed{\hat{V}|\psi^+_{\vec{k}}\rangle = \hat{T}^+(E)|\phi_{\vec{k}}\rangle}$ with $E = \frac{(\hbar k)^2}{2\mathcal{M}}$ and using the above-derived iterative expression

$$
\hat{T}^+(E) = \hat{V} + \hat{V}\tfrac{1}{E-\hat{H}_0+i\hbar\epsilon}\hat{V} + \hat{V}\tfrac{1}{E-\hat{H}_0+i\hbar\epsilon}\hat{V}\tfrac{1}{E-\hat{H}_0+i\hbar\epsilon}\hat{V} + \cdots\cdots,
$$

we obtain the so-called Born series of the scattering amplitude:

$$
\begin{aligned}
f_{\vec{k}}(\vec{k}\,') = \; & -\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\,\langle\phi_{\vec{k}'}|\hat{T}^+(E)|\phi_{\vec{k}}\rangle = \lim_{m\to\infty}\underbrace{\sum_{n=1}^{m} f_{n\vec{k}}(\vec{k}\,')}_{f^{(m)}_{\vec{k}}(\vec{k}\,')} \\
& f_{1\vec{k}}(\vec{k}\,') = -\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\,\langle\phi_{\vec{k}'}|\hat{V}|\phi_{\vec{k}}\rangle \\
& f_{2\vec{k}}(\vec{k}\,') = -\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\,\langle\phi_{\vec{k}'}|\hat{V}\tfrac{1}{E-\hat{H}_0+i\hbar\eta}\hat{V}|\phi_{\vec{k}}\rangle \\
& f_{3\vec{k}}(\vec{k}\,') = -\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\,\langle\phi_{\vec{k}'}|\hat{V}\tfrac{1}{E-\hat{H}_0+i\hbar\eta}\hat{V}\tfrac{1}{E-\hat{H}_0+i\hbar\eta}\hat{V}|\phi_{\vec{k}}\rangle \\
& \cdots\cdots
\end{aligned}
$$

Interpretation through a sequence of free evolutions and point interactions



▸ Relation to non-stationary perturbation theory

We confine the system into a **finite box** of linear size L. A normalized plane wave in the box is given by $\boxed{|\tilde{\phi}_{\vec{k}}\rangle \equiv \frac{1}{L^{\frac{3}{2}}}\, e^{i\vec{k}\cdot\vec{x}}}$ with $\vec{k} = \frac{2\pi}{L}\vec{n}$, where $\vec{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$ satisfies the quantization condition $n_x, n_y, n_z = 0, 1, 2, \ldots$

The $|\tilde{\phi}_{\vec{k}}\rangle \to |\tilde{\phi}_{\vec{k}\,'}\rangle$ transition rate can be obtained from the Fermi golden rule, as well as from the corresponding differential cross section:

$$\boxed{\mathcal{R}_{\vec{k}\to\vec{k}'} = \tfrac{2\pi}{\hbar}\, |\langle\tilde{\phi}_{\vec{k}'}|\hat{V}|\tilde{\phi}_{\vec{k}}\rangle|^2\, \varrho_f(E) = |\vec{j}_{\rm in}|\, \left(\tfrac{d\sigma}{d\Omega}\right)_{\vec{k}}(\vec{k}\,')\, d\Omega}$$

(a) $|\langle\tilde{\phi}_{\vec{k}'}|\hat{V}|\tilde{\phi}_{\vec{k}}\rangle|^2 = \frac{1}{L^6}\left|\int e^{i(\vec{k}-\vec{k}\,')\cdot\vec{x}\,'} V(\vec{x}\,')\, d\vec{x}\,'\right|^2$

(b) $\varrho_f(E) = \frac{dN}{dE} = \frac{\left(\frac{L}{2\pi}\right)^3 k^2\, dk\, d\Omega}{\frac{\hbar^2 k}{\mathcal{M}} dk} = \left(\frac{L}{2\pi}\right)^3 \frac{\mathcal{M}k}{\hbar^2}\, d\Omega \quad$ with $E = \frac{(\hbar k)^2}{2\mathcal{M}}$

(c) $|\vec{j}_{\rm in}| = \frac{\hbar k}{L^3\mathcal{M}}$

$$\Rightarrow \quad \left(\tfrac{d\sigma}{d\Omega}\right)_{\vec{k}}(\vec{k}\,') = \left(\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\right)^2 \left|\tfrac{1}{(2\pi)^3}\int e^{i(\vec{k}-\vec{k}\,')\cdot\vec{x}\,'} V(\vec{x}\,')\, d\vec{x}\,'\right|^2 \equiv |f^{(1)}_{\vec{k}}(\vec{k}\,')|^2$$

Therefore, we see that the nonstationary perturbation theory in the first order yields the same expression as the first-order Born approximation.

▸ Convergence criteria

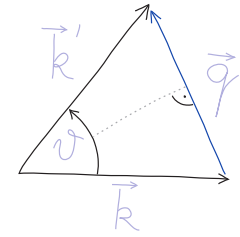
The Born series for scattering amplitude converges for finite-range potentials. For infinite-range potentials, the series may converge if the potential decreases "fast enough". For a given potential $V(\vec{x})$ there exists a function of energy $\lambda_{\max}(E)$ (convergence radius) such that the Born series of a scaled potential $V_\lambda(\vec{x}) \equiv \lambda V(\vec{x})$ converges for $\lambda \le \lambda_{\max}(E)$.

▸ First Born approximation for spherically symmetric potentials

For potentials depending just on $r = |\vec{x}|$ the integration in each term of the Born series is reduced. For the first term, in particular, we proceed as follows:

$$f^{(1)}_{\vec{k}}(\vec{k}\,') = -\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\, \tfrac{1}{(2\pi)^3}\int e^{i(\vec{k}-\vec{k}\,')\cdot\vec{x}\,'} V(|\vec{x}\,'|)\, d\vec{x}\,' \qquad \textbf{Fourier transform of } V$$

transferred momentum $\boxed{\hbar\vec{q} = \hbar(\vec{k}\,'-\vec{k})}$



$$q = |\vec{k}\,'-\vec{k}| = \sqrt{k'^2 + k^2 - 2k'k\cos\vartheta} = \sqrt{2k^2(1-\cos\vartheta)} = 2k\sin\tfrac{\vartheta}{2}$$

We introduce a local coordinate system (x', y', z') with z' along $\vec{q}$ and then spherical coordinates (r', θ', ϕ'):

$$f^{(1)}_{\vec{k}}(\vec{k}\,') = -\tfrac{\mathcal{M}}{2\pi\hbar^2}\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-iqr'\cos\theta'} V(r')\, r'^2 \sin\theta'\, d\phi'\, d\theta'\, dr' =$$

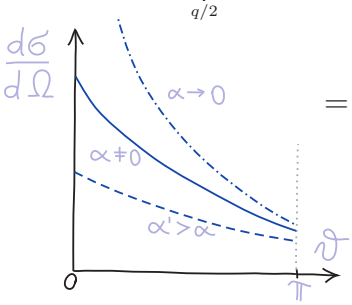
$$-\frac{\mathcal{M}}{\hbar^2}\int_0^\infty \underbrace{\left[\frac{e^{-iqr'\cos\theta'}}{-iqr'}\right]_0^\pi}_{-\frac{2\sin qr'}{qr'}} V(r')\,r'^2 dr' \Rightarrow \boxed{f_{\vec{k}}^{(1)}(\vec{k}\,') = \frac{\mathcal{M}}{\hbar^2 k\sin\frac{\vartheta}{2}}\int_0^\infty r' V(r')\sin\left(2kr'\sin\tfrac{\vartheta}{2}\right)dr'}$$

We see that the scattering amplitude depends only on angle ϑ (not on φ), which remains valid for all terms of the Born series. This can be seen directly from the axial symmetry of the problem with an isotropic potential around the incoming-particle direction.

▶ Yukawa scattering

Scattering by Yukawa potential $\boxed{V(r) = K\,\frac{e^{-\alpha r}}{r}}$ with $\alpha > 0$

$$f_{\vec{k}}^{(1)}(\vec{k}\,') = \frac{K\mathcal{M}}{\hbar^2 \underbrace{k\sin\frac{\vartheta}{2}}_{q/2}}\int_0^\infty e^{-\alpha r'}\underbrace{\sin\left(2kr'\sin\tfrac{\vartheta}{2}\right)}_{\frac{1}{2i}[e^{+iqr'}-e^{-iqr'}]}dr'$$



$$= \frac{2K\mathcal{M}}{\hbar^2}\frac{1}{2iq}\Bigg[\overbrace{\int_0^\infty e^{(-\alpha+iq)r'}dr' - \int_0^\infty e^{(-\alpha-iq)r'}dr'}^{\frac{+2iq}{\alpha^2+q^2}}\Bigg] = \frac{2K\mathcal{M}}{\hbar^2}\frac{1}{\alpha^2+4k^2\sin^2\frac{\vartheta}{2}}$$

$$\Rightarrow \quad \boxed{\left(\frac{d\sigma}{d\Omega}\right)_k^{(1)}(\vartheta) = \left(\frac{2K\mathcal{M}}{\hbar^2}\right)^2 \frac{1}{\left[\alpha^2+4k^2\sin^2\frac{\vartheta}{2}\right]^2}}$$

The $\alpha \to 0$ limit $\Rightarrow$ **Rutherford formula**: $\left(\frac{d\sigma}{d\Omega}\right)_p(\vartheta) = \left(\frac{\mathcal{M}}{2}\,\frac{q\,q'}{4\pi\epsilon_0}\right)^2 \frac{1}{p^4\sin^4\frac{\vartheta}{2}}$

This formula can be obtained classically (it does not contain $\hbar$). However, **Coulomb scattering** cannot be described by the spherical-wave asymptotics used here, as this asymptotics is applicable only for finite-range or quickly decreasing potentials (cf. Sec. 13).

◀ Historical remark

1911: E. Rutherford derives classically the cross-section formula for Coulomb scattering to describe the 1909 experiment by H. Geiger & E. Marsden

1926: M. Born describes the scattering processes within QM; he derives explicitly the first approximation of a general scattering amplitude

1935: H. Yukawa introduces the potential for meson-mediated interaction of nucleons; this potential is now used to describe screened Coulomb interactions

13. SCATTERING: PARTIAL WAVES

We turn now to another method of analyzing scattering processes. It relies on the assumption of **spherical symmetry** of all terms of the total Hamiltonian. This

allows one to express the cross section as a series of contributions associated with orbital angular momentum quantum numbers $l = 0, 1, 2, \ldots$ The series is formally infinite, but for finite-range potentials and a finite projectile energy E it is effectively terminated above a certain maximal value $l = l_{\max}(E)$ corresponding to the maximal orbital angular momentum for which the projectile passes through the interaction region. So we again deal with a kind of expansion, but of a completely different nature than the above perturbative expansion.

■ Elastic scattering via partial waves

The basic idea of the method is to express the scattered particle wavefunction in terms of states with different conserved values (for spherically symmetric potentials) of the orbital angular momentum.

▶ **Expansion of the asymptotic wavefunction** $\psi_{\vec{k}}(\vec{x}) \approx \frac{1}{(2\pi)^{\frac{3}{2}}}\left[e^{ikz} + f_k(\vartheta)\frac{e^{ikr}}{r}\right]$ for a general **isotropic potential** $V(r)$ in the **orbital-momentum basis**:

$\boxed{|klm\rangle \propto R_{kl}(r)Y_{lm}(\vartheta,\varphi)}$ with $l, m \equiv$ conserved quantum numbers.

Since z is associated with the direction of the linear momentum of the incoming particle, the angular-momentum projection to z is $0 \Rightarrow$ only $\boxed{m = 0}$ components $Y_{l0}(\vartheta,\varphi) \propto P_l(\cos\vartheta)$ $[\equiv P_{l0}(\cos\vartheta)]$ contribute to the expansion:

(a) Expansion of the **incoming plane wave** into spherical waves:

$$\boxed{e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\vartheta) \approx \sum_{l=0}^{\infty}(2l+1)\frac{e^{+ikr}-e^{-i(kr-l\pi)}}{2ikr}P_l(\cos\vartheta)}$$

where we used asymptotics of Bessel functions for $r \gg \frac{1}{k} = \frac{\hbar}{p} = \frac{\lambda}{2\pi}$:

$$j_l(kr) \sim \frac{\sin\left(kr - l\frac{\pi}{2}\right)}{kr} = \frac{e^{+i\left(kr-l\frac{\pi}{2}\right)} - e^{-i\left(kr-l\frac{\pi}{2}\right)}}{2ikr}$$

(b) Expansion of **scattering amplitude**:

$$\boxed{f_k(\vartheta) = \sum_{l=0}^{\infty}(2l+1)F_l(k)P_l(\cos\vartheta)}$$

This is a general expansion of an arbitrary function of angle ϑ, the unknown coefficients $F_l(k)$ expressing the individual **partial-wave amplitudes**

The entire asymptotic wavefunction then reads as:

$$\boxed{\psi_{\vec{k}}(\vec{x}) \approx \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0}^{\infty}(2l+1)\frac{1}{2ik}\left\{\underbrace{[1+2ikF_l(k)]}_{S_l(k)}\frac{e^{+ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right\}P_l(\cos\vartheta)}$$

▶ **S-matrix element**

Parameter $S_l(k)$ in the above expression is the diagonal element of the S-matrix in the basis $|+klm\rangle$ of outgoing spherical waves with given l, k. We derive

a relation of $S_l(k)$ to the S-matrix in the plane-wave basis. From Sec. 12 we know: $\langle\Phi_{E'n'}|\hat{S}|\Phi_{En}\rangle = \delta(E-E')\big[\delta_{nn'} - 2i\pi\,\langle\Phi_{E'n'}|\hat{T}^+(E)|\Phi_{En}\rangle\big]$

$$\Rightarrow \quad \langle\phi_{\vec{k}'}|\hat{S}|\phi_{\vec{k}}\rangle = \delta(\vec{k}-\vec{k}') - 2i\pi\,\frac{\mathcal{M}}{\hbar^2 k}\,\delta(k-k')\,\underbrace{\langle\phi_{\vec{k}'}|\hat{T}^+(E)|\phi_{\vec{k}}\rangle}_{-\frac{\hbar^2}{4\pi^2\mathcal{M}}f_{\vec{k}}(\vec{k}')}$$

$\boxed{\cos\vartheta = \frac{\vec{k}'\cdot\vec{k}}{k'k}}$ $\qquad\qquad \sum_l (2l+1)\frac{S_l(k)-1}{2ik}P_l(\cos\vartheta)$

$$\Rightarrow \quad \langle\phi_{\vec{k}'}|\hat{S}|\phi_{\vec{k}}\rangle = \delta(\vec{k}-\vec{k}') + \frac{i}{2\pi k}\,\delta(k-k')\,\overbrace{f_{\vec{k}}(\vec{k}')} \quad =$$

$$= \underbrace{\delta(\vec{k}-\vec{k}')}_{\frac{1}{2\pi k^2}\delta(k-k')\delta(\cos\vartheta-1)} - \frac{1}{4\pi k^2}\delta(k-k')\underbrace{\sum_l (2l+1)P_l(\cos\vartheta)}_{2\delta(\cos\vartheta-1)} + \frac{1}{4\pi k^2}\delta(k-k')\sum_l (2l+1)S_l(k)P_l(\cos\vartheta)$$

$\Leftarrow$ completeness of Legendre polyns.

$\int_0^\infty\int_0^\pi\int_0^{2\pi} \frac{1}{2\pi k^2}\delta(k-k')\delta(\cos\vartheta-1)k^2\sin\vartheta\,dk\,d\vartheta\,d\varphi = 1$ $\qquad \sum_l (2l+1)P_l(x)P_l(y) = 2\delta(x-y)$

$$\boxed{\langle\phi_{\vec{k}'}|\hat{S}|\phi_{\vec{k}}\rangle = \delta(k-k')\,\frac{1}{4\pi k^2}\sum_l (2l+1)S_l(k)P_l(\cos\vartheta)}$$

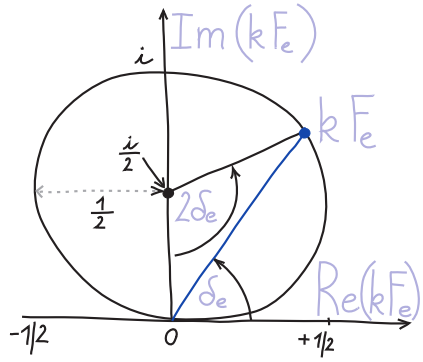
expansion of S-matrix to Lagendre polynomials

▶ Equivalent parametrizations of the scattering amplitude

The continuity equation ⇒ incoming flux = outgoing flux (this is sometimes called the **unitarity condition**) ⇒ coefficients for each l at $\frac{e^{+ikr}}{r}$ and $\frac{e^{-ikr}}{r}$ differ just by a phase ⇒ $\boxed{|S_l(k)| = 1}$

$$\boxed{1 + 2ikF_l(k) = S_l(k) = e^{2i\delta_l(k)} \quad \Leftrightarrow \quad F_l(k) = \frac{S_l(k)-1}{2ik} = e^{i\delta_l(k)}\frac{\sin\delta_l(k)}{k}}$$

$\delta_l(k) \equiv$ a relative **phase shift** of the outgoing partial wave l



The above relations define alternative (equivalent) parametrizations of the scattering amplitude & elastic cross section via quantities $F_l(k) \longleftrightarrow S_l(k) \longleftrightarrow \delta_l(k)$

The scattering amplitude:

$$\boxed{f_k(\vartheta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[S_l(k)-1]P_l(\cos\vartheta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l(k)}\sin\delta_l(k)P_l(\cos\vartheta)}$$

▶ Differential cross section of elastic scattering $= |f_k(\vartheta)|^2$

$$\left(\tfrac{d\sigma}{d\Omega}\right)_k(\vartheta) = \sum_{l,l'}(2l+1)(2l+1)F_l(k)F_{l'}^*(k)P_l(\cos\vartheta)P_{l'}(\cos\vartheta)$$

$$= \tfrac{1}{4k^2}\sum_{l,l'}(2l+1)(2l'+1)[S_l(k)-1][S_{l'}^*(k)-1]P_l(\cos\vartheta)P_{l'}(\cos\vartheta)$$

$$= \tfrac{1}{k^2}\sum_{l,l'}(2l+1)(2l'+1)\sin\delta_l(k)\sin\delta_{l'}(k)e^{i[\delta_l(k)-\delta_{l'}(k)]}P_l(\cos\vartheta)P_{l'}(\cos\vartheta)$$

▶ Integral cross section of elastic scattering

Integrating the differential cross section over the full space angle we obtain the integral cross section:

$$\sigma^{\rm el}(k) = \int_0^{2\pi}\int_0^{\pi} |f_k(\vartheta)|^2 \sin\vartheta \, d\varphi \, d\vartheta$$

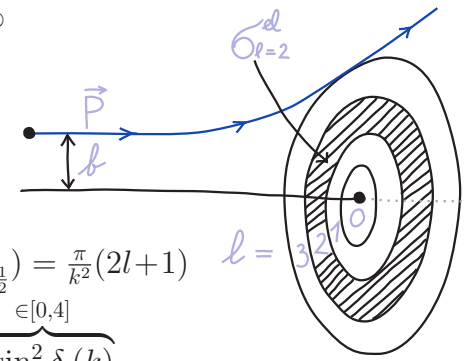
$$\sigma^{\rm el}(k) = 2\pi \sum_{l,l'} (2l+1)(2l'+1) F_l(k) F_l^*(k) \overbrace{\int_0^{\pi} P_l(\cos\vartheta) P_{l'}(\cos\vartheta) \underbrace{\sin\vartheta \, d\vartheta}_{d(\cos\vartheta)}}^{\frac{2}{2l+1}\delta_{ll'}}$$

$$\boxed{\sigma^{\rm el}(k) = 4\pi \sum_{l=0}^{\infty} (2l+1) |F_l(k)|^2 = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |S_l(k)-1|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\delta_l(k)}$$

$$\sigma^{\rm el}(k) = \sum_{l=0}^{\infty} \sigma_l^{\rm el}(k) \qquad \sigma_l^{\rm el}(k) = 0 \text{ for } [\, F_l(k) = 0 \;\Leftrightarrow\; \sin\delta_l(k) = 0 \;\Leftrightarrow\; S_l(k) = 1 \,]$$

▶ Classical calculation via the impact factor

The above expressions of the integral cross sections can be interpreted in a classical language, making use of the so-called impact factor b defined as the transverse projectile–target distance for $z \to -\infty$



Orbital momentum $\underbrace{L}_{\sqrt{\hbar^2 l(l+1)}} = b \underbrace{p}_{\hbar k}$

$\Rightarrow$ for given l we have: $b_l(k) \approx \frac{\sqrt{l(l+1)}}{k}$

Estimated cross section of $l^{\rm th}$ part. wave:

$$\sigma_l^{\rm el}(k) = \pi(b_{l+\frac{1}{2}}^2 - b_{l-\frac{1}{2}}^2) = \tfrac{\pi}{k^2}(2l+1)$$

In the quantum calculation we obtained:

$$\sigma_l^{\rm el}(k) = \tfrac{\pi}{k^2}(2l+1) \overbrace{4\sin^2\delta_l(k)}^{\in[0,4]}$$

The quantum factor $4\sin^2\delta_l(k)$ expresses constructive/destructive interference effects in each term $\sigma_l^{\rm el}(k)$

▶ Estimate of maximal angular momentum

The classical impact-factor considerations make it possible to estimate the upper value of l where the cross-section series can be cut off. This value is obtained from the maximal angular momentum for which the particle still hits the finite spatial region of nonzero potential. For a potential satisfying $V(r) \approx 0$ for $r > R$ we expect $\boxed{\sigma_l^{\rm el}(k) \approx 0 \text{ for } l > l_{\max}(k) \approx kR}$

In this way, all infinite sums become effectively **finite sums**: $\boxed{\sum_{l=0}^{\infty} \longrightarrow \sum_{l=0}^{l_{\max}}}$

▶ Determination of phase shifts from the actual solution

If we happen to know the *actual unbound solution* of the Schrödinger equation for the given potential (with the given energy in the continuous spectrum),

we can directly calculate the required phase shifts & amplitudes of individual partial waves:

Radial Schrödinger equation $\boxed{\frac{d^2u_{kl}(r)}{dr^2} - \left[\frac{2\mathcal{M}}{\hbar^2}V(r) + \frac{l(l+1)}{r^2}\right]u_{kl}(r) + k^2 u_{kl}(r) = 0}$

Solution $\boxed{R_{kl}(r) = \frac{u_{kl}(r)}{r}}$ outside the range of the potential (for $r \geq R$):

$$= a_l\, j_l(kr) + b_l\, n_l(kr) = c_l^+\, h_l^+(kr) + c_l^-\, h_l^-(kr)$$

$j_l(kr)$, $n_l(kr)$ $\equiv$ **Bessel, Neumann functions** with asymptotics:	$h_l^{\pm}(kr) = j_l(kr) \pm i n_l(kr)$ $\equiv$ **Hankel functions** with asymptotics:
$j_l(kr) \approx \frac{1}{kr}\sin\left(kr - l\frac{\pi}{2}\right) = \frac{1}{kr}\cos\left[kr-(l+1)\frac{\pi}{2}\right]$ $n_l(kr) \approx -\frac{1}{kr}\cos\left(kr - l\frac{\pi}{2}\right) = \frac{1}{kr}\sin\left[kr-(l+1)\frac{\pi}{2}\right]$	$h_l^+(kr) \approx \frac{1}{kr}e^{+i\left[kr-(l+1)\frac{\pi}{2}\right]}$ $h_l^-(kr) \approx \frac{1}{kr}e^{-i\left[kr-(l+1)\frac{\pi}{2}\right]}$

The general form of $r \geq R$ wavefunction yielding $\psi_{kl}(\vec{x}) = \frac{1}{(2\pi)^{3/2}}e^{ikz}$ for $V(r)=0$:

$$\psi_{kl}(\vec{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0}^{\infty}(2l+1)i^l \overbrace{\left[c_l^+ h_l^+(kr) + c_l^- h_l^-(kr)\right]}^{R_{kl}(r)} P_l(\cos\vartheta)$$

$$\approx \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0}^{\infty}(2l+1)\frac{1}{ik}\left[c_l^+\frac{e^{+ikr}}{r} - c_l^-\frac{e^{-i(kr-l\pi)}}{r}\right]P_l(\cos\vartheta)$$

This is compared with the required asymptotics:

$$\psi_{\vec{k}}(\vec{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0}^{\infty}(2l+1)\frac{1}{2ik}\left[e^{2i\delta_l(k)}\frac{e^{+ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right]P_l(\cos\vartheta)$$

$\Rightarrow$ $r \geq R$ solution of radial Schrödinger eq. expressed in terms of $\delta_l(k)$:

$\boxed{c_l^+ = \frac{e^{2i\delta_l(k)}}{2},\quad c_l^- = \frac{1}{2}}$ $\Rightarrow$ $R_{kl}(r) = \frac{e^{2i\delta_l(k)}}{2}[j_l(kr) + i n_l(kr)] + \frac{1}{2}[j_l(kr) - i n_l(kr)]$

$$\boxed{R_{kl}(r) = e^{i\delta_l(k)}\left[\cos\delta_l(k)\; j_l(kr) - \sin\delta_l(k)\; n_l(kr)\right]}$$

For $kr \gg l$ we get: $R_{kl}(r) \approx \frac{e^{i\delta_l(k)}}{kr}\left[\cos\delta_l(k)\sin(kr - l\frac{\pi}{2}) - \sin\delta_l(k)\cos(kr - l\frac{\pi}{2})\right] =$

$$\boxed{\frac{e^{i\delta_l(k)}}{kr}\sin\left(kr - l\tfrac{\pi}{2} + \delta_l(k)\right) \overset{r\to\infty}{\approx} R_{kl}(r)}$$

So $\delta_l(k)$ is really a phase shift of the asymptotic partial wave with respect to the $V=0$ solution, which has $\delta_l(k)=0\ \forall l$ because $n_l(kr)$ is not in e^{ikz}.

Conclusion: If one writes the actual asymptotic solution of the radial Schrödinger equation in the above form (using Bessel & Neumann or Hankel functions), the phase shifts $\delta_l(k)$ for all partial waves are read out from that expression.

▶ Phase shifts for a sharp finite-range potential

The above-described general method yields explicit results for potentials that *vanish identically* outside the range R:

$$V(r)\begin{cases} \neq 0 & \text{for } r \leq R \quad \text{(inside)} \\ = 0 & \text{for } r > R \quad \text{(outside)} \end{cases}$$

We require continuous connection of "inside-outside" **logarithmic derivative**

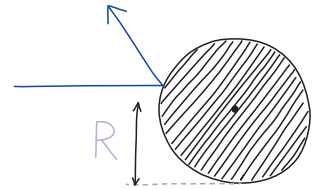
$$\beta_{kl}(R) \equiv R\frac{d}{dr}\ln R_{kl}(r)\Big|_{r=R} = R\,\frac{R'_{kl}(r)}{R_{kl}(r)}\Big|_{r=R} \qquad \forall\, l=0,1,2\ldots$$

$$\beta_{kl}(R)=kR\frac{\cos\delta_l(k)\,\frac{dj_l}{dr}(kR)-\sin\delta_l(k)\,\frac{dn_l}{dr}(kR)}{\cos\delta_l(k)\,j_l(kR)-\sin\delta_l(k)\,n_l(kR)} \;\Leftrightarrow\; \boxed{\tan\delta_l(k)=\frac{kR\,\frac{dj_l}{dr}(kR)-\beta_{kl}(R)\,j_l(kR)}{kR\,\frac{dn_l}{dr}(kR)-\beta_{kl}(R)\,n_l(kR)}}$$

Calculating the values of the logarithmic derivative $\beta_{kl}(R)$ from the **inside solution**, we can determine all phase shifts $\delta_l(k) \Rightarrow$ solve the scattering problem.

▶ **Hard-sphere scattering**

$$\boxed{V(r)=\begin{cases}\infty & \text{for } r\le R\\ 0 & \text{for } r>R\end{cases}}$$



$$R_{kl}(R)=e^{i\delta_l(k)}\big[\cos\delta_l(k)\;j_l(kR)-\sin\delta_l(k)\;n_l(kR)\big]=0 \;\Rightarrow\; \boxed{\tan\delta_l(k)=\frac{j_l(kR)}{n_l(kR)}}$$

$$l{=}0{:}\quad j_0(kR){=}\tfrac{\sin kR}{kR},\;\; n_0(kR){=}-\tfrac{\cos kR}{kR} \;\Rightarrow\; \boxed{\delta_0(k)=-kR}$$

(a) High-energy case $(kR\gg 1)$

$$\boxed{l\ll kR \;\Rightarrow\; j_l(kR)\approx\tfrac{1}{kR}\sin(kR-l\tfrac{\pi}{2}),\quad n_l(kR)\approx-\tfrac{1}{kR}\cos(kR-l\tfrac{\pi}{2})}$$

$\Rightarrow \tan\delta_l(k)=-\tan\left(kR-l\frac{\pi}{2}\right) \Rightarrow$ the l^{th} and $(l{+}1)^{\text{th}}$ phase shifts differ by $\frac{\pi}{2}$

$\Rightarrow$ their contrib. to σ^{el} is $\frac{4\pi}{k^2}\left[(2l{+}1)\sin^2\delta_l(k)+(2l{+}3)\cos^2\delta_l(k)\right]\approx\frac{4\pi}{k^2}(2l{+}2)$

$\Rightarrow$ each l-term of the series contributes by $\approx\frac{4\pi}{k^2}\frac{2l+2}{2}$

$$\boxed{l\gg kR \;\Rightarrow\; j_l(kR)\approx\tfrac{(kR)^l}{(2l+1)!!},\quad n_l(kR)\approx-\tfrac{(2l-1)!!}{(kR)^{l+1}}}$$

$$\Rightarrow \tan\delta_l(k)\approx-\tfrac{(kR)^{2l+1}}{(2l+1)!!(2l-1)!!} \Rightarrow \tan\delta_{l+1}(k)\approx\underbrace{\left(\tfrac{kR}{2l}\right)^2}_{\ll 1}\tan\delta_l(k) \Rightarrow \text{decrease with } l$$

Assume $\boxed{l_{\max}\approx kR}$

$$\sigma^{\text{el}}(k)\approx\tfrac{4\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l{+}1)\sin^2\delta_l(k)\approx\tfrac{4\pi}{k^2}\underbrace{\sum_{l=0}^{kR}\tfrac{2l+2}{2}}_{\approx\frac{(kR)^2}{2}}\approx\boxed{2\pi R^2\approx\sigma^{\text{el}}} \qquad \ldots 2\times\ \pi R^2$$

(b) Low-energy case $(kR\ll 1)$

Only the $l{=}0$ term works: $\delta_0(k)=-kR\approx\sin\delta_0(k)$

$$\sigma^{\text{el}}(k)\approx\tfrac{4\pi}{k^2}\sin^2\delta_0(k)\approx\boxed{4\pi R^2\approx\sigma^{\text{el}}} \qquad \ldots 4\times\ \pi R^2$$

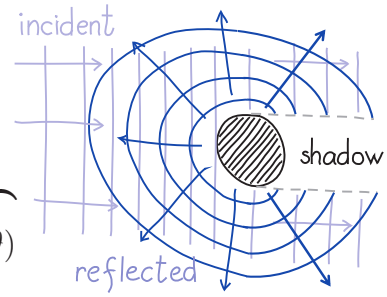
In no case the classical geometrical cross section $\boxed{\sigma_{\text{clas}}=\pi R^2}$ was obtained. The reason for low energy is a quantum interference phenomenon, but why is it so for high energy, when one would expect the classical behavior?

▶ **Shadow scattering**

The answer to the above question concerning the geometric cross section in high-E case: For $\sigma^{\text{el}}{=}0$ the wavefunction would be $\psi(\vec{x})\propto e^{ikz}$, which is nonzero

everywhere, including the region behind the sphere, where we classically expect a shadow (zero probability of finding the particle). Just to generate $\psi(\vec{x})=0$ in the shadow region behind the sphere, the cross section must be $\sigma^{\text{shad}} \approx \pi R^2$. The reflected part of $\psi(\vec{x})$ produces another contribution $\sigma^{\text{refl}} \approx \pi R^2$.
Together: $\sigma^{\text{el}} = \sigma^{\text{shad}} + \sigma^{\text{refl}} \approx 2\pi R^2$

Reflected & shadow parts identified in:



$$f_k(\vartheta) = \sum_{l=0}^{\infty}(2l+1)\underbrace{\tfrac{e^{2i\delta_l(k)}-1}{2ik}}_{F_l(k)} P_l(\cos\vartheta) =$$

$$= \overbrace{\tfrac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)e^{2i\delta_l(k)}P_l(\cos\vartheta)}^{f_k^{\text{refl}}(\vartheta)} \overbrace{-\tfrac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)}^{f_k^{\text{shad}}(\vartheta)}$$

$$\sigma^{\text{refl}}(k) = \iint |f_k^{\text{refl}}(\vartheta)|^2 \sin\vartheta d\varphi d\vartheta =$$

$$= \tfrac{1}{4k^2}\sum_{l,l'}(2l+1)(2l'+1)e^{i[\delta_l(k)-\delta_{l'}(k)]}\tfrac{4\pi}{2l+1}\delta_{ll'} = \tfrac{\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1) \approx \pi R^2$$

$$\sigma^{\text{shad}}(k) = \iint |f_k^{\text{shad}}(\vartheta)|^2 \sin\vartheta d\varphi d\vartheta = \cdots\cdots \qquad \cdots\cdots \approx \pi R^2$$

$$\sigma^{\text{interf}}(k) = \iint 2\text{Re}[f_k^{\text{refl}}(\vartheta) f_k^{\text{shad}*}(\vartheta)] \sin\vartheta d\varphi d\vartheta = \cdots = \tfrac{2\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1)\cos[2\delta_l(k)] \approx 0$$

▶ Coulomb scattering

Coulomb potential is a **long-range** one, hence the asymtotic solution of the Schrödinger equation cannot be required in the above-applied familiar form. A **special treatment** is needed. Here we just very briefly outline the method of solution without performing all calculations (which are rather sophisticated). We consider the **repulsive Coulomb potential** $V(r) = +\tfrac{q\,q'}{4\pi\epsilon_0}\tfrac{1}{r}$ with $\left\{\begin{matrix} q=Ze \\ q'=Z'e \end{matrix}\right\}$:

$$\left[-\tfrac{\hbar^2}{2\mathcal{M}}\Delta + \tfrac{q\,q'}{4\pi\epsilon_0}\tfrac{1}{r} - \tfrac{(\hbar k)^2}{2\mathcal{M}}\right]\psi_k(\vec{x}) = 0 \quad \Leftrightarrow \quad \left[\Delta + k^2 - \tfrac{2\gamma k}{r}\right]\psi_k(\vec{x}) = 0$$

$$\gamma = \tfrac{q\,q'\mathcal{M}}{4\pi\epsilon_0\hbar^2 k} = \underbrace{\tfrac{e^2}{4\pi\epsilon_0(\hbar c)}}_{\alpha \doteq \frac{1}{137}} \underbrace{\tfrac{c\mathcal{M}}{\hbar k}}_{\left(\frac{v}{c}\right)^{-1}} ZZ' \qquad \left[\tfrac{d^2}{dr^2} + k^2 - \tfrac{2\gamma k}{r} - \tfrac{l(l+1)}{r^2}\right] u_{kl}(r) = 0$$

The Schrödinger equation is solved analytically in terms of **hypergeometric functions**. This yields the following **asymptotic solution**:

$$\psi_k(\vec{x}) \overset{r\to\infty}{\propto} e^{i[kz-\gamma\ln k(r-z)]} + f_k(\vartheta)\tfrac{e^{i(kr-\gamma\ln 2kr)}}{r}$$

$$\propto \tfrac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\left[e^{2i\delta_l(k)}\tfrac{e^{i(kr-\gamma\ln 2kr)}}{r} - \tfrac{e^{-i(kr-\gamma\ln 2kr-l\pi)}}{r}\right]$$

with known amplitude $f_k(\vartheta) = -\gamma\tfrac{e^{-i\left[\gamma\ln\left(\sin^2\frac{\vartheta}{2}\right)-2\delta_0(k)\right]}}{2k\sin^2\frac{\vartheta}{2}}$ and phase shifts $\delta_l(k)$

$$\vec{j}_{\text{in}} \propto -\tfrac{\hbar\gamma}{\mathcal{M}}\tfrac{x}{r(r-z)}\vec{n}_x - \tfrac{\hbar\gamma}{\mathcal{M}}\tfrac{y}{r(r-z)}\vec{n}_y + \left(\tfrac{\hbar k}{\mathcal{M}} - \tfrac{\hbar\gamma}{\mathcal{M}}\tfrac{1}{r}\right)\vec{n}_z \overset{r\to\infty}{\longrightarrow} \tfrac{\hbar k}{\mathcal{M}}\vec{n}_z$$

$\vec{j}_{\rm out} \propto \frac{|f_k(\vartheta)|^2}{r^2}\left(\frac{\hbar k}{\mathcal{M}} - \frac{\hbar\gamma}{\mathcal{M}}\frac{1}{r}\right)\vec{n}_r \quad \stackrel{r\to\infty}{\longrightarrow} \quad |f_k(\vartheta)|^2\,\frac{\hbar k}{\mathcal{M}r^2}\,\vec{n}_r$

Differential cross section:

$$\left(\frac{d\sigma}{d\Omega}\right)_k(\vartheta) = |f_k(\vartheta)|^2 = \left|\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l(k)}\sin\delta_l(k)P_l(\cos\vartheta)\right|^2 = \alpha^2\frac{ZZ'}{16}\left(\frac{\hbar c}{E}\right)^2\frac{1}{\sin^4\frac{\vartheta}{2}}$$

So the **Rutherford formula** is reproduced. Recall that this formula can be obtained from classical mechanics and that we have "derived" it (in the 1st Born approx.) from the Yukawa scattering (Sec. 12). The fact that the correct calculation with hypergeometric functions yields the same result can be seen as a lucky coincidence. The situation is more difficult in case of a superposition of the Coulomb potential with an additional (finite-range) potential (as, e.g.,in elastic scattering of nuclei). Then the above modified asymptotics must be used, in which the phase shifts $\delta_l(k)$ are to be determined numerically.

■ Inclusion of inelastic scattering

The method of partial waves makes it easy to include into the description the presence of inelastic scattering. More precisely, the inelastic scattering is included only through its *influence on elastic scattering*, the method providing nothing more but just a convenient phenomenological *parametrization*. A microscopic description requires to keep under control all the segments of the full Hilbert space where products of various inelastic channels appear, which is a hard problem. Nevertheless, even with these limitations, the parametrization provided by the partial-wave method has rather important consequences.

► Elastic scattering in presence of inelastic channels

The S-matrix element is no more a complex unity but satisfies: $|S_l(k)| \in [0,1]$:

$$\boxed{S_l(k) = \underbrace{\eta_l(k)}_{\in[0,1]}\,e^{2i\delta_l(k)}} \Rightarrow \boxed{\begin{aligned} F_l(k) &= \tfrac{S_l(k)-1}{2ik} \\ &= \tfrac{1}{2k}\Big\{\eta_l(k)\sin 2\delta_l(k) + i\,[1-\eta_l(k)\cos 2\delta_l(k)]\Big\}\end{aligned}}$$

The scattering amplitude: $\quad f_k(\vartheta) = \sum_{l=0}^{\infty}(2l+1)F_l(k)P_l(\cos\vartheta)$

The integral cross section of elastic scattering:

$$\boxed{\sigma^{\rm el}(k) = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\,|S_l(k)-1|^2 = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\Big[1+\eta_l^2(k)-2\eta_l(k)\cos 2\delta_l(k)\Big]}$$

► Integral cross section of inelastic processes

The integral inelastic cross section can be calculated through the balance of the overall incoming & outgoing flows derived from the asymptotic wavefunction:

$$\psi_{\vec{k}}(\vec{x}) \approx \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0}^{\infty}(2l+1)\frac{1}{2ik}\left\{S_l(k)\,\frac{e^{+ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right\}P_l(\cos\vartheta)$$

The radial flow at point $\vec{x}$: $\vec{j}_r(\vec{x}) = \frac{1}{\mathcal{M}} \operatorname{Re}\left(\psi^*_{\vec{k}}(\vec{x}) \underbrace{\left[-i\hbar\frac{\partial}{\partial r} - \frac{i\hbar}{r}\right]}_{\hat{p}_r \text{ rad. momentum}} \psi_{\vec{k}}(\vec{x})\right) \vec{n}_r =$

$= \frac{1}{\mathcal{M}} \frac{1}{(2\pi)^3} \vec{n}_r \sum_{l,l'} (2l+1)(2l'+1) P_l(\cos\vartheta) P_{l'}(\cos\vartheta) \times$

$\times \operatorname{Re} \frac{1}{-2ik} \left\{ S_l^*(k) \frac{e^{-ikr}}{r} - \frac{e^{+i(kr-l\pi)}}{r} \right\} \frac{\hbar k}{2ik} \left\{ S_l(k) \frac{e^{+ikr}}{r} + \frac{e^{-i(kr-l\pi)}}{r} \right\}$

$= \frac{1}{\mathcal{M}} \frac{1}{(2\pi)^3} \vec{n}_r \sum_{l,l'} (2l+1)(2l'+1) P_l(\cos\vartheta) P_{l'}(\cos\vartheta) \frac{\hbar}{4kr^2} \left[|S_l(k)|^2 - 1\right]$

The integral flow through a sphere with radius r (total rate of scattering events):

$J^{\text{el}}(k) = \iint j_r(r,\vartheta,\varphi) r^2 \sin\vartheta d\varphi d\vartheta = -\frac{1}{(2\pi)^3} \frac{\pi\hbar}{\mathcal{M}k} \sum_{l=0}^{\infty} (2l+1) \left[1 - |S_l(k)|^2\right] \le 0$

The $J^{\text{el}}(k) \le 0$ value represents the part of the incoming flow which is not compensated by the outgoing flow because of inelastic processes $\Rightarrow$ the integral cross section of inelastic process is:

$$\sigma^{\text{inel}}(k) = \frac{\mathcal{R}^{\text{inel}}(k)}{j_{\text{in}}(k)} = \frac{-J^{\text{el}}(k)}{\frac{1}{(2\pi)^3}\frac{\hbar k}{\mathcal{M}}} \quad \Rightarrow \quad \boxed{\sigma^{\text{inel}}(k) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left[1 - \underbrace{|S_l(k)|^2}_{\eta_l^2(k)}\right]}$$

Total cross section

$\sigma^{\text{tot}}(k) = \sigma^{\text{el}}(k) + \sigma^{\text{inel}}(k) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left\{ |S_l(k) - 1|^2 + \left[1 - |S_l(k)|^2\right] \right\}$

Note that the above considerations do *not* allow one to calculate the differential cross section of inelastic processes. For this task, the $\eta_l(k)$ parameters alone are not sufficient.

$$\boxed{\sigma^{\text{tot}}(k) = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left[1 - \underbrace{\operatorname{Re} S_l(k)}_{\eta_l(k)\cos 2\delta_l(k)}\right]}$$

► **Relation between elastic and inelastic cross sections**

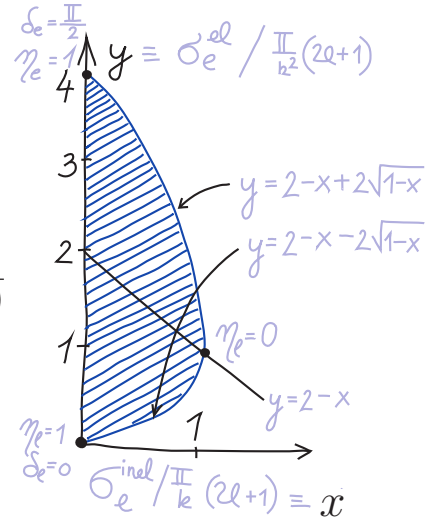
Let us define variables $\begin{cases} x_l(k) \equiv \frac{\sigma_l^{\text{inel}}(k)}{\frac{\pi}{k^2}(2l+1)} = 1 - \eta_l^2(k) & \in [0,1] \\ y_l(k) \equiv \frac{\sigma_l^{\text{el}}(k)}{\frac{\pi}{k^2}(2l+1)} = 1 + \eta_l^2(k) - 2\eta_l(k)\cos 2\delta_l(k) & \in [0,4] \end{cases}$

$$\Rightarrow \quad \boxed{y_l(k) = 2 - x_l(k) - 2\sqrt{1 - x_l(k)}\cos 2\delta_l(k)}$$

Considering $-1 \le \cos 2\delta_l(k) \le +1$ we obtain:

$$2 - x_l(k) - 2\sqrt{1 - x_l(k)} \le y_l(k) \le 2 - x_l(k) + 2\sqrt{1 - x_l(k)}$$

This represents an important **constraint** upon the possible values of elastic & inelastic integral cross sections for a given partial wave. In particular, we see that $\sigma_l^{\text{inel}}(k) > 0$ implies $\sigma_l^{\text{el}}(k) > 0$. Even in case of the total absorption,



$\eta_l(k)=0$, when $\sigma_l^{\text{inel}}(k)$ is at its maximum, we obtain $\sigma_l^{\text{el}}(k)=\sigma_l^{\text{inel}}(k)$, which is a consequence of the shadow scattering (see above).

▶ Optical theorem

Statement: Imaginary part of the **elastic forward scattering amplitude** $\propto$ **total cross section** including all processes: $\boxed{\text{Im}\, f_k^{\text{el}}(\vartheta=0)=\frac{k}{4\pi}\sigma^{\text{tot}}(k)}$

Proof for **isotropic potentials**:

$$\text{Im} f_k^{\text{el}}(\vartheta=0)=\sum_{l=0}^{\infty}(2l+1)\underbrace{\text{Im}\, F_l(k)}_{\frac{1}{2k}[1-\eta_l(k)\cos 2\delta_l(k)]}\overbrace{P_l(1)}^{1}=\frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)\big[1-\underbrace{\eta_l(k)\cos 2\delta_l(k)}_{\text{Re}S_l(k)}\big]$$
$$=\frac{k}{4\pi}\sigma^{\text{tot}}(k)$$

This relation is valid in the **most general case**, i.e., also for anisotropic potentials (beyond the method of partial waves). For elastic scattering by a general potential, it can be proven from the Lippmann-Schwinger equation that:

$$\underbrace{-\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\,\text{Im}\langle\phi_{\vec{k}}|\hat{T}^+(E)|\phi_{\vec{k}}\rangle}_{\text{Im}f_{\vec{k}}(\vec{k})}=\underbrace{\frac{k}{4\pi}\Big(\tfrac{4\pi^2\mathcal{M}}{\hbar^2}\Big)^2\int|\langle\phi_{\vec{k}'}|\hat{T}^+(E)|\phi_{\vec{k}}\rangle|^2\,\delta\big(k'-\sqrt{\tfrac{2\mathcal{M}E}{\hbar^2}}\,\big)k'^2dk'd\Omega'}_{\sigma^{\text{el}}(k)}$$

Elementary **interpretation** of the optical theorem for elastic scattering: The asymptotic wavefunction $\psi_k(\vec{x})=e^{ikz}+f_k(\vartheta)\frac{e^{ikr}}{r}$ is approximated for $\boxed{z\gg x,y}$

using $r=\sqrt{x^2+y^2+z^2}\approx z+\frac{x^2+y^2}{2z}\quad\Rightarrow\quad|\psi_k(\vec{x})|^2\approx 1+\frac{2}{z}\,\text{Re}\big[f_k(\vartheta)e^{ik\frac{x^2+y^2}{2z}}\big]$

Integration over a small distant rectangle $\Delta x\times\Delta y$ at $z=\text{const.}\gg\Delta x,\Delta y$:

$$I\equiv\iint\limits_{\Delta x\times\Delta y}|\psi_k(\vec{x})|^2dx\,dy\;\approx\;\Delta x\Delta y+\frac{2}{z}\,\text{Re}f_k(0)\underbrace{\int\limits_{-\frac{\Delta x}{2}}^{+\frac{\Delta x}{2}}e^{ik\frac{x^2}{2z}}dx}_{\sqrt{2\pi(-\frac{z}{ik})}}\underbrace{\int\limits_{-\frac{\Delta y}{2}}^{+\frac{\Delta y}{2}}e^{ik\frac{y^2}{2z}}dy}_{\text{dtto}}$$

$$\approx\Delta x\Delta y+\frac{4\pi}{k}\overbrace{\text{Re}[if_k(0)]}^{-\text{Im}f_k(0)}$$

$\mathcal{R}=j_{\text{in}}(k)I\equiv$ the actual rate of particles passing through the rectangle

$\mathcal{R}_0=j_{\text{in}}(k)\Delta x\Delta y\equiv$ the free rate

$$\mathcal{R}_0-\mathcal{R}=j_{\text{in}}(k)\sigma^{\text{tot}}(k)\quad\Rightarrow\quad\text{optical theorem}\quad\sigma^{\text{tot}}(k)=\tfrac{4\pi}{k}\text{Im}f_k(0)$$

An intuitive analogue of the optical theorem can be formulated within the (non)stationary perturbation theory: The amplitude of the initial unperturbed state in the final state is given — through the normalization condition — by the summed admixtures of all other unperturbed states in the final state.

▶ High-energy scattering on a black sphere

We assume $\boxed{\begin{array}{lll}S_l=0 & \text{for } l\le l_{\max} & \text{full absorption}\\ S_l=1 & \text{for } l>l_{\max} & \text{no scattering}\end{array}}$ with $l_{\max}\approx kR\gg 1$

Integral cross sections:

$$\sigma^{\text{inel}}(k) = \tfrac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-|S_l|^2] = \tfrac{\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1) = \tfrac{\pi}{k^2}(l_{\max}+1)^2 \approx \pi R^2$$

$$\sigma^{\text{tot}}(k) = \tfrac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-\text{Re}S_l] = \tfrac{2\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1) = \tfrac{2\pi}{k^2}(l_{\max}+1)^2 \approx 2\pi R^2$$

$$\sigma^{\text{el}}(k) = \sigma^{\text{tot}}(k) - \sigma^{\text{inel}}(k) \approx \pi R^2 \quad \text{shadow scattering}$$

■ Low-energy & resonance scattering

We conclude this section by sketching two additional topics: The low-energy scattering, which is a tool to determine basic properties of interaction, and resonance scattering, which indicates the existence of metastable states. Both these topic became much expanded in more advanced courses of QM.

▸ Low-energy limit of scattering amplitude

For $k\to 0$, only the $l=0$ partial wave is active, so in absence of inelastic scattering there is just a single real parameter which determines the cross section:

$$\boxed{a \equiv \lim_{k\to 0}\left[-\frac{\sin\delta_0(k)}{k}\right]} \quad \textbf{scattering length} \quad \Rightarrow \quad \begin{cases} \lim\limits_{k\to 0}\sigma^{\text{el}}(k) = \lim\limits_{k\to 0}\ \frac{4\pi}{k^2}\sin^2\delta_0(k) \\ \boxed{\sigma^{\text{el}}(k\to 0) = 4\pi a^2} \end{cases}$$

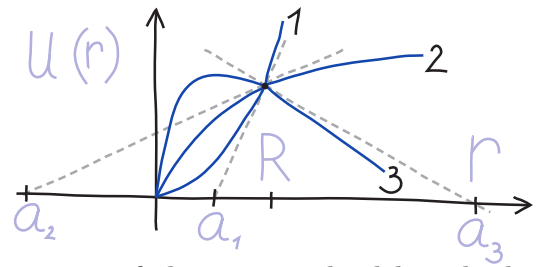
The visual meaning of the scattering length is derived from the wavefunction form at $r > R$:

$$R_{k,l=0}(r) = e^{i\delta_0(k)}\left[\cos\delta_0(k)\overbrace{j_0(kr)}^{\frac{\sin kr}{kr}} - \sin\delta_0(k)\overbrace{n_0(kr)}^{-\frac{\cos kr}{kr}}\right] = \frac{e^{i\delta_0(k)}}{kr}\sin\left[kr+\delta_0(k)\right]$$

$$\simeq \frac{e^{i\delta_0(k)}}{kr}\sin[k(r-a)] \equiv \frac{u_k(r)}{r}$$

$$\Rightarrow \quad u_k(r)\big|_{k\to 0} \propto (r-a) \quad \text{for } r \geq R$$

$$\Rightarrow \quad \text{the tangent at } r=R \text{ crosses zero at } r=a$$



The value of a indicates some basic properties of the potential, although the information it gives is usually not unique:

$$\left.\begin{array}{c} 0 < a < R \\ a \lesssim R \\ \hline -\infty < a < +\infty \\ a < 0 \\ R \ll a \end{array}\right\} \Leftrightarrow \begin{cases} \text{repulsive potential (convex} \to \text{concave wf.)} \\ \text{strong repulsive potential}(a = R \text{ for hard sphere}) \\ \hline \text{attractive potential} \\ \text{shallow attractive potential} \\ \text{attractive potential with weakly bound state } E \lesssim 0 \end{cases}$$

▸ Isolated resonance

Essential insight into the scattering theory can be gained via a **complex extension** of the S-matrix. Mathematical properties of analytic functions in the

complex plane can then be used to disclose some general physical features of scattering processes. Here we assume elastic scattering on an isotropic potential, for which all information is contained in a set of S-matrix elements $\{S_l(k)\}_{l=0}^{\infty}$. These elements are now considered to be complex functions of the complex momentum variable $k \in \mathbb{C}$. On the real-k axis, all $S_l(k)$ should be smooth functions, but in the complex plane they can have some poles. Let us look what happens if such a pole is located near the real axis. We assume:

$\boxed{S_l(k) = \dfrac{k - k_{\rm R}^*}{k - k_{\rm R}}}$ function satisfying $|S_l(k)| = 1$ for $k \in \mathbb{R}$ with a **simple pole** at $k = k_{\rm R}$ given by $\boxed{\frac{(\hbar k_{\rm R})^2}{2\mathcal{M}} = E_0 - i\,\frac{\Gamma}{2} \equiv E_{\rm R}}$

$$k_{\rm R} = \sqrt{\tfrac{2\mathcal{M}E_{\rm R}}{\hbar^2}} = \sqrt{\tfrac{2\mathcal{M}E_0}{\hbar^2}}\sqrt{1 - i\,\tfrac{\Gamma}{2E_0}} \approx \overbrace{\sqrt{\tfrac{2\mathcal{M}E_0}{\hbar^2}}}^{k_0} - i\overbrace{\sqrt{\tfrac{\mathcal{M}\Gamma^2}{8\hbar^2 E_0}}}^{\kappa} \quad \text{for } \Gamma \ll E_0$$

For complex energy the evolution is not unitary. The survival probability of a state $|\psi_{\rm R}(0)\rangle$ with $E = E_{\rm R} \in \mathbb{C}$ exponentially decreases:

$$\mathfrak{p}_0(t) = |\langle\psi_{\rm R}(0)|\psi_{\rm R}(t)\rangle|^2 = \left|e^{-\frac{i}{\hbar}\left(E_0 - i\,\frac{\Gamma}{2}\right)t}\right|^2 = e^{-\frac{\Gamma}{\hbar}t} \qquad = \langle\psi_{\rm R}(t)|\psi_{\rm R}(t)\rangle \ \text{ norm}$$

This corresponds to a **quasistationary state** with the mean lifetime $\boxed{\tau = \frac{\hbar}{\Gamma}}$ for which the decay products go outside the initial Hilbert space $\mathcal{H}$

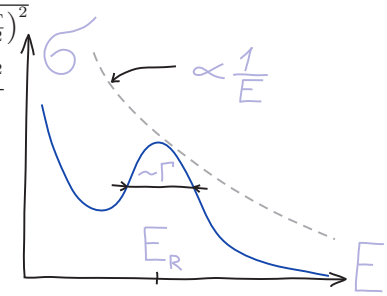
Only the outgoing wave is present at $k = k_{\rm R}$ since $S_l(k_{\rm R}) = \infty \;\Rightarrow$ scattering wavefunction $\psi_k(\vec{x}) \propto \frac{e^{+ik_{\rm R}r}}{r} \approx \frac{e^{+ik_0 r}}{r}\, e^{+\kappa r}$ has modulus increasing with r

Approximation of the cross section for $E - E_0 \ll E_0$:

$$\sigma_l^{\rm el}(k) = \tfrac{\pi}{k^2}(2l+1)\left|S_l(k) - 1\right|^2 = \tfrac{\pi}{k^2}(2l+1)\left|\tfrac{k_{\rm R} - k_{\rm R}^*}{k - k_{\rm R}}\right|^2 \approx \tfrac{\pi}{k^2}(2l+1)\overbrace{\left|\tfrac{-2i\kappa}{(k-k_0)+i\kappa}\right|^2}^{\frac{4\kappa^2}{(k-k_0)^2+\kappa^2}} =$$

$$\tfrac{4\pi}{k^2}(2l+1)\,\frac{\frac{\mathcal{M}}{2\hbar^2}\left(\frac{\Gamma}{2}\right)^2}{\frac{2\mathcal{M}}{\hbar^2}E_0\left(\sqrt{E}-\sqrt{E_0}\right)^2 + \frac{\mathcal{M}}{2\hbar^2}\left(\frac{\Gamma}{2}\right)^2} \approx \tfrac{4\pi}{k^2}(2l+1)\,\frac{\left(\frac{\Gamma}{2}\right)^2}{(E-E_0)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

with $\left(\sqrt{E} - \sqrt{E_0}\right)^2 \approx \frac{(E-E_0)^2}{4E_0}$



Breit-Wigner resonance

$$\boxed{\sigma_l^{\rm el}(k) \approx \frac{4\pi\hbar^2}{2\mathcal{M}E}(2l+1)\frac{\left(\frac{\Gamma}{2}\right)^2}{(E-E_0)^2 + \left(\frac{\Gamma}{2}\right)^2}}$$

◀ Historical remark

1870-90's: Lord Rayleigh develops the scattering theory for electromagnetic & sound waves, deriving the "optical theorem" and elaborating the partial-wave expansion
1927: H. Faxen & J. Holtsmark apply the partial-wave expansion in QM
1928: G. Gamow applies the complex energy formalism to unstable systems
1929: G. Breit & E. Wigner describe resonant states via the B.-W. distribution
1939: N. Bohr, R. Peierls, G. Placzek apply the Rayleigh optical relation in QM

14. BOSONIC & FERMIONIC SYSTEMS

It the following two sections, we will deal with systems consisting of a number (fixed or variable) of mutually interacting particles. In the main focus will be the systems of *indistinguishable particles*, either bosons or fermions. The concept of indistinguishability and its various consequences were already discussed at several places of this course, starting from Sec. 1b. Now we intend to formulate a general language describing all non-relativistic many-particle systems like atoms, nuclei, molecules, condensates etc.

In this section, we will introduce the principal mathematical gear of many-body physics: the operators that can create or annihilate particles in a given state. These operators make it possible to generate a basis of the whole Fock space and to express any physical operator in this space. Moreover, basic algebraic properties of the creation/annihilation operators capture elegantly the difference between bosons and fermions. As a by product, we will learn how to quantize the electromagnetic field, preparing the ground for the relativistic theory of quantum fields (which is unfortunately beyond the scope of this course).

■ Hilbert space of bosons & fermions

Let us first recall the relevant properties of bosonic and fermionic subspaces of a general many-particle Hilbert space. We define a so-called representation of occupation numbers in these subspaces, which is a natural starting point for introduction of the creation/annihilation operators.

▶ Indistinguishable particles

Let us recall some facts from Sec. 1b. Hilbert space of N identical but distinguishable particles is $\mathcal{H}^{(N)}=\mathcal{H}_1\otimes\mathcal{H}_2\otimes\cdots\otimes\mathcal{H}_N$, where all $\mathcal{H}_k$ are identical single-particle spaces. If the particles are indistinguishable, we need to perform a projection to bosonic or fermionic subspaces $\mathcal{H}_\pm^{(N)}\subset\mathcal{H}^{(N)}$. It is expressed via sums over **particle permutations** $\boxed{(1,2,\dots N)\to(k_1^\pi,k_2^\pi,\dots k_N^\pi)\quad \pi=1,2,\dots N!}$

$\boxed{\textbf{bosons}:\ \hat{P}_+=\frac{1}{N!}\sum_{\pi=1}^{N!}\hat{\mathcal{E}}_\pi}$ Factor $\frac{1}{N!}$ ensures projector property $\hat{P}_\pm^2=\hat{P}_\pm$

$\boxed{\textbf{fermions}:\ \hat{P}_-=\frac{1}{N!}\sum_{\pi=1}^{N!}\underbrace{\sigma_\pi}_{\pm1}\hat{\mathcal{E}}_\pi}$ permutation sign

▶ Bases in the bosonic & fermionic spaces

Separable (non-entangled) basis in $\mathcal{H}^{(N)}$: $|\Phi_{i_1i_2\dots i_N}\rangle\equiv|\phi_{i_1}\rangle_1|\phi_{i_2}\rangle_2\dots|\phi_{i_N}\rangle_N$

where $|\phi_i\rangle_k\equiv i^{\text{th}}$ basis state in the k^{th} single-particle space

Simplified notation: $|\Phi_{i_1i_2\dots i_N}\rangle\to\boxed{|\Phi_{12\dots N}\rangle\equiv|\phi_1\rangle_1|\phi_2\rangle_2\dots|\phi_N\rangle_N}$ $\begin{cases}\text{with}\\ |\phi_k\rangle_k\equiv|\phi_{i_k}\rangle_k\end{cases}$

so $|\phi_k\rangle_k$ is *any* (not the k^{th}) basis state of the k^{th}particle

Action of permutation operators: $\hat{\mathcal{E}}_\pi|\Phi_{12\ldots N}\rangle \equiv |\phi_{k_1^\pi}\rangle_1|\phi_{k_2^\pi}\rangle_2\ldots|\phi_{k_N^\pi}\rangle_N$

Projections of the separable basis $\{|\Phi_{12\ldots N}\rangle\}$ to $\mathcal{H}_\pm^{(N)} \quad \Rightarrow$

(a) basis in boson space: $\mathcal{N}_+\hat{P}_+|\Phi_{12\ldots N}\rangle = \frac{\mathcal{N}_+}{N!}\sum_{\pi=1}^{N!}|\phi_{k_1^\pi}\rangle_1|\phi_{k_2^\pi}\rangle_2\ldots|\phi_{k_N^\pi}\rangle_N$

(b) basis in fermion space: $\mathcal{N}_-\hat{P}_-|\Phi_{12\ldots N}\rangle = \frac{\mathcal{N}_-}{N!}\underbrace{\sum_{\pi=1}^{N!}\sigma_\pi|\phi_{k_1^\pi}\rangle_1|\phi_{k_2^\pi}\rangle_2\ldots|\phi_{k_N^\pi}\rangle_N}$

antisymmetry of the determinant under any exchange of columns or rows

$$\text{Det}\begin{pmatrix} |\phi_1\rangle_1 & |\phi_1\rangle_2 & \ldots & |\phi_1\rangle_N \\ |\phi_2\rangle_1 & |\phi_2\rangle_2 & \ldots & |\phi_2\rangle_N \\ \vdots & & & \vdots \\ |\phi_N\rangle_1 & |\phi_N\rangle_2 & \ldots & |\phi_N\rangle_N \end{pmatrix}$$ **Slater determinant**

Normalization coefficients $\boxed{\mathcal{N}_+ = \sqrt{\frac{N!}{n_1!\,n_2!\,n_3!\ldots}} \qquad \mathcal{N}_- = \sqrt{N!}}$

$n_k \equiv$ number of repetitions of the state $|\phi_k\rangle$ in the ensemble, i.e., number of particles in the state $|\phi_k\rangle$ (bosons: n_k=0,1,2,3…, fermions: n_k=0,1)

$\Rightarrow \quad \boxed{n_1 + n_2 + n_3 + \cdots = N}$

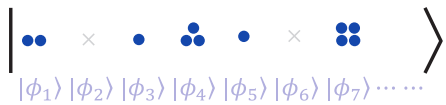
Reasoning:
We first note that $\mathcal{N}_- = \mathcal{N}_+$ if $n_k \in \{0,1\}\ \forall k$ (as follows from the Pauli principle valid for fermions). So we only need to derive $\mathcal{N}_+$:

$$\mathcal{N}_+\hat{P}_+|\Phi_{12\ldots N}\rangle \equiv \mathcal{N}_+\tfrac{1}{N!} \times \big[\text{sum of } N! \text{ states, partly identical}\big]$$
$$= \underbrace{\mathcal{N}_+\tfrac{n_1!\,n_2!\,n_3!\ldots}{N!}}_{\sqrt{\frac{n_1!\,n_2!\,n_3!\ldots}{N!}}} \times \big[\text{sum of } \tfrac{N!}{n_1!\,n_2!\,n_3!\ldots} \text{ orthogonal terms}\big]$$
$$\Rightarrow \quad \mathcal{N}_+ = \sqrt{\tfrac{N!}{n_1!\,n_2!\,n_3!\ldots}}$$

► **Representation of occupation numbers**

We introduce the following notation:

$$\boxed{\mathcal{N}_\pm\hat{P}_\pm|\Phi_{12\ldots N}\rangle \equiv |n_1, n_2, n_3, \cdots, n_k, \cdots\rangle_\pm}$$



with $n_k \equiv \left\{\begin{array}{l}\text{occupation number of the} \\ \text{basis state } |\phi_k\rangle \text{ (with } k\text{=1,2,3,}\ldots\infty)\end{array}\right\} = \left\{\begin{array}{ll} 0,1,2,3\ldots & \text{for bosons} \\ 0,1 & \text{for fermions}\end{array}\right.$

These vectors form a basis in the space of indistinguishable particles (bosons or fermions) ≡ representation of occupation numbers

■ Bosonic & fermionic creation/annihilation operators

Creation and annihilation operators, respectively, increase and decrease the number of particles in a given single-particle state by one, forming a system of "ladder" operators in the Fock space. Their repeated application enables one to generate any basis state in the occupation-number representation from a unique state called *vacuum*. Mutual permutations of these operators obey

simple commutation or anticommutation rules, depending on the bosonic or fermionic nature of the particles involved.

► Definition of creation/annihilation operators

Action in the Fock space (Hilbert space with indefinite particle number N):

$$\mathcal{H}_\pm = \mathcal{H}_\pm^{(0)} \oplus \mathcal{H}_\pm^{(1)} \oplus \mathcal{H}_\pm^{(2)} \oplus \cdots \mathcal{H}_\pm^{(N-1)} \oplus \mathcal{H}_\pm^{(N)} \oplus \mathcal{H}_\pm^{(N+1)} \cdots$$

Particle creation operators: $\mathcal{H}_\pm^{(N)} \to \mathcal{H}_\pm^{(N+1)}$

Particle annihilation operators: $\mathcal{H}_\pm^{(N-1)} \leftarrow \mathcal{H}_\pm^{(N)}$ and $0 \leftarrow \mathcal{H}_\pm^{(0)}$

Creation operators

$$\boxed{\begin{array}{ll} \text{Bosons:} & \hat{b}_k^\dagger |n_1, ..n_k, ...\rangle_+ = \sqrt{n_k+1}\, |n_1, ..(n_k+1), ...\rangle_+ \\ \text{Fermions:} & \hat{a}_k^\dagger |n_1, ..n_k, ...\rangle_- = \begin{cases} \overbrace{\sqrt{n_k+1}}^{1}\, |n_1, ..(n_k+1), ...\rangle_- & \text{for } n_k = 0 \\ 0 & \text{for } n_k = 1 \end{cases} \end{array}}$$

So $\hat{b}_k^\dagger$ or $\hat{a}_k^\dagger$ (unified notation $\hat{c}_k^\dagger$) create 1 boson or fermion in state $|\phi_k\rangle$. For fermions, if the state is already occupied ($n_k = 1$), the application of $\hat{a}_k^\dagger$ yields zero (which guarantees the satisfaction of Pauli principle).

Annihilation operators

$$\boxed{\begin{array}{ll} \text{Bosons:} & \hat{b}_k |n_1, ..n_k, ..\rangle_+ = \sqrt{n_k}\, |n_1, ..(n_k-1), ...\rangle_+ \\ \text{Fermions:} & \hat{a}_k |n_1, ..n_k, ..\rangle_- = \sqrt{n_k}\, |n_1, ..(n_k-1), ...\rangle_- \end{array}}$$

So $\hat{b}_k$ or $\hat{a}_k$ (unified notation $\hat{c}_k$) annihilate 1 boson or fermion in state $|\phi_k\rangle$. Note that for $n_k = 0$ the application of $\hat{c}_k$ yields zero.

Defined in this way, the annihilation operators are Hermitian conjugates of creation operators:

$$\underbrace{{}_+\langle n_1', ..n_k', ..|\hat{b}_k|n_1, ..n_k, ..\rangle_+}_{\sqrt{n_k}\ \delta_{n_1' n_1} \cdots \delta_{n_k' (n_k-1)} \cdots} = \underbrace{{}_+\langle n_1, ..n_k, ..|\hat{b}_k^\dagger|n_1', ..n_k', ..\rangle_+^*}_{\sqrt{n_k'+1}\ \delta_{n_1 n_1'} \cdots \delta_{n_k (n_k'+1)} \cdots}$$

$$\overbrace{{}_-\langle n_1', ..n_k', ..|\hat{a}_k|n_1, ..n_k, ..\rangle_-} = \overbrace{{}_-\langle n_1, ..n_k, ..|\hat{a}_k^\dagger|n_1', ..n_k', ..\rangle_-^*}$$

Square-root coefficients included in the above definitions ensure simple algebraic properties; see below and in Sec. 3b (the ladder operators and particularly the phonon creation/annihilation operators for the harmonic oscillator).

► Commutation relations for boson operators

$$\boxed{[\hat{b}_k^\dagger, \hat{b}_l^\dagger] = 0 = [\hat{b}_k, \hat{b}_l]}$$ (order of creation/annihilation of 2 bosons is irrelevant)

Proof for $k = l$ is trivial and for $k \neq l$ follows from:

$\hat{b}_k^\dagger \hat{b}_l^\dagger |..n_k..n_l...\rangle_+ = \hat{b}_l^\dagger \hat{b}_k^\dagger |..n_k..n_l...\rangle_+ = \sqrt{(n_k+1)(n_l+1)}\, |..(n_k+1)..(n_l+1)...\rangle_+$

The relation for annihilation operators obtained by the Hermitian conjugation.

$\boxed{[\hat{b}_k, \hat{b}_l^\dagger] = \delta_{kl}}$ (do not commute for $k=l$)

Proof for $k=l$: $\big(\hat{b}_k\hat{b}_k^\dagger - \hat{b}_k^\dagger\hat{b}_k\big)|..n_k..\rangle_+ = \overbrace{\big(\sqrt{(n_k+1)^2} - \sqrt{n_k^2}\,\big)}^{1}\,|..n_k..\rangle_+$

For $k\neq l$: $\hat{b}_k\hat{b}_l^\dagger|..n_k..n_l..\rangle_+ = \hat{b}_l^\dagger\hat{b}_k|..n_k..n_l..\rangle_+ = \sqrt{n_k(n_l+1)}\,|..(n_k-1)..(n_l+1)..\rangle_+$

▶ Anticommutation relations for fermion operators

Fermionic relations expressed through **anticommutators**: $\{\hat{A},\hat{B}\} \equiv \hat{A}\hat{B}+\hat{B}\hat{A}$

Pauli principle $\Rightarrow$ $\hat{a}_k^\dagger\hat{a}_k^\dagger|..n_k..\rangle_- = 0 = \hat{a}_k\hat{a}_k|..n_k..\rangle_-$

$\Rightarrow$ $\hat{a}_k^\dagger\hat{a}_k^\dagger = 0 = \hat{a}_k\hat{a}_k$ $\Rightarrow$ $\boxed{\{\hat{a}_k^\dagger, \hat{a}_k^\dagger\} = 0 = \{\hat{a}_k, \hat{a}_k\}}$

$\hat{a}_k\hat{a}_k^\dagger|..n_k..\rangle_- = \begin{cases} 0 & \text{for } n_k=1 \\ |..n_k..\rangle_- & \text{for } n_k=0 \end{cases}$ $\qquad$ $\hat{a}_k^\dagger\hat{a}_k|..n_k..\rangle_- = \begin{cases} |..n_k..\rangle_- & \text{for } n_k=1 \\ 0 & \text{for } n_k=0 \end{cases}$

$\Rightarrow$ $\underbrace{(\hat{a}_k\hat{a}_k^\dagger + \hat{a}_k^\dagger\hat{a}_k)}_{\{\hat{a}_k,\hat{a}_k^\dagger\}}|..n_k..\rangle_- = |..n_k..\rangle_- \Rightarrow$ $\boxed{\{\hat{a}_k, \hat{a}_k^\dagger\} = \hat{I}}$

We require more general relations:

$\boxed{\{\hat{a}_k^\dagger, \hat{a}_l^\dagger\} = 0 = \{\hat{a}_k, \hat{a}_l\}}$

$\boxed{\{\hat{a}_k, \hat{a}_l^\dagger\} = \delta_{kl}}$

The validity for $k=l$ was just proven. For $k\neq l$ these relations represent some *satisfiable requirements upon the phases*, namely:

$\hat{a}_k^\dagger\hat{a}_l^\dagger\,|..\overbrace{n_k}^{0}..\overbrace{n_l}^{0}...\rangle_- = -\hat{a}_l^\dagger\hat{a}_k^\dagger\,|..\overbrace{n_k}^{0}..\overbrace{n_l}^{0}...\rangle_-$

$\hat{a}_k\hat{a}_l^\dagger\,|..\underbrace{n_k}_{1}..\underbrace{n_l}_{0}...\rangle_- = -\hat{a}_l^\dagger\hat{a}_k\,|..\underbrace{n_k}_{1}..\underbrace{n_l}_{0}...\rangle_-$

In this way, the fermionic creation/annihilation operators are fully analogous to the bosonic ones except that the commutators are replaced by anticommutators.

▶ Particle number operators

Number of particles in the single-particle state $|\phi_k\rangle$:

bosons $\boxed{\hat{N}_k = \hat{b}_k^\dagger\hat{b}_k}$ $\qquad$ fermions $\boxed{\hat{N}_k = \hat{a}_k^\dagger\hat{a}_k}$

$\hat{b}_k^\dagger\hat{b}_k\,|..n_k..\rangle_+ = \underbrace{\sqrt{n_k^2}}_{n_k}\,|..n_k..\rangle_+$ $\qquad$ $\hat{a}_k^\dagger\hat{a}_k\,|..n_k..\rangle_- = \underbrace{\sqrt{n_k^2}}_{n_k=0,1}\,|..n_k..\rangle_-$

$\Rightarrow$ **total number of particles**:

bosons $\boxed{\hat{N} = \sum_k \hat{b}_k^\dagger\hat{b}_k}$ $\qquad$ fermions $\boxed{\hat{N} = \sum_k \hat{a}_k^\dagger\hat{a}_k}$

We identify standard commutation relations of ladder operators (Sec. 3b):

$$\begin{cases} \big[\hat{N}_k, \hat{b}_l^\dagger\big] = \delta_{kl}\hat{b}_l^\dagger & \big[\hat{N}_k, \hat{b}_l\big] = -\delta_{kl}\hat{b}_l \\ \big[\hat{N}, \hat{b}_l^\dagger\big] = +\hat{b}_l^\dagger & \big[\hat{N}, \hat{b}_l\big] = -\hat{b}_l \\ \big[\hat{N}_k, \hat{a}_l^\dagger\big] = \delta_{kl}\hat{a}_l^\dagger & \big[\hat{N}_k, \hat{a}_l\big] = -\delta_{kl}\hat{a}_l \\ \big[\hat{N}, \hat{a}_l^\dagger\big] = +\hat{a}_l^\dagger & \big[\hat{N}, \hat{a}_l\big] = -\hat{a}_l \end{cases}$$

▶ Creation of basis states from the vacuum

Consecutive creation of individual particles into the occupied single-particle states:

$$\boxed{|n_1,n_2,n_3...\rangle_\pm = \begin{cases} \frac{1}{\sqrt{n_1!n_2!n_3!...}}(\hat{b}_1^\dagger)^{n_1}(\hat{b}_2^\dagger)^{n_2}(\hat{b}_3^\dagger)^{n_3}\cdots|0\rangle & \text{for bosons} \\ (\hat{a}_1^\dagger)^{n_1}(\hat{a}_2^\dagger)^{n_2}(\hat{a}_3^\dagger)^{n_3}\cdots|0\rangle & \text{for fermions} \end{cases}}$$

Here, $|0\rangle$ represents the **vacuum state**, which is the only state forming the subspace $\mathcal{H}_\pm^{(0)}$ (no particle present). This state satisfies: $\boxed{\hat{b}_k|0\rangle = 0 = \hat{a}_k|0\rangle}$

▶ Relation between spin and statistics

How to decide whether a given particle is a boson or a fermion? For the reasons explained in Sec. 15, belonging to the boson or fermion family is referred to as "statistics". In relativistic quantum field theory it is possible to prove that all elementary particles (which are excitations of some particular types of fields) satisfy the following relation between spin and statistics:

Particles with $\boldsymbol{s}$ **= half-integer** are **fermions**. These are the electron, muon, tauon, all neutrinos, and all quarks, i.e., all leptons & hadrons forming matter. All these particles have $s=\frac{1}{2}$.

Particles with $\boldsymbol{s}$ **= integer** are **bosons**. These are the photon ($s=1$), intermediate W & Z bosons ($s=1$), gluons ($s=1$), and hopefully also the yet undiscovered graviton ($s=2$?), i.e., the mediators of all fundamental interactions. Also the Higgs boson, which plays a special role in the Standard Model, is a boson with $s=0$.

How about composite particles formed by several elementary constituents? The spin–statistics theorem holds even for such objects, but only in a limited sense. Indeed: (a) An object composed of any number of bosons (integer-spin particles) has an integer spin and the bosonic character (a wavefunction of a pair of such objects is symmetric under the exchange of objects). (b) An object composed of an even number of fermions (half-integer-spin particles) has again an integer spin and also the bosonic character (a two-object wavefunction is exchange-symmetric due to even number of sign changes involved in the exchange of objects). (c) An object composed of an odd number of fermions has a half-integer spin and the fermionic character (a two-object wavefunction is antisymmetric under the exchange of objects due to odd number of sign changes). However, the problem gets more complicated if checking (anti)commutation relations of the corresponding creation/annihilation operators.

▶ Bifermions vs. bosons

Bifermion ≡ a **pair of fermions**. Example: meson (quark-antiquark). Any bifermion must have an integer spin. Question: Is it a real boson?

Exchange of 2 bifermions $\Rightarrow$ 2$\times$ change of sign $\Rightarrow$ boson-like behavior

However, consider the creation/annihilation operators of a general bifermion:

$$\left.\begin{array}{c}\hat{A}^\dagger=\sum_{k,l}\alpha_{kl}\hat{a}_k^\dagger\hat{a}_l^\dagger \\ \text{creation}\end{array}\right\}\Leftrightarrow\left\{\begin{array}{c}\hat{A}=\sum_{k,l}\alpha_{kl}^*\hat{a}_l\hat{a}_k \\ \text{annihilation}\end{array}\right.$$

Antisymmetry : $\alpha_{kl}=-\alpha_{lk}$

Normalization : $\sum_{k,l}|\alpha_{kl}|^2=\frac{1}{2}$

Normalization: $1=\langle 0|\hat{A}\hat{A}^\dagger|0\rangle=\sum_{k,l}\sum_{k',l'}\alpha_{k'l'}^*\alpha_{kl}\langle 0|\hat{a}_{l'}\hat{a}_{k'}\hat{a}_k^\dagger\hat{a}_l^\dagger|0\rangle=2\sum_{k,l}|\alpha_{kl}|^2$

Commutator:

rearrange to the form of the 1st term

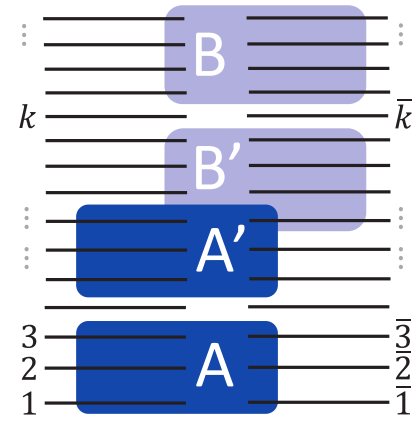
$$[\hat{A},\hat{A}^\dagger]=\sum_{k,l}\sum_{k',l'}\alpha_{k'l'}^*\alpha_{kl}[\hat{a}_{l'}\hat{a}_{k'},\hat{a}_k^\dagger\hat{a}_l^\dagger]=\sum_{k,l}\sum_{k',l'}\alpha_{k'l'}^*\alpha_{kl}\big(\hat{a}_{l'}\hat{a}_{k'}\hat{a}_k^\dagger\hat{a}_l^\dagger-\overbrace{\hat{a}_k^\dagger\hat{a}_l^\dagger\hat{a}_{l'}\hat{a}_{k'}}\big)$$

$$=\sum_{k,l}\sum_{k',l'}\alpha_{k'l'}^*\alpha_{kl}\big(-\delta_{kk'}\hat{a}_l^\dagger\hat{a}_{l'}+\delta_{kl'}\hat{a}_l^\dagger\hat{a}_{k'}+\delta_{lk'}\hat{a}_k^\dagger\hat{a}_{l'}-\delta_{ll'}\hat{a}_k^\dagger\hat{a}_{k'}+\delta_{kk'}\delta_{ll'}-\delta_{kl'}\delta_{lk'}\big)$$

$$=\hat{I}+\underbrace{4\sum_{l,l'}\Big(\sum_k\alpha_{l'k}^*\alpha_{kl}\Big)\hat{a}_l^\dagger\hat{a}_{l'}}_{\hat{\Delta}}$$

correction to the boson-type commutator

Its effect for a given many-body state $|\Psi\rangle$ depends on the expectation value $\langle\Psi|\hat{\Delta}|\Psi\rangle$.



Example:

Consider a set of fermionic states that appear in pairs $(k,\bar{k})\equiv(1,\bar{1}),(2,\bar{2}),...$ (e.g., quark-antiquark states in a meson, or time-reversal conjugate states of electrons or nucleons in a superconductor or in a nucleus) and define

2 bifermions

$$\left\{\begin{array}{ll}\hat{A}^\dagger=\frac{1}{\sqrt{4n_\mathrm{A}}}\sum_{k\in\mathcal{S}_\mathrm{A}}\big(\hat{a}_k^\dagger\hat{a}_{\bar{k}}^\dagger-\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger\big) & \mathcal{S}_\mathrm{A}\equiv\begin{array}{l}\text{subset of } k\text{-states}\\ \text{with } n_\mathrm{A} \text{ members}\end{array}\\ \hat{B}^\dagger=\frac{1}{\sqrt{4n_\mathrm{B}}}\sum_{k\in\mathcal{S}_\mathrm{B}}\big(\hat{a}_k^\dagger\hat{a}_{\bar{k}}^\dagger-\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger\big) & \mathcal{S}_\mathrm{B}\equiv\begin{array}{l}\text{subset of } k\text{-states}\\ \text{with } n_\mathrm{B} \text{ members}\end{array}\end{array}\right.$$

We first assume that the subsets $\mathcal{S}_\mathrm{A}$ and $\mathcal{S}_\mathrm{B}$ do not overlap: $\boxed{\mathcal{S}_\mathrm{A}\cap\mathcal{S}_\mathrm{B}=\emptyset}$

Then we can easily prove the bosonic commutation relations:

$$\boxed{[\hat{A}^\dagger,\hat{B}^\dagger]=[\hat{A},\hat{B}]=[\hat{A},\hat{B}^\dagger]=[\hat{A}^\dagger,\hat{B}]=0}$$

However, we get:

$$\boxed{\begin{array}{l}\big[\hat{A},\hat{A}^\dagger\big]=\hat{I}-\frac{1}{n_\mathrm{A}}\hat{N}_\mathrm{A}\\ \big[\hat{B},\hat{B}^\dagger\big]=\hat{I}-\frac{1}{n_\mathrm{B}}\hat{N}_\mathrm{B}\end{array}}\quad\text{with }\hat{N}_\bullet=\sum_{k\in\mathcal{S}_\bullet}\big(\hat{a}_k^\dagger\hat{a}_k+\hat{a}_{\bar{k}}^\dagger\hat{a}_{\bar{k}}\big)$$

The last relations show limitations in the repeated creation of bifermions of both A- and B-types. The numbers of these bifermions is limited by the Pauli principle, i.e., by the capacity of the corresponding $\mathcal{S}_\mathrm{A}$ and $\mathcal{S}_\mathrm{B}$ fermionic state subsets. Consider for instance the A-bifermion: If $N_\mathrm{A}=0$ (no particle in states $\in\mathcal{S}_\mathrm{A}$), we get $[\hat{A},\hat{A}^\dagger]=\hat{I}\ \Rightarrow\ [\hat{A}^\dagger\hat{A},\hat{A}^\dagger]=+\hat{A}^\dagger\ \Rightarrow\ \hat{A}^\dagger$ behaves as a creation

operator with respect to the "number operator" $\hat{A}^\dagger\hat{A}$. However, as the states $\hat{A}^\dagger|0\rangle$, $(\hat{A}^\dagger)^2|0\rangle$, $(\hat{A}^\dagger)^3|0\rangle$, ... yield $N_{\rm A}=2,4,6,...$, the repeated action of the operator $\hat{A}^\dagger$ gradually changes its character. Once the state subset $\mathcal{S}_{\rm A}$ is full, $N_{\rm A}=2n_{\rm A}$, we get $[\hat{A},\hat{A}^\dagger]=-\hat{I}\ \Rightarrow\ [\hat{A}^\dagger\hat{A},\hat{A}^\dagger]=-\hat{A}^\dagger\ \Rightarrow\ \hat{A}^\dagger$ behaves effectively as an *annihilation* operator with respect to $\hat{A}^\dagger\hat{A}$.

If the subsets $\mathcal{S}_{\rm A}$ and $\mathcal{S}_{\rm B}$ overlap $\boxed{\mathcal{S}_{\rm A}\cap\mathcal{S}_{\rm B}\neq\emptyset}$ (see the A' & B' case in the above figure), we still keep the bosonic commutation relations $[\hat{A}^\dagger,\hat{B}^\dagger]=[\hat{A},\hat{B}]=0$, but in addition to the above non-bosonic relations $[\hat{A},\hat{A}^\dagger]=\hat{I}-\frac{1}{n_{\rm A}}\hat{N}_{\rm A}$ and $[\hat{B},\hat{B}^\dagger]=\hat{I}-\frac{1}{n_{\rm B}}\hat{N}_{\rm B}$ we also get $\boxed{[\hat{A},\hat{B}^\dagger]=[\hat{B},\hat{A}^\dagger]=\frac{1}{\sqrt{n_{\rm A}n_{\rm B}}}(n_{\rm AB}\hat{I}-\hat{N}_{\rm AB})}$ with $n_{\rm AB}\equiv$ the number of k-states in the $\mathcal{S}_{\rm A}\cap\mathcal{S}_{\rm B}$ set and $\hat{N}_{\rm AB}=\sum\limits_{k\in\mathcal{S}_{\rm A}\cap\mathcal{S}_{\rm A}}(\hat{a}_k^\dagger\hat{a}_k+\hat{a}_{\bar{k}}^\dagger\hat{a}_{\bar{k}})$. So not even a single pair of the A- and B-bifermions behaves as a pair of true bosons.

Conclusion: Bifermions may resemble bosons only if they do not overlap with each other (i.e., if they do not share the same fermionic states) and if their numbers are very low compared to the overall capacity of the corresponding part of the fermionic Hilbert space.

► Transformations of creation/annihilation operators

Consider 2 single-particle bases: $\big\{|\phi_j\rangle\big\}_j\overset{\hat{U}}{\leftrightarrow}\big\{|\tilde{\phi}_i\rangle\big\}_i\ \Leftrightarrow\ |\tilde{\phi}_i\rangle=\sum\limits_{i'}\underbrace{\langle\phi_{i'}|\tilde{\phi}_i\rangle}_{U_{ii'}}|\phi_{i'}\rangle$

$\hat{U}$ represents a unitary operator relating the two bases, which also constitutes the transformation between boson & fermion creation/annihilation operators:

$$\boxed{\hat{\tilde{b}}_i^\dagger\equiv\sum_{i'}\langle\phi_{i'}|\tilde{\phi}_i\rangle\hat{b}_{i'}^\dagger}\quad\boxed{\hat{\tilde{b}}_j\equiv\sum_{j'}\langle\tilde{\phi}_j|\phi_{j'}\rangle\hat{b}_{j'}}\quad\boxed{\hat{\tilde{a}}_i^\dagger\equiv\sum_{i'}\langle\phi_{i'}|\tilde{\phi}_i\rangle\hat{a}_{i'}^\dagger}\quad\boxed{\hat{\tilde{a}}_j\equiv\sum_{j'}\langle\tilde{\phi}_j|\phi_{j'}\rangle\hat{a}_{j'}}$$

$$\Big[\hat{\tilde{b}}_j,\hat{\tilde{b}}_i^\dagger\Big]=\sum_{j',i'}\langle\tilde{\phi}_j|\phi_{j'}\rangle\langle\phi_{i'}|\tilde{\phi}_i\rangle\overbrace{\Big[\hat{b}_{j'},\hat{b}_{i'}^\dagger\Big]}^{\delta_{i'j'}}=\delta_{ij}\qquad\Big\{\hat{\tilde{a}}_j,\hat{\tilde{a}}_i^\dagger\Big\}=\sum_{j',i'}\langle\tilde{\phi}_j|\phi_{j'}\rangle\langle\phi_{i'}|\tilde{\phi}_i\rangle\overbrace{\Big\{\hat{a}_{j'},\hat{a}_{i'}^\dagger\Big\}}^{\delta_{i'j'}}=\delta_{ij}$$

$\Rightarrow$ commutation/anticommutation relations remain the same

► Second quantization

A transformation of creation/annihilation operators for general particles to the **coordinate & spin eigenbasis** $\big\{|\tilde{\phi}_{\vec{x},m_s}\rangle\big\}$

$$\hat{\tilde{b}}_{\vec{x},m_s}^\dagger\equiv\hat{\psi}_+^\dagger(\vec{x},m_s)=\sum_i\overbrace{\langle\phi_i|\tilde{\phi}_{\vec{x},m_s}\rangle}^{\phi_i^*(\vec{x},m_s)}\hat{b}_i^\dagger\qquad\hat{\tilde{a}}_{\vec{x},m_s}^\dagger\equiv\hat{\psi}_-^\dagger(\vec{x},m_s)=\sum_i\overbrace{\langle\phi_i|\tilde{\phi}_{\vec{x},m_s}\rangle}^{\phi_i^*(\vec{x},m_s)}\hat{a}_i^\dagger$$

$$\hat{\tilde{b}}_{\vec{x},m_s}\equiv\hat{\psi}_+(\vec{x},m_s)=\sum_j\underbrace{\langle\tilde{\phi}_{\vec{x},m_s}|\phi_j\rangle}_{\phi_j(\vec{x},m_s)}\hat{b}_j\qquad\hat{\tilde{a}}_{\vec{x},m_s}\equiv\hat{\psi}_-(\vec{x},m_s)=\sum_j\underbrace{\langle\tilde{\phi}_{\vec{x},m_s}|\phi_j\rangle}_{\phi_j(\vec{x},m_s)}\hat{a}_j$$

The new single-particle basis is not discrete (countable) ⇒ commutation/ anticommutation relations will contain the δ-function:

Commutation relations (bosons)		Anticommutation relations (fermions)
$\left[\hat{\psi}_+^\dagger(\vec{x},m_s),\hat{\psi}_+^\dagger(\vec{x}\,',m_s')\right]$	$=0=$	$\left\{\hat{\psi}_-^\dagger(\vec{x},m_s),\hat{\psi}_-^\dagger(\vec{x}\,',m_s')\right\}$
$\left[\hat{\psi}_+(\vec{x},m_s),\hat{\psi}_+(\vec{x}\,',m_s')\right]$	$=0=$	$\left\{\hat{\psi}_-(\vec{x},m_s),\hat{\psi}_-(\vec{x}\,',m_s')\right\}$
$\left[\hat{\psi}_+(\vec{x},m_s),\hat{\psi}_+^\dagger(\vec{x}\,',m_s')\right]$	$=\delta(\vec{x}-\vec{x}')\delta_{m_sm_s'}=$	$\left\{\hat{\psi}_-(\vec{x},m_s),\hat{\psi}_-^\dagger(\vec{x}\,',m_s')\right\}$

Proof of the last line:

$$\left[\hat{\psi}_+(\vec{x},m_s),\hat{\psi}_+^\dagger(\vec{x}\,',m_s')\right]=\sum_{i,j}\langle\tilde{\phi}_{\vec{x},m_s}|\phi_j\rangle\langle\phi_i|\tilde{\phi}_{\vec{x}\,',m_s'}\rangle\overbrace{[\hat{b}_j,\hat{b}_i^\dagger]}^{\delta_{ij}}=\overbrace{\langle\tilde{\phi}_{\vec{x},m_s}|\tilde{\phi}_{\vec{x}\,',m_s'}\rangle}^{\delta(\vec{x}-\vec{x}')\delta_{m_sm_s'}}$$

$$\left\{\hat{\psi}_-(\vec{x},m_s),\hat{\psi}_-^\dagger(\vec{x}\,',m_s')\right\}=\sum_{i,j}\langle\tilde{\phi}_{\vec{x},m_s}|\phi_j\rangle\langle\phi_i|\tilde{\phi}_{\vec{x}\,',m_s'}\rangle\underbrace{\{\hat{a}_j,\hat{a}_i^\dagger\}}_{\delta_{ij}}=\underbrace{\langle\tilde{\phi}_{\vec{x},m_s}|\tilde{\phi}_{\vec{x}\,',m_s'}\rangle}_{\delta(\vec{x}-\vec{x}')\delta_{m_sm_s'}}$$

Particle number operator:

$$\hat{N}_\pm=\sum_{m_s}\int\underbrace{\hat{\psi}_\pm^\dagger(\vec{x},m_s)\hat{\psi}_\pm(\vec{x},m_s)}_{\hat{n}_\pm(\vec{x},m_s)\ \text{particle density}}d\vec{x}$$

The above procedure is often referred to as the "second quantization", in analogy to the "first quantization", in which physical quantities became operators. In view of the above particle-number formula we can say that the second quantization induces the transition: $\left.\begin{matrix}\text{wavefunction}\\ \psi^*(\vec{x},m_s)\\ \psi(\vec{x},m_s)\end{matrix}\right\}\mapsto\left\{\begin{matrix}\hat{\psi}_\pm^\dagger(\vec{x},m_s)\\ \hat{\psi}_\pm(\vec{x},m_s)\end{matrix}\right.\ \text{operator}$

What used to be the single-particle probability density $|\psi(\vec{x},m_s)|^2$ is now the density of particles expressed by operator $\hat{n}_\pm(\vec{x},m_s)$, and what used to be just the normalization condition $\sum_{m_s}\int d\vec{x}\,|\psi(\vec{x},m_s)|^2=1$ is now an operator expression of the total number of particles $\hat{N}_\pm$. The Hilbert space of interest is no more that of a single particle, but the Fock space with any number of particles, including zero. This is one of the entry points to the quantum field theory, which treats all elementary particles as quantum excitations of some specific fields. Let us stress that this is the only way how to marriage quantum theory with special relativity, which allows to transform the rest mass to energy and vice versa, and therefore cannot in general guarantee conservation of the number of particles. But we must keep this gate closed (however tempting it may be) and continue with our tour of non-relativistic quantum problems.

■ Operators in bosonic & fermionic *N*-particle spaces

Creation/annihilation operators enable one to express *any* operator acting in the whole Fock space. In particular, the operators that conserve the total number of particles (those keeping the subspaces $\mathcal{H}_\pm^{(N)}$ invariant) can be written

through products containing the same number of creation and annihilation operators. This results in an important classification of such operators according to the number of particles ($n = 1, 2, 3 \ldots$) they influence in a single action. We talk about n-body operators, e.g., 1-body, 2-body or 3-body terms of a Hamiltonian describing independent motions and mutual interactions of particles in a bound quantum system (an atom, nucleus or quantum dot).

▶ General operator expressed via creation/annihilation operators

Creation/annihilation operators of bosons or fermions **unified notation**:
$$\begin{cases} \hat{c}_k^\dagger \equiv \hat{b}_k^\dagger \text{ or } \hat{a}_k^\dagger \\ \hat{c}_k \equiv \hat{b}_k \text{ or } \hat{a}_k \end{cases}$$

Consider operator $\hat{O}$ conserving the particle number $\Rightarrow \boxed{[\hat{O}, \hat{N}] = 0}$

$\hat{O}$ acts within any N-particle subspace $\mathcal{H}^{(N)}$, where it can be expressed as:

$$\hat{O} = \sum_{i_1,..i_N} \sum_{i'_1,..i'_N} \langle \phi_{i_1}..\phi_{i_N}|\hat{O}|\phi_{i'_1}..\phi_{i'_N}\rangle |\phi_{i_1}..\phi_{i_N}\rangle\langle\phi_{i'_1}..\phi_{i'_N}|$$

Assume that the operator (observable) $\hat{O}$ is physical for *indistinguishable particles* $\Rightarrow$ it acts inside $\mathcal{H}_\pm^{(N)} \Rightarrow \boxed{[\hat{O}, \hat{P}_\pm] = 0}$

$$\hat{O}\hat{P}_\pm = \hat{P}_\pm\hat{O}\hat{P}_\pm = \sum_{i_1,..i_N} \sum_{i'_1,..i'_N} \langle \phi_{i_1}..\phi_{i_N}|\hat{O}|\phi_{i'_1}..\phi_{i'_N}\rangle \underbrace{\hat{P}_\pm|\phi_{i_1}..\phi_{i_N}\rangle}_{\sqrt{\frac{n_1!n_2!..}{N!}}|n_1,n_2,..\rangle} \underbrace{\langle\phi_{i'_1}..\phi_{i'_N}|\hat{P}_\pm}_{\langle n'_1,n'_2,..|\sqrt{\frac{n'_1!n'_2!..}{N!}}}$$

$$= \frac{1}{N!} \sum_{i_1,..i_N} \sum_{i'_1,..i'_N} \langle \phi_{i_1}..\phi_{i_N}|\hat{O}|\phi_{i'_1}..\phi_{i'_N}\rangle\, \hat{c}_{i_1}^\dagger \hat{c}_{i_2}^\dagger..\hat{c}_{i_N}^\dagger \underbrace{|0\rangle\langle 0|}_{\hat{P}^{(0)}} \hat{c}_{i'_N}..\hat{c}_{i'_2}\hat{c}_{i'_1}$$

within the space $\mathcal{H}^{(N)}$... ...can be removed

$$\boxed{\hat{P}_\pm\hat{O}\hat{P}_\pm = \frac{1}{N!} \sum_{i_1,...i_N} \sum_{i'_1,...i'_N} \langle \phi_{i_1}..\phi_{i_N}|\hat{O}|\phi_{i'_1}..\phi_{i'_N}\rangle\, \hat{c}_{i_1}^\dagger \hat{c}_{i_2}^\dagger..\hat{c}_{i_N}^\dagger \hat{c}_{i'_N}..\hat{c}_{i'_2}\hat{c}_{i'_1}}$$

This is the most general expression in the N-particle subspace of an operator respecting particle indistinguishability and conserving particle number. However, as shown below, for some classes of operators this can be further simplified.

▶ One-body operators

Operator defined in the $N=1$ subspace through: $\boxed{(\hat{T})_k|\psi\underbrace{\rangle_k}_{\substack{\text{particle}\\ \text{index}}} = \sum_{i_k}\langle\phi_{i_k}|\hat{T}|\psi\rangle|\phi_{i_k}\rangle_k}$

Examples: the kinetic energy of a particle and its potential energy in an external field

The action of $\hat{T}$ is extended to all $N > 1$ subspaces via summation over all particles:

$$\boxed{\hat{O}^{(1)} = \sum_{k=1}^{N}(\hat{T})_k} \equiv \sum_{k=1}^{N}\big(\hat{I}_1 \otimes \cdots \hat{I}_{k-1} \otimes \underbrace{\hat{T}}_{k^{\text{th}}\text{place}} \otimes \hat{I}_{k+1} \cdots \otimes \hat{I}_N\big)$$

The defining property of the 1-body operator in an N-particle subspace is expressed as:

$$\hat{O}^{(1)}\underbrace{\hat{P}_{\pm}|\phi_1\cdots\phi_k\cdots\phi_N\rangle}_{\frac{1}{\sqrt{N!}}\hat{c}_1^\dagger\cdots\hat{c}_k^\dagger\cdots\hat{c}_N^\dagger|0\rangle}=\sum_{k=1}^{N}\sum_{i_k}\langle\phi_{i_k}|\hat{T}|\phi_k\rangle\underbrace{\hat{P}_{\pm}|\phi_1\cdots\phi_{i_k}\cdots\phi_N\rangle}_{\frac{1}{\sqrt{N!}}\hat{c}_1^\dagger\cdots\hat{c}_{i_k}^\dagger\cdots\hat{c}_N^\dagger|0\rangle}$$

We consider an operator defined as $\hat{O}^{(1)}\equiv\sum_{i,i'}\langle\phi_i|\hat{T}|\phi_{i'}\rangle\,\hat{c}_i^\dagger\hat{c}_{i'}$ and show that it satisfies the above property:

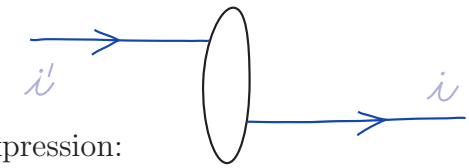
Note that: $[\hat{O}^{(1)},\hat{c}_k^\dagger]=\sum_{i,i'}\langle\phi_i|\hat{T}|\phi_{i'}\rangle\overbrace{[\hat{c}_i^\dagger\hat{c}_{i'},\hat{c}_k^\dagger]}^{\delta_{i'k}\hat{c}_i^\dagger}=\sum_{i}\langle\phi_i|\hat{T}|\phi_k\rangle\hat{c}_i^\dagger$

$$\hat{O}^{(1)}\hat{c}_1^\dagger..\hat{c}_k^\dagger..\hat{c}_N^\dagger|0\rangle=\Big\{\underbrace{\big([\hat{O}^{(1)},\hat{c}_1^\dagger]}_{\sum_{i_1}\langle\phi_{i_1}|\hat{T}|\phi_1\rangle\hat{c}_{i_1}^\dagger}\hat{c}_2^\dagger..\hat{c}_N^\dagger\big)+\cdots+\big(\hat{c}_1^\dagger..\hat{c}_{k-1}^\dagger\underbrace{[\hat{O}^{(1)},\hat{c}_k^\dagger]}_{\sum_{i_k}\langle\phi_{i_k}|\hat{T}|\phi_k\rangle\hat{c}_{i_k}^\dagger}..\hat{c}_N^\dagger\big)$$
$$+\cdots+\big(\hat{c}_1^\dagger..\hat{c}_{N-1}^\dagger\overbrace{[\hat{O}^{(1)},\hat{c}_N^\dagger]}^{\sum_{i_N}\langle\phi_{i_N}|\hat{T}|\phi_N\rangle\hat{c}_{i_N}^\dagger}\big)\Big\}|0\rangle=\sum_{k=1}^{N}\sum_{i_k}\langle\phi_{i_k}|\hat{T}|\phi_k\rangle\hat{c}_1^\dagger..\hat{c}_{i_k}^\dagger..\hat{c}_N^\dagger|0\rangle$$

The above defining property is verified, so the 1-body operator is given by:

$$\boxed{\hat{O}^{(1)}\equiv\sum_{i,i'}\langle\phi_i|\hat{T}|\phi_{i'}\rangle\,\hat{c}_i^\dagger\hat{c}_{i'}}$$

Graphical representation of this expression:



▶ Two-body operators

Operator defined in the $N=2$ subspace through:

$$(\hat{V})_{kl}|\psi\rangle\underbrace{{}_{kl}}_{\substack{\text{particle}\\\text{indices}}}=\sum_{i_k,i_l}\langle\phi_{i_k}\phi_{i_l}|\hat{V}|\psi\rangle_{kl}|\phi_{i_k}\phi_{i_l}\rangle_{kl}$$

Example: an interaction energy of two particles. With respect to the exchange symmetry we require: $\langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle=\langle\phi_j\phi_i|\hat{V}|\phi_{j'}\phi_{i'}\rangle$. The action of $\hat{V}$ is extended to all $N>2$ subspaces via summation over all particle pairs:

$$\boxed{\hat{O}^{(2)}=\sum_{k=1}^{N}\sum_{l=k+1}^{N}(\hat{V})_{kl}}=\sum_{\substack{k\\l>k}\}=1}^{N}\hat{I}_1\otimes\cdots\hat{I}_{k-1}\otimes\hat{I}_{k+1}\otimes\cdots\hat{I}_{l-1}\otimes\hat{I}_{l+1}\otimes\cdots\hat{I}_N\otimes(\hat{V})_{kl}$$

The defining property of the 2-body operator in an N subspace reads as:

$$\hat{O}^{(2)}\hat{c}_1^\dagger..\hat{c}_k^\dagger..\hat{c}_l^\dagger..\hat{c}_N^\dagger|0\rangle=\sum_{\substack{k\\l>k}\}=1}^{N}\sum_{i_k,j_l}\langle\phi_{i_k}\phi_{j_l}|\hat{V}|\phi_k\phi_l\rangle\;\hat{c}_1^\dagger..\hat{c}_{i_k}^\dagger..\hat{c}_{j_l}^\dagger..\hat{c}_N^\dagger|0\rangle$$

We consider an operator defined as $\hat{O}^{(2)}\equiv\frac{1}{2}\sum_{i,i'}\sum_{j,j'}\langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle\,\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{j'}\hat{c}_{i'}$ and show that it satisfies the above property:

First note that: $[\hat{O}^{(2)},\hat{c}_k^\dagger]=\frac{1}{2}\sum_{i,i'}\sum_{j,j'}\langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle\overbrace{[\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{j'}\hat{c}_{i'},\hat{c}_k^\dagger]}^{\delta_{i'k}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{j'}\pm\delta_{j'k}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{i'}}}=$

$$=\frac{1}{2}\sum_{i,j,j'}\langle\phi_i\phi_j|\hat{V}|\phi_k\phi_{j'}\rangle\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{j'}+\frac{1}{2}\sum_{i,i',j}\langle\phi_j\phi_i|\hat{V}|\phi_k\phi_{i'}\rangle\hat{c}_j^\dagger\hat{c}_i^\dagger\hat{c}_{i'}=\sum_{i,j,l}\langle\phi_i\phi_j|\hat{V}|\phi_k\phi_l\rangle\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_l$$

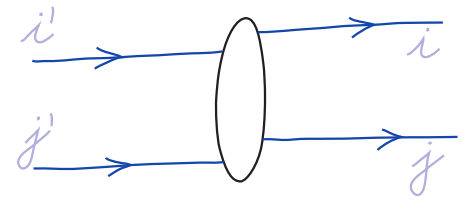
$$\hat{O}^{(2)}\hat{c}_1^\dagger..\hat{c}_k^\dagger..\hat{c}_l^\dagger..\hat{c}_N^\dagger|0\rangle = \Big\{ \underbrace{\big([\hat{O}^{(2)},\hat{c}_1^\dagger]\,\hat{c}_2^\dagger..\hat{c}_N^\dagger\big)}_{\sum_{i_1,j_1,l_1}\langle\phi_{i_1}\phi_{j_1}|\hat{V}|\phi_1\phi_{l_1}\rangle\hat{c}_{i_1}^\dagger\hat{c}_{j_1}^\dagger\hat{c}_{l_1}} + \cdots + \underbrace{\big(\hat{c}_1^\dagger..\hat{c}_{k-1}^\dagger\,[\hat{O}^{(2)},\hat{c}_k^\dagger]..\hat{c}_N^\dagger\big)}_{\sum_{i_k,j_k,l_k}\langle\phi_{i_k}\phi_{j_k}|\hat{V}|\phi_k\phi_{l_k}\rangle\hat{c}_{i_k}^\dagger\hat{c}_{j_k}^\dagger\hat{c}_{l_k}}$$
$$+\cdots+\underbrace{\big(\hat{c}_1^\dagger..\hat{c}_{N-1}^\dagger\,[\hat{O}^{(2)},\hat{c}_N^\dagger]\big)}_{\sum_{i_N,j_N,l_N}\langle\phi_{i_N}\phi_{j_N}|\hat{V}|\phi_N\phi_{l_N}\rangle\hat{c}_{i_N}^\dagger\hat{c}_{j_N}^\dagger\hat{c}_{l_N}}\Big\}|0\rangle = \sum_{\substack{k\\ l>k}\}=1}^{N}\sum_{i_k,j_l}\langle\phi_{i_k}\phi_{j_l}|\hat{V}|\phi_k\phi_l\rangle\;\hat{c}_1^\dagger..\hat{c}_{i_k}^\dagger..\hat{c}_{j_l}^\dagger..\hat{c}_N^\dagger|0\rangle$$

The last equality results from the fact that $\hat{c}_{l_k}$ in the commutator expressions can only annihilate a state already created (otherwise the result=0) $\Rightarrow$ l_k=$(k+1)$ or $(k+2)$ or … N. The pair $\hat{c}_{j_k}^\dagger\hat{c}_{l_k}$ commutes to the right to the position of the $\hat{c}_{l_k}^\dagger$ and the whole combination $\hat{c}_{j_k}^\dagger\hat{c}_{l_k}\hat{c}_{l_k}^\dagger$ is replaced by $\hat{c}_{j_k}^\dagger$. The last expression verifies the above property of 2-body operators.

So the 2-body operator is expressed by:

$$\hat{O}^{(2)} \equiv \tfrac{1}{2}\sum_{i,i'}\sum_{j,j'}\langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle\;\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{j'}\hat{c}_{i'}$$

Graphical representation of this expression:



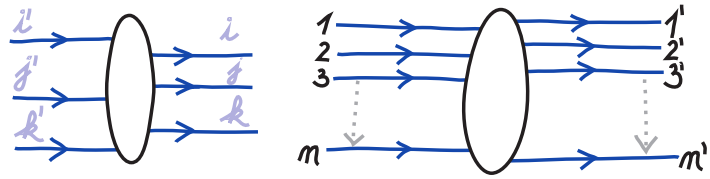
▶ Higher-order operators

An analogous procedure can be applied (though with increasing intricacy) to any n-body operator.

Example, **three-body**:

$$\hat{O}^{(3)} = \sum_{k=1}^{N}\sum_{l=k+1}^{N}\sum_{m=l+1}^{N}(\hat{W})_{klm}$$
$$= \tfrac{1}{3!}\sum_{i,i'}\sum_{j,j'}\sum_{k,k'}\langle\phi_i\phi_j\phi_k|\hat{W}|\phi_{i'}\phi_{j'}\phi_{k'}\rangle\;\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_k^\dagger\hat{c}_{k'}\hat{c}_{j'}\hat{c}_{i'}$$

Graphical representation of 3- & n-body operators:



▶ **Normal ordering** of the products of creation/annihilation operators

Matrix elements of an n-body operator in the N-body space are expressed in terms of the following vacuum expectation values:

$$\langle 0|\underbrace{\hat{c}_{j_1}\cdots\hat{c}_{j_N}}_{N\times}\underbrace{\hat{c}_{k_1}^\dagger\cdots\hat{c}_{k_n}^\dagger}_{n\times}\underbrace{\hat{c}_{l_1}\cdots\hat{c}_{l_n}}_{n\times}\underbrace{\hat{c}_{i_N}^\dagger\cdots\hat{c}_{i_1}^\dagger}_{N\times}|0\rangle$$

The product inside is standardly rewritten in the normal-ordered form:

$$:\underbrace{\hat{c}_{i_1}^\dagger\cdots\hat{c}_{j_1}\cdots\hat{c}_{i_k}^\dagger\cdots\hat{c}_{j_l}\cdots\hat{c}_{j_m}\cdots\hat{c}_{i_n}^\dagger}_{\text{unsorted product of } n\times\hat{c}_\bullet^\dagger \text{ and } m\times\hat{c}_\circ}: = \underbrace{\sigma}_{\pm}\underbrace{\hat{c}_{i_1}^\dagger\cdots\hat{c}_{i_k}^\dagger\cdots\hat{c}_{i_n}^\dagger}_{n\times\hat{c}_\bullet^\dagger}\underbrace{\hat{c}_{j_1}\cdots\hat{c}_{j_l}\cdots\hat{c}_{j_m}}_{m\times\hat{c}_\circ}$$

$$\sigma=\begin{cases}+1 & \text{bosons}\\ \pm 1=\sigma_\pi & \text{fermions: sign of permut. } (i_1..j_1..i_k..j_l..j_m..i_n)\to(i_1..i_k..i_nj_1..j_l..j_m)\end{cases}$$

Examples:
$$\begin{cases} :\hat b_i\hat b_j^\dagger: = \hat b_j^\dagger\hat b_i & :\hat a_i\hat a_j^\dagger: = -\hat a_j^\dagger\hat a_i\\ :\hat b_i^\dagger\hat b_j\hat b_k^\dagger: = \hat b_i^\dagger\hat b_k^\dagger\hat b_j & :\hat a_i^\dagger\hat a_j\hat a_k^\dagger: = -\hat a_i^\dagger\hat a_k^\dagger\hat a_j\\ \qquad = \hat b_k^\dagger\hat b_i^\dagger\hat b_j & \qquad = +\hat a_k^\dagger\hat a_i^\dagger\hat a_j\end{cases}$$

▶ Wick theorem

There exists a systematic way how a product of creation/annihilation operators can be transformed into the normal-ordered form. It makes use of so-called **contraction**, which for an operator product $\hat A\hat B$ is defined as the vacuum expectation value $\boxed{\langle\hat A\hat B\rangle_0=\langle 0|\hat A\hat B|0\rangle}$

Examples:
$$\begin{cases}\langle\hat b_i\hat b_j^\dagger\rangle_0=\delta_{ij}=\langle\hat a_i\hat a_j^\dagger\rangle_0\\ \langle\hat b_j^\dagger\hat b_i\rangle_0=0=\langle\hat a_j^\dagger\hat a_i\rangle_0\\ \langle\hat b_j^\dagger\hat b_i^\dagger\rangle_0=\langle\hat b_j\hat b_i\rangle_0=0=\langle\hat a_j\hat a_i\rangle_0=\langle\hat a_j^\dagger\hat a_i^\dagger\rangle_0\end{cases}$$

Statement:

Product of creation & annihilation operators $=$
$$\sum_{k=0,1,2,...}\ \underbrace{\sigma}_{\pm}$$
(normal ordered product with k pairs removed) $\equiv :\bullet_k:$
$\times$ (product of k contractions of the removed pairs) $\equiv c_k$

The proof not given here, instead we give some examples

Examples : **bosons**| |**fermions**

$\hat b_i\hat b_j^\dagger = \underbrace{:\hat b_i\hat b_j^\dagger:}_{\hat b_j^\dagger\hat b_i}+\underbrace{\langle\hat b_i\hat b_j^\dagger\rangle_0}_{\delta_{ij}}$ | $\hat a_i\hat a_j^\dagger = \underbrace{:\hat a_i\hat a_j^\dagger:}_{-\hat a_j^\dagger\hat a_i}+\underbrace{\langle\hat a_i\hat a_j^\dagger\rangle_0}_{\delta_{ij}}$

$\hat b_i^\dagger\hat b_j\hat b_k\hat b_l^\dagger=\hat b_i^\dagger\hat b_l^\dagger\hat b_j\hat b_k+\delta_{kl}\hat b_i^\dagger\hat b_j+\delta_{jl}\hat b_i^\dagger\hat b_k$ | $\hat a_i^\dagger\hat a_j\hat a_k\hat a_l^\dagger=\hat a_i^\dagger\hat a_l^\dagger\hat a_j\hat a_k+\delta_{kl}\hat a_i^\dagger\hat a_j-\delta_{jl}\hat a_i^\dagger\hat a_k$

General product :

$\hat A\hat B\hat C\hat D=:\hat A\hat B\hat C\hat D:+\langle\hat A\hat B\rangle_0:\hat C\hat D:$ | $\hat A\hat B\hat C\hat D=:\hat A\hat B\hat C\hat D:+\langle\hat A\hat B\rangle_0:\hat C\hat D:$

$+\langle\hat A\hat C\rangle_0:\hat B\hat D:+\langle\hat A\hat D\rangle_0:\hat B\hat C:$ | $-\langle\hat A\hat C\rangle_0:\hat B\hat D:+\langle\hat A\hat D\rangle_0:\hat B\hat C:$

$+\langle\hat B\hat C\rangle_0:\hat A\hat D:+\langle\hat B\hat D\rangle_0:\hat A\hat C:$ | $+\langle\hat B\hat C\rangle_0:\hat A\hat D:-\langle\hat B\hat D\rangle_0:\hat A\hat C:$

$+\langle\hat C\hat D\rangle_0:\hat A\hat B:+\langle\hat A\hat B\rangle_0\langle\hat C\hat D\rangle_0$ | $+\langle\hat C\hat D\rangle_0:\hat A\hat B:+\langle\hat A\hat B\rangle_0\langle\hat C\hat D\rangle_0$

$+\langle\hat A\hat C\rangle_0\langle\hat B\hat D\rangle_0+\langle\hat A\hat D\rangle_0\langle\hat B\hat C\rangle_0$ | $-\langle\hat A\hat C\rangle_0\langle\hat B\hat D\rangle_0+\langle\hat A\hat D\rangle_0\langle\hat B\hat C\rangle_0$

If the **vacuum expectation value** of an operator product is to be evaluated, one makes use of the obvious fact that $\boxed{\langle 0|:\bullet_k:|0\rangle=0}$ Only the terms composed solely of contractions (if $\neq 0$) may contribute to the result.

▶ Two-state correlations

The N-body state $|\Psi\rangle$ contains complete information on the system, including information on statistical distributions and mutual correlations of all occupation numbers n_i associated with single-particle states $|\phi_i\rangle$. For any $|\Psi\rangle$, these properties can be described by means of the following general quantities:

(a) Average: $\langle n_i\rangle_\Psi = \langle\Psi|\hat{c}_i^\dagger\hat{c}_i|\Psi\rangle$

(b) Dispersion: $\langle\langle n_i^2\rangle\rangle_\Psi = \langle n_i^2\rangle_\Psi - \langle n_i\rangle_\Psi^2 = \underbrace{\langle\Psi|\hat{c}_i^\dagger\hat{c}_i\hat{c}_i^\dagger\hat{c}_i|\Psi\rangle}_{\langle\Psi|\hat{b}_i^\dagger\hat{b}_i^\dagger\hat{b}_i\hat{b}_i|\Psi\rangle+\langle\Psi|\hat{b}_i^\dagger\hat{b}_i|\Psi\rangle \quad \text{(bosons)}} - \langle\Psi|\hat{c}_i^\dagger\hat{c}_i|\Psi\rangle^2$

(c) Correlation between occupation numbers of states $|\phi_i\rangle, |\phi_j\rangle$ (for $i \neq j$): $\langle\Psi|\hat{a}_i^\dagger\hat{a}_i|\Psi\rangle \quad \text{(fermions)}$

$$\boxed{\langle\langle n_i n_j\rangle\rangle_\Psi = \underbrace{\langle n_i n_j\rangle_\Psi - \langle n_i\rangle_\Psi\langle n_j\rangle_\Psi}_{\left\langle (n_i-\langle n_i\rangle_\Psi)(n_j-\langle n_j\rangle_\Psi)\right\rangle_\Psi}} = \underbrace{\langle\Psi|\hat{c}_i^\dagger\hat{c}_i\hat{c}_j^\dagger\hat{c}_j|\Psi\rangle}_{\langle\Psi|\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_j\hat{c}_i|\Psi\rangle} - \langle\Psi|\hat{c}_i^\dagger\hat{c}_i|\Psi\rangle\langle\Psi|\hat{c}_j^\dagger\hat{c}_j|\Psi\rangle$$

Normalized correlation coefficient: $C_{ij}(\Psi) = \begin{cases} +1 & \text{for perfect correlation} \\ 0 & \text{for null correlation} \\ -1 & \text{for perfect anticorrelation} \end{cases}$

$$\boxed{C_{ij}(\Psi) \equiv \frac{\langle\langle n_i n_j\rangle\rangle_\Psi}{\sqrt{\langle\langle n_i^2\rangle\rangle_\Psi \langle\langle n_j^2\rangle\rangle_\Psi}} \in [-1,+1]}$$

► Many-body Hamiltonian

General expression of a Hamiltonian with **1-body terms** (kinetic energies of individual particles + potential energies in an external potential field) and **2-particle interactions**:

$$\hat{H} = \sum_{i,i'} \varepsilon_{ii'}\,\hat{c}_i^\dagger\hat{c}_{i'} + \frac{1}{2}\sum_{\substack{i,i'\\ j,j'}} \nu_{iji'j'}\,\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_{j'}\hat{c}_{i'}$$

where $\varepsilon_{ii'} = \langle\phi_i|\hat{T}|\phi_{i'}\rangle$ and $\nu_{iji'j'} = \langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle$ are matrix elements in the space of *distinguishable* particles. The 3-particle and higher interactions can also be included by the respective n-body expressions.

► Coordinate form of Hamiltonian

If the many-body Hamiltonian is expressed in terms of coordinates $\hat{\vec{x}}_k$ and spin projections $\hat{s}_{zk}$ of individual particles (k=1,...N), it is useful to utilize the coordinate form of creation & annihilation operators.

$$\hat{H} = \underbrace{\sum_{k=1}^{N}\overbrace{\left(-\tfrac{\hbar^2}{2M}\Delta_k\right)}^{(\hat{T})_k}}_{\text{kinetic term } \hat{O}^{(1)}_{\text{kin}}} + \underbrace{\sum_{k=1}^{N}\overbrace{U(\hat{\vec{x}}_k,\hat{s}_{zk})}^{(\hat{U})_k}}_{\text{external potential } \hat{O}^{(1)}_{\text{pot}}} + \underbrace{\sum_{\substack{k\\ l>k}\}=1}^{N}\overbrace{V(\hat{\vec{x}}_k,\hat{s}_{zk};\hat{\vec{x}}_l,\hat{s}_{zl})}^{(\hat{V})_{kl}}}_{\text{interaction } \hat{O}^{(2)}_{\text{int}}}$$

$$\hat{O}^{(1)}_{\text{kin}} + \hat{O}^{(1)}_{\text{pot}} = \sum_{i,i'}\langle\phi_i|(\hat{T}+\hat{U})|\phi_{i'}\rangle\hat{c}_i^\dagger\hat{c}_{i'}$$

$$= \sum_{i,i'}\left\{\sum_{m_s}\int \phi_i^*(\vec{x},m_s)\left[-\tfrac{\hbar^2}{2M}\Delta + U(\vec{x},m_s)\right]\phi_{i'}(\vec{x},m_s)d\vec{x}\right\}\hat{c}_i^\dagger\hat{c}_{i'}$$

$$= \sum_{m_s}\int \underbrace{\left[\sum_i \phi_i^*(\vec{x},m_s)\hat{c}_i^\dagger\right]}_{\hat{\psi}^\dagger_\pm(\vec{x},m_s)}\left[-\tfrac{\hbar^2}{2M}\Delta + U(\vec{x},m_s)\right]\underbrace{\left[\sum_{i'}\phi_{i'}(\vec{x},m_s)\hat{c}_{i'}\right]}_{\hat{\psi}_\pm(\vec{x},m_s)}d\vec{x}$$

$$\hat{O}^{(2)}_{\rm int} = \tfrac{1}{2}\sum_{i,i',j,j'} \langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle \hat{c}^\dagger_i\hat{c}^\dagger_j\hat{c}_{j'}\hat{c}_{i'} = \tfrac{1}{2}\times$$

$$\sum_{\substack{i,i'\\ j,j'}}\left\{\sum_{\substack{m_s\\ m'_s}}\iint \phi^*_i(\vec{x},m_s)\phi^*_j(\vec{x}',m'_s)V(\vec{x},m_s;\vec{x},'\,m'_s)\phi_{i'}(\vec{x},m_s)\phi_{j'}(\vec{x}',m'_s)d\vec{x}d\vec{x}'\right\}\hat{c}^\dagger_i\hat{c}^\dagger_j\hat{c}_{j'}\hat{c}_{i'}$$

$$= \tfrac{1}{2}\sum_{\substack{m_s\\ m'_s}}\iint \hat{\psi}^\dagger_\pm(\vec{x},m_s)\hat{\psi}^\dagger_\pm(\vec{x}',m'_s)V(\vec{x},m_s;\vec{x}',m'_s)\hat{\psi}_\pm(\vec{x}',m'_s)\hat{\psi}_\pm(\vec{x},m_s)d\vec{x}d\vec{x}'$$

The final expression is of the **field-theory type**:

$$\hat{H} = \sum_{m_s}\int \hat{\psi}^\dagger_\pm(\vec{x},m_s)\big[-\tfrac{\hbar^2}{2M}\Delta + U(\vec{x},m_s)\big]\hat{\psi}_\pm(\vec{x},m_s)\;d\vec{x}$$
$$+\tfrac{1}{2}\sum_{\substack{m_s\\ m'_s}}\iint \hat{\psi}^\dagger_\pm(\vec{x},m_s)\hat{\psi}^\dagger_\pm(\vec{x}',m'_s)V(\vec{x},m_s;\vec{x}',m'_s)\hat{\psi}_\pm(\vec{x}',m'_s)\hat{\psi}_\pm(\vec{x},m_s)\;d\vec{x}\,d\vec{x}'$$

■ Quantization of electromagnetic field

The above-described formalism of the second quantization will now be applied in a concrete task to quantize the electromagnetic field. We know that electromagnetic quanta — the photons — have spin $s=1$, so they are bosons. The quantized elmg. field enables one to describe all processes connected with the electromagnetic interaction of matter, including, e.g., spontaneous decays of many-body systems accompanied by the emission of photons.

▸ Photon creation/annihilation operators

The general solution of the wave equation $\vec{\nabla}^2\vec{A} - \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = 0$ for the elmg. vector potential $\vec{A}(\vec{x},t)$ in vacuum ($c=\frac{1}{\sqrt{\epsilon_0\mu_0}}$) is a superposition of planar waves:

$$\vec{A}(\vec{x},t) = \sum_{\nu=\pm}\int \mathcal{N}_{Vk}\left\{\underbrace{\alpha_{\vec{k}\nu}}_{\mapsto\ \hat{b}_{\vec{k}\nu}}\ \vec{e}_{\vec{k}\nu}e^{+i(\vec{k}\cdot\vec{x}-\omega_k t)} + \underbrace{\alpha^*_{\vec{k}\nu}}_{\mapsto\ \hat{b}^\dagger_{\vec{k}\nu}}\ \vec{e}^{\,*}_{\vec{k}\nu}e^{-i(\vec{k}\cdot\vec{x}-\omega_k t)}\right\}d\vec{k}$$

with $\omega_k = c|\vec{k}|$ and:

(a) $\mathcal{N}_{Vk} \equiv$ a scaling factor for each mode which will be determined later

(b) $\boxed{\vec{e}_{\vec{k}\pm} = \mp\frac{1}{\sqrt{2}}\left[\vec{e}_{\vec{k}x} \pm i\vec{e}_{\vec{k}y}\right]} \equiv$ **circular polarization** vectors composed of unit vectors of linear polarization satisfying the Coulomb gauge condition: $\vec{e}_{\vec{k}x}\cdot\vec{k} = 0 = \vec{e}_{\vec{k}y}\cdot\vec{k} \;\Rightarrow\; \boxed{\vec{e}^{\,*}_{\vec{k}\nu}\cdot\vec{e}_{\vec{k}\nu'} = \delta_{\nu\nu'}}$

(c) $\alpha_{\vec{k}\nu} \equiv$ arbitrary coefficients

Field quantization:

The field function $\vec{A}(\vec{x},t)\in\mathbb{R}^3$ becomes a quantum observable described by a selfadjoint vector operator $\hat{\vec{A}}(\vec{x},t) = \hat{\vec{A}}^\dagger(\vec{x},t) \;\Rightarrow$ We work in the **Heisenberg picture** $\Rightarrow \hat{\vec{A}}$ is time-dependent.

$$\begin{array}{rcl}\alpha_{\vec{k}\nu} & \mapsto & \hat{b}_{\vec{k}\nu}\\ \alpha^*_{\vec{k}\nu} & \mapsto & \hat{b}^\dagger_{\vec{k}\nu}\end{array}$$

Operators $\hat{b}^\dagger_{\vec{k}\nu}$ and $\hat{b}_{\vec{k}\nu}$, respectively, create and annihilate **photons** with **momentum** $\vec{p}_\gamma = \hbar\vec{k}$ and **spin projection** $s_{\vec{k}} = \nu\hbar = \pm\hbar$ to the flight direction $\vec{k}/k$:

$$\hat{b}^\dagger_{\vec{k}\nu}|0\rangle_\gamma = |\vec{k}\nu\rangle_\gamma$$
$$\hat{b}_{\vec{k}\nu}|\vec{k}\nu\rangle_\gamma = |0\rangle_\gamma$$

The reasoning of this statement follows from evaluation of the total field energy:

► **Energy of the electromagnetic field**

Classical expression for energy: $\mathcal{E} = \frac{1}{2}\int\limits_V \left[\epsilon_0 |\overbrace{\vec{E}(\vec{x},t)}^{-\frac{\partial\vec{A}}{\partial t}}|^2 + \mu_0^{-1}|\overbrace{\vec{B}(\vec{x},t)}^{\vec{\nabla}\times\vec{A}}|^2\right] d\vec{x}$

$$-\tfrac{\partial}{\partial t}\vec{A} = \sum_{\nu=\pm}\int \mathcal{N}_{Vk}\left\{ i\alpha_{\vec{k}\nu}\omega_k\vec{e}_{\vec{k}\nu}e^{+i(\vec{k}\cdot\vec{x}-\omega_k t)} - i\alpha^*_{\vec{k}\nu}\omega_k\vec{e}^{\,*}_{\vec{k}\nu}e^{-i(\vec{k}\cdot\vec{x}-\omega_k t)}\right\} d\vec{k}$$

$$c[\vec{\nabla}\times\vec{A}] = \sum_{\nu=\pm}\int \mathcal{N}_{Vk}\left\{ i\alpha_{\vec{k}\nu}\overbrace{[c\vec{k}\times\vec{e}_{\vec{k}\nu}]}^{i\nu\omega_k\vec{e}_{\vec{k}\nu}}e^{+i(\vec{k}\cdot\vec{x}-\omega_k t)} - i\alpha^*_{\vec{k}\nu}\overbrace{[c\vec{k}\times\vec{e}^{\,*}_{\vec{k}\nu}]}^{-i\nu\omega_k\vec{e}^{\,*}_{\vec{k}\nu}}e^{-i(\vec{k}\cdot\vec{x}-\omega_k t)}\right\} d\vec{k}$$

For $V\to\infty$ the spatial integration yields: $\int\limits_V e^{i(\vec{k}\pm\vec{k}')\cdot\vec{x}}d\vec{x} \approx V\delta_{\vec{k},\mp\vec{k}'}$

The resulting expression for energy: $\mathcal{E} = V\epsilon_0\sum\limits_\nu\int(\mathcal{N}_{Vk}\omega_k)^2\left(\alpha^*_{\vec{k}\nu}\alpha_{\vec{k}\nu} + \alpha_{\vec{k}\nu}\alpha^*_{\vec{k}\nu}\right)d\vec{k}$

This after the quantization, with the choice of $\mathcal{N}_{Vk} = \sqrt{\frac{\hbar}{2V\epsilon_0\omega_k}}$, leads to:

$$\hat{\mathcal{E}} = \sum_{\nu=\pm}\int \hbar\omega_k\left(\hat{b}^\dagger_{\vec{k}\nu}\hat{b}_{\vec{k}\nu} + \tfrac{1}{2}\right)d\vec{k}$$

Hamiltonian of a system of independent harmonic oscillators, each of them associated with a single field mode $\vec{k}\nu$

So the free electromagnetic field is equivalent to **an infinite (continuous) system of independent (uncoupled) harmonic oscillators!** Photons with a given momentum $\hbar\vec{k}$ and polarization ν are quanta ("phonons") of the oscillator associated with the corresponding mode.

Note: The energy term associated with zero-point motion yields diverging contribution and must be removed (this is a mere shift of the energy axis).

► **Photon emission & absorption**

In Sec. 11, we outlined the theory of transitions stimulated by classical elmg. waves in systems of charged particles. Now this theory can be extended to describe interactions of matter with general, also *non-classical* field states.

Example: Any field state $|\Psi_\gamma\rangle$ with a definite photon number N_γ is non-classical. Indeed, any such state yields *vanishing averages* of field intensities: $\langle\Psi_\gamma|\hat{\vec{E}}(\vec{x},t)|\Psi_\gamma\rangle = 0 = \langle\Psi_\gamma|\hat{\vec{B}}(\vec{x},t)|\Psi_\gamma\rangle$ (both $\hat{\vec{E}}$ & $\hat{\vec{B}}$ are composed of terms containing a single operator $\hat{b}^\dagger_{\vec{k}\nu}$ or $\hat{b}_{\vec{k}\nu}$ ⇒ change of N_γ on one side of the scalar product). However, the dispersions of the field intensities in $|\Psi_\gamma\rangle$ are nonzero.

In particular, such general theory applies to the processes of single-photon absorption and spontaneous single-photon emission.

Consider a system composed of N particles with charges q_k and masses M_k. The **matter-field interaction Hamiltonian** (cf. Sec. 11):

$$\hat{H}'(t) = -\sum_{k=1}^{N} \tfrac{q_k}{M_k} \big[\hat{\vec{A}}(\hat{\vec{x}}_k, t) \cdot \hat{\vec{p}}_k \big]$$

where $\hat{\vec{A}}(\hat{\vec{x}}_k, t)$ is taken from the above general expression with the $\left\{ \begin{smallmatrix} \alpha_{\vec{k}\nu} \mapsto \hat{b}_{\vec{k}\nu} \\ \alpha^*_{\vec{k}\nu} \mapsto \hat{b}^\dagger_{\vec{k}\nu} \end{smallmatrix} \right\}$ substitutions

The Hilbert space is $\mathcal{H} = \mathcal{H}_\mathrm{a} \otimes \mathcal{H}_\gamma$. The atom/nucleus space $\mathcal{H}_\mathrm{a}$ is spanned by energy eigenstates $|E_{0i}\rangle_\mathrm{a}$. The full Fock space of photons $\mathcal{H}_\gamma = \bigoplus_{N_\gamma=1}^{\infty} \mathcal{H}_\gamma^{(N_\gamma)}$ can be reduced (for the single-photon processes) just to the segment $\mathcal{H}_\gamma^{(0)} \oplus \mathcal{H}_\gamma^{(1)}$ spanned by vectors $|0\rangle_\gamma$ and $\{|\vec{k}\nu\rangle_\gamma\}$. Transition probabilities for photon absorptions & emissions are calculated with the aid of the Fermi golden rule:

Process	Initial state $\lvert\psi_{0i}\rangle$		Final state $\lvert\psi_{0j}\rangle$	Active term in $\hat{H}'(t)$
emission	$\lvert E_{0i}\rangle_\mathrm{a} \lvert 0\rangle_\gamma$	$\longrightarrow$	$\lvert E_{0j}\rangle_\mathrm{a} \lvert\vec{k}\nu\rangle_\gamma$	one with $\hat{b}^\dagger_{\vec{k}\nu}$
absorption	$\lvert E_{0i}\rangle_\mathrm{a} \lvert\vec{k}\nu\rangle_\gamma$	$\longrightarrow$	$\lvert E_{0j}\rangle_\mathrm{a} \lvert 0\rangle_\gamma$	one with $\hat{b}_{\vec{k}\nu}$

From this point on, the calculation of transition amplitudes is rather analogous to that presented in Sec. 11 (using either just the dipole approximation or the whole multipole expansion). For spontaneous emissions, the density of final states must include also the state density $\varrho_\gamma(E_\gamma)$ of the emitted photon. This is calculated as the energy derivative of the number of elmg. modes in a box of volume $V \to \infty$ (cf. Sec. 12). Details can be found in many textbooks.

◀ Historical remark

1927: Paul Dirac shows the equivalence of an ensemble of non-interacting bosons with indefinite particle number (elmg. field) with a system of harmonic oscillators (the use of occupation-number representation & creation/annihilation operators)
1928: Pascual Jordan & Eugene Wigner generalize Dirac's results to fermions (the use of anticommutators) & ensembles of interacting particles
1932: Vladimir Fock introduces the Hilbert space for q. fields/ many-body systems
1939,40: Markus Fierz and Wolfgang Pauli formulate the spin-statistics theorem
1950: G.-C. Wick provides a method for evaluating products of creat./annih. opers.

15. MANY-BODY TECHNIQUES

We are ready now to apply the above-derived general formalism in some sophisticated approximation methods, which are extremely useful for the description of various quantum many-body systems — atomic nuclei, atoms, molecules, molecular aggregates and nanoscale metal clusters, quantum dots etc..

■ Fermionic mean field & Hartree-Fock method

All elementary constituents (bosonic and/or fermionic particles) of a typical bound many-body system interact with each other. This usually makes the exact solution of such systems very difficult, practically intractable. However,

this difficult problem can be often effectively approximated — at least as far as the system's *ground-state* properties are considered — by solving a much simpler problem of individual particles moving in a *single-particle mean field*. For any selected particle of the system, the mean field expresses the influence of all the other particles averaged over their quantum-mechanical distribution in space. We first treat the essence of the mean-field method in systems composed of fermions, e.g., in electron shells of atoms or in atomic nuclei.

▶ Hartree-Fock ansatz for the ground-state wavefunction

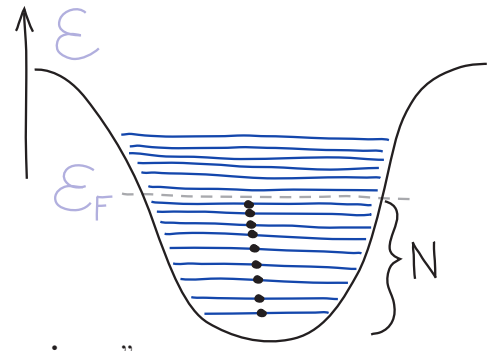
Fermionic **Hamiltonian** with **one + two body** terms written in an arbitrary basis:

$$\hat{H} = \sum_{k,k'} \varepsilon_{kk'} \hat{a}_k^\dagger \hat{a}_{k'} + \tfrac{1}{2} \sum_{\substack{k,k' \\ l,l'}} \nu_{klk'l'} \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_{l'} \hat{a}_{k'}$$

The ground state of an N-particle system is searched as the **Slater-determinant** type of the wavefunction

$$|\Psi_{\rm HF}\rangle = \hat{a}_N^\dagger \cdots \hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle$$

where $\hat{a}_N^\dagger, \ldots, \hat{a}_2^\dagger, \hat{a}_1^\dagger$ create some orthonormal single-particle states interpreted as the lowest eigenstates of an unknown **one-body Hamiltonian = mean field**



⇒ the ground state can be seen as the "**Fermi sea**" (N lowest levels of the mean-field Hamiltonian occupied, higher levels empty)

▶ Variation of the HF state

The unknown mean-field states $|\phi_i\rangle = \hat{a}_i^\dagger|0\rangle$ entering into $|\Psi_{\rm HF}\rangle$ will be determined by the **stationary variational method**:

Infinitesimal unitary variation $|\phi_i\rangle \mapsto |\phi_i\rangle + |\delta\phi_i\rangle$

$$|\phi_i\rangle \mapsto \underbrace{\sum_j u_{ij}|\phi_j\rangle}_{e^{i\hat{\epsilon}}|\phi_i\rangle} \approx |\phi_i\rangle + \underbrace{i\sum_j \epsilon_{ij}|\phi_j\rangle}_{|\delta\phi_i\rangle} \quad \Rightarrow \quad \hat{a}_i^\dagger \mapsto \hat{a}_i^\dagger + \underbrace{i\sum_j \epsilon_{ij}\hat{a}_j^\dagger}_{\delta\hat{a}_i^\dagger} \qquad \epsilon_{ij} = \epsilon_{ji}^*$$

$$|\Psi_{\rm HF}\rangle = \hat{a}_N^\dagger \cdots \hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle \quad \mapsto \quad \left(\hat{a}_N^\dagger + \delta\hat{a}_N^\dagger\right) \cdots \left(\hat{a}_2^\dagger + \delta\hat{a}_2^\dagger\right) \left(\hat{a}_1^\dagger + \delta\hat{a}_1^\dagger\right) |0\rangle$$

$$\approx |\Psi_{\rm HF}\rangle + (\underbrace{\delta\hat{a}_N^\dagger}_{i\sum_j \epsilon_{Nj}\hat{a}_j^\dagger} \cdots \hat{a}_2^\dagger \hat{a}_1^\dagger)|0\rangle + \cdots\cdots + (\hat{a}_N^\dagger \cdots \underbrace{\delta\hat{a}_2^\dagger}_{i\sum_j \epsilon_{2j}\hat{a}_j^\dagger} \hat{a}_1^\dagger)|0\rangle + (\hat{a}_N^\dagger \cdots \hat{a}_2^\dagger \underbrace{\delta\hat{a}_1^\dagger}_{i\sum_j \epsilon_{1j}\hat{a}_j^\dagger})|0\rangle$$

Ket variation:

$$|\Psi_{\rm HF}\rangle \mapsto |\Psi_{\rm HF}\rangle + \underbrace{i\sum_{i=1}^{N}\sum_{j=N+1}^{\infty} \epsilon_{ij}\hat{a}_j^\dagger \hat{a}_i |\Psi_{\rm HF}\rangle}_{|\delta\Psi_{\rm HF}\rangle}$$

Bra variation (independent coefficients $\epsilon'_{ij} = \epsilon'^*_{ji}$):

$$\langle\Psi'_{\rm HF}| \mapsto \langle\Psi_{\rm HF}| - \underbrace{i\sum_{i=1}^{N}\sum_{j=N+1}^{\infty} \epsilon'_{ji}\langle\Psi_{\rm HF}|\hat{a}_i^\dagger \hat{a}_j}_{\langle\delta\Psi'_{\rm HF}|}$$

▶ Variational condition

The condition for $|\Psi_{\rm HF}\rangle$ reads as follows:

$$\langle\Psi_{\rm HF}|\hat{H}|\delta\Psi_{\rm HF}\rangle+\langle\delta\Psi'_{\rm HF}|\hat{H}|\Psi_{\rm HF}\rangle=i\sum_{i\le N}\sum_{j>N}\langle\Psi_{\rm HF}|\epsilon_{ij}\hat{H}\hat{a}_j^\dagger\hat{a}_i-\epsilon'_{ji}\hat{a}_i^\dagger\hat{a}_j\hat{H}|\Psi_{\rm HF}\rangle\overset{!}{=}0\ \forall\begin{Bmatrix}\epsilon_{ij}\\ \epsilon'_{ji}\end{Bmatrix}$$

$$\Rightarrow\quad\boxed{\langle\Psi_{\rm HF}|\hat{H}\hat{a}_j^\dagger\hat{a}_i|\Psi_{\rm HF}\rangle\overset{!}{=}0\quad\forall\begin{Bmatrix}i\le N\\ j>N\end{Bmatrix}}$$

Assuming without loss of generality that $\hat{H}=\sum_{k,k'}\varepsilon_{kk'}\hat{a}_k^\dagger\hat{a}_{k'}+\frac{1}{2}\sum_{k,k',l,l'}\nu_{klk'l'}\hat{a}_k^\dagger\hat{a}_l^\dagger\hat{a}_{l'}\hat{a}_{k'}$ is written in terms of the creation & annihilation operators of the states involved in the desired state $|\Psi_{\rm HF}\rangle$ we get:

$$\boxed{\left\langle\Psi_{\rm HF}\middle|\left(\sum_{k,k'}\varepsilon_{kk'}\hat{a}_k^\dagger\hat{a}_{k'}+\tfrac{1}{2}\sum_{\substack{k,k'\\l,l'}}\nu_{klk'l'}\hat{a}_k^\dagger\hat{a}_l^\dagger\hat{a}_{l'}\hat{a}_{k'}\right)\hat{a}_j^\dagger\hat{a}_i\middle|\Psi_{\rm HF}\right\rangle=0\quad\forall\begin{Bmatrix}i\le N\\ j>N\end{Bmatrix}}$$

Evaluation of both terms: anticommutation of $\hat{a}_j^\dagger$ or $\hat{a}_i$ to the leftmost position (the resulting matrix element $=0$ since $j>N$ and $i\le N$)

(a) One-body term: $\sum_{k,k'}\varepsilon_{kk'}\langle\Psi_{\rm HF}|\hat{a}_k^\dagger\hat{a}_{k'}\hat{a}_j^\dagger\hat{a}_i|\Psi_{\rm HF}\rangle=$

$$=\sum_{k,k'}\varepsilon_{kk'}\left(\underbrace{\langle\Psi_{\rm HF}|\hat{a}_j^\dagger\hat{a}_k^\dagger\hat{a}_{k'}\hat{a}_i|\Psi_{\rm HF}\rangle}_{0}+\delta_{jk'}\underbrace{\langle\Psi_{\rm HF}|\hat{a}_k^\dagger\hat{a}_i|\Psi_{\rm HF}\rangle}_{\langle\Psi_{\rm HF}|\hat{a}_i\hat{a}_k^\dagger|\Psi_{\rm HF}\rangle+\delta_{ik}\langle\Psi_{\rm HF}|\Psi_{\rm HF}\rangle}\right)=\sum_{k,k'}\varepsilon_{kk'}\delta_{jk'}\delta_{ik}=\varepsilon_{ij}$$

(b) Two-body term: $\frac{1}{2}\sum_{\substack{k,k'\\l,l'}}\nu_{klk'l'}\langle\Psi_{\rm HF}|\hat{a}_k^\dagger\hat{a}_l^\dagger\hat{a}_{l'}\hat{a}_{k'}\hat{a}_j^\dagger\hat{a}_i|\Psi_{\rm HF}\rangle=$

$$=\tfrac{1}{2}\sum_{\substack{k,k'\\l,l'}}\nu_{klk'l'}\Bigg[\delta_{jk'}\delta_{ik}\underbrace{\langle\Psi_{\rm HF}|\hat{a}_l^\dagger\hat{a}_{l'}|\Psi_{\rm HF}\rangle}_{\substack{\delta_{ll'}\text{ for }l\le N\\ 0\text{ for }l,l'>N}}+\delta_{jl'}\delta_{il}\underbrace{\langle\Psi_{\rm HF}|\hat{a}_k^\dagger\hat{a}_{k'}|\Psi_{\rm HF}\rangle}_{\substack{\delta_{kk'}\text{ for }k\le N\\ 0\text{ for }k,k'>N}}$$

$$-\delta_{jk'}\delta_{il}\overbrace{\langle\Psi_{\rm HF}|\hat{a}_k^\dagger\hat{a}_{l'}|\Psi_{\rm HF}\rangle}^{\substack{\delta_{kl'}\text{ for }k\le N\\ 0\text{ for }k,k'>N}}-\delta_{jl'}\delta_{ik}\overbrace{\langle\Psi_{\rm HF}|\hat{a}_l^\dagger\hat{a}_{k'}|\Psi_{\rm HF}\rangle}^{\substack{\delta_{lk'}\text{ for }l\le N\\ 0\text{ for }l,l'>N}}\Bigg]=$$

$$=\tfrac{1}{2}\Bigg[\sum_{k\le N}\underbrace{(\nu_{ikjk}+\nu_{kikj})}_{2\nu_{kikj}}-\sum_{k\le N}\underbrace{(\nu_{ikkj}+\nu_{kijk})}_{2\nu_{ikkj}}\Bigg]=\sum_{k\le N}(\nu_{kikj}-\nu_{ikkj})$$

Together: $\boxed{\boxed{\varepsilon_{ij}+\sum_{k\le N}(\nu_{kikj}-\nu_{ikkj})=0\qquad\forall\begin{Bmatrix}i\le N\\ j>N\end{Bmatrix}}}$

This represents a coupled set of conditions for the Hamiltonian matrix elements in the HF basis which must be satisfied to minimize the energy functional

▶ Mean-field equation

We know that $\varepsilon_{ij}\equiv\langle\phi_i|\hat{T}|\phi_j\rangle$. The above set of equations can be formally solved by introducing another one-body operator $\hat{V}_{\rm HF}$, which is defined through

its matrix elements in the HF basis as follows: $\boxed{\langle\phi_i|\hat{V}_{\rm HF}|\phi_j\rangle \equiv \sum_{k\le N}(\nu_{kikj}-\nu_{ikkj})}$

It represents the **Hartree-Fock mean field**

$\Rightarrow$ The above variational condition reads as: $\langle\phi_i|(\hat{T}+\hat{V}_{\rm HF})|\phi_j\rangle = 0$ for $\left\{\begin{smallmatrix} i\le N \\ j>N\end{smallmatrix}\right.$

This can be replaced by a stronger condition that $(\hat{T}+\hat{V}_{\rm HF})$ is diagonal in the basis $\{|\phi_n\rangle\}$, i.e: $\boxed{\boxed{\big(\hat{T}+\hat{V}_{\rm HF}\big)|\phi_n\rangle = \varepsilon_n|\phi_n\rangle}}$ **one-body eigenvalue equation**

So the state $|\Psi_{\rm HF}\rangle$, which approximates the exact many-body ground state, is determined through eigensolutions of a one-body problem! However, the mean field $\hat{V}_{\rm HF}$ contained in this one-body problem is expressed vis the eigensolutions *that we want to determine*:

$$\hat{V}_{\rm HF}|\phi_n\rangle = \sum_m \langle\phi_m|\hat{V}_{\rm HF}|\phi_n\rangle|\phi_m\rangle = \sum_m \left[\sum_{k\le N}\Big(\langle\phi_k\phi_m|\hat{V}|\phi_k\phi_n\rangle - \langle\phi_m\phi_k|\hat{V}|\phi_k\phi_n\rangle\Big)\right]|\phi_m\rangle$$

$\Rightarrow$ **selfconsistent problem**

The solution can be searched in an **iterative procedure**: an initial "randomly selected" basis $\{|\phi_n^{(0)}\rangle\}$ $\Rightarrow$ $0^{\rm th}$order mean field $\hat{V}_{\rm HF}^{(0)}$ $\Rightarrow$ new basis $\{|\phi_n^{(1)}\rangle\}$ $\Rightarrow$ $1^{\rm st}$order mean field $\hat{V}_{\rm HF}^{(1)}$ $\Rightarrow$ new basis $\{|\phi_n^{(2)}\rangle\}$ $\Rightarrow$ $2^{\rm nd}$order mean field $\hat{V}_{\rm HF}^{(2)}$ $\Rightarrow$ .....

One may hope in a fast convergence (facilitated by a good choice of $\{|\phi_n^{(0)}\rangle\}$).

▶ Coordinate representation of the mean field

Meaning of the above-defined mean field operator becomes more intuitive in the coordinate representation. The action of $\hat{V}_{\rm HF}$ on the HF single-particle basis read as: $\hat{V}_{\rm HF}\,\phi_n(\vec{x},\mu) =$ (two-body interaction)

$$\sum_m\Big[\sum_{k\le N}\sum_{\mu_1\mu_2}\iint\phi_k^*(\vec{x}_1,\mu_1)\phi_m^*(\vec{x}_2,\mu_2)\overbrace{V(\vec{x}_1,\vec{x}_2)}\,\phi_k(\vec{x}_1,\mu_1)\phi_n(\vec{x}_2,\mu_2)d\vec{x}_1d\vec{x}_2\Big]\phi_m(\vec{x},\mu)$$

$$-\sum_m\Big[\sum_{k\le N}\sum_{\mu_1\mu_2}\iint\phi_m^*(\vec{x}_1,\mu_1)\phi_k^*(\vec{x}_2,\mu_2)V(\vec{x}_1,\vec{x}_2)\phi_k(\vec{x}_1,\mu_1)\phi_n(\vec{x}_2,\mu_2)d\vec{x}_1d\vec{x}_2\Big]\phi_m(\vec{x},\mu)$$

Using $\sum_m \phi_m^*(\vec{x}_\bullet,\mu_\bullet)\phi_m(\vec{x},\mu) = \delta(\vec{x}_\bullet-\vec{x})\delta_{\mu_\bullet\mu}$ (with $\bullet$=1,2) we obtain:

$$\hat{V}_{\rm HF}\,\phi_n(\vec{x},\mu) = \underbrace{\left[\int\sum_{k\le N}\sum_{\mu_1}|\phi_k(\vec{x}_1,\mu_1)|^2V(\vec{x}_1,\vec{x})d\vec{x}_1\right]}_{V_{\rm HF}(\vec{x})\ \textbf{local potential}}\phi_n(\vec{x},\mu) \quad + \quad \overbrace{\int\sum_{\mu_2}\underbrace{\left[\sum_{k\le N}\phi_k^*(\vec{x}_2,\mu_2)V(\vec{x},\vec{x}_2)\phi_k(\vec{x},\mu)\right]}_{W_{\rm HF}(\vec{x},\mu,\vec{x}_2,\mu_2)\ \text{transformation kernel}}\phi_n(\vec{x}_2,\mu_2)d\vec{x}_2}^{\textbf{nonlocal potential}\ \int\sum_{\mu_2}W_{\rm HF}(\vec{x},\mu,\vec{x}_2,\mu_2)\phi_n(\vec{x}_2,\mu_2)d\vec{x}_2}$$

The local mean-field potential $V_{\rm HF}(\vec{x})$ is given by averaging of the two-body potential $V(\vec{x}_1,\vec{x})$ at position $\vec{x}$ over a cloud of all constituent particles with spatial density $\varrho(\vec{x}_1) = \sum_{k\le N}\sum_{\mu_1}|\phi_k(\vec{x}_1,\mu_1)|^2$.

The nonlocal, so-called **exchange term** with the kernel $W_{\rm HF}(\vec{x},\mu,\vec{x}_2,\mu_2)$ results from the antisymmetrization of two-body wavefunctions.

▶ Ground-state energy

From the HF wavefunction obtained from a converged mean-field procedure we estimate the ground-state energy as:

$$E_0 \approx \langle \Psi_{\rm HF}|\hat{H}|\Psi_{\rm HF}\rangle = \cdots\cdots = \sum_{k\le N} \varepsilon_{kk} + \tfrac{1}{2}\sum_{k\le N}\sum_{l\le N}(\nu_{klkl} - \nu_{lkkl})$$

However, summation of single-particle energies of the occupied mean-field states yields a different value:

$$\sum_{k\le N}\varepsilon_k = \sum_{k\le N}\langle\phi_k|(\hat{T}+\hat{V}_{\rm HF})|\phi_k\rangle = \sum_{k\le N}\varepsilon_{kk} + \sum_{k\le N}\sum_{l\le N}(\nu_{klkl}-\nu_{lkkl})$$

Comparison of the above expressions:

$$\boxed{E_0 \approx \sum_{k\le N}\Big[\varepsilon_k - \underbrace{\tfrac{1}{2}\sum_{l\le N}(\nu_{klkl}-\nu_{lkkl})}_{\langle\phi_k|\hat{V}_{\rm HF}|\phi_k\rangle}\Big]}$$

The correction $\Delta\varepsilon_k = \frac{1}{2}\langle\phi_k|\hat{V}_{\rm HF}|\phi_k\rangle$ of energy ε_k, present in the last formula, compensates the double counting of particle interaction energies (e.g., the sum $\varepsilon_1+\varepsilon_2$ contains all interaction between particles $1\leftrightarrow k$ and $2\leftrightarrow k$, so the term $1\leftrightarrow 2 = 2\leftrightarrow 1$ is counted twice)

◀ Historical remark

1927: D.R. Hartree introduces a self-consistent method to solve many-body Sch. eq.
1930: V. Fock and J.C. Slater modify the Hartree method to respect antisymmetry
1935: D.R. Hartree reformulates the method in a way suitable for computations

■ Bosonic condensates & Hartree-Bose method

The Hartree-Fock method has its bosonic counterpart, called after Hartree and Bose. It relies on the same principle, but is much simpler technically since bosons do not obey the Pauli exclusion law. So in the mean-field approximation, the ground state is formed by all constituent bosons sitting in the same state.

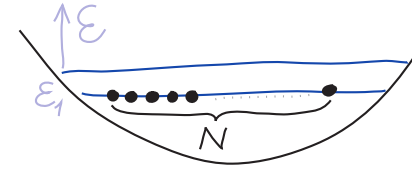
▶ Bosonic condensate

Bosonic Hamiltonian with one + two body terms:

$$\boxed{\hat{H} = \sum_{k,k'}\varepsilon_{kk'}\hat{b}_k^\dagger\hat{b}_{k'} + \tfrac{1}{2}\sum_{\substack{k,k'\\l,l'}}\nu_{klk'l'}\hat{b}_k^\dagger\hat{b}_l^\dagger\hat{b}_{l'}\hat{b}_{k'}}$$

Ground state of the N-particle system searched in the form of the **condensate** type of wavefunction: $\boxed{|\Psi_{\rm HB}\rangle = \frac{1}{\sqrt{N!}}(\hat{B}^\dagger)^N|0\rangle}$

with $\boxed{\hat{B}^\dagger \equiv \sum_k \beta_k\hat{b}_k^\dagger}$ creating the boson into a general single-particle state $|\psi_B\rangle = \sum_k \beta_k|\phi_k\rangle$



with unknown coefficients subject to normalization: $\sum_k |\beta_k|^2 = 1$

▶ Energy functional

To perform the variational procedure, we need to express the energy functional $\langle\Psi_{\rm HB}|\hat{H}|\Psi_{\rm HB}\rangle$ as a function of coefficients $\{\beta_k\}$. First we evaluate commutators:

$$\left.\begin{array}{l}\underbrace{[\hat{b}_k,\hat{B}^\dagger]}_{\hat{C}_1}=\beta_k\\ \underbrace{[\hat{b}_k,(\hat{B}^\dagger)^N]}_{\hat{C}_N}=\underbrace{[\hat{b}_k,\hat{B}^\dagger]}_{\beta_k}(\hat{B}^\dagger)^{N-1}+\hat{B}^\dagger\underbrace{[\hat{b}_k,(\hat{B}^\dagger)^{N-1}]}_{\hat{C}_{N-1}}\end{array}\right\}\Rightarrow\left\{\begin{array}{l}[\hat{b}_k,(\hat{B}^\dagger)^N]=N\beta_k(\hat{B}^\dagger)^{N-1}\\ [(\hat{B})^N,\hat{b}_k^\dagger]=N\beta_k^*(\hat{B})^{N-1}\end{array}\right.$$

From these relations we calculate the following averages:

$$\langle\Psi_{\rm HB}|\hat{b}_k^\dagger\hat{b}_{k'}|\Psi_{\rm HB}\rangle=\tfrac{1}{N!}\langle0|(\hat{B})^N\hat{b}_k^\dagger\hat{b}_{k'}(\hat{B}^\dagger)^N|0\rangle=\beta_k^*\beta_{k'}\tfrac{N^2}{N!}\langle0|(\hat{B})^{N-1}(\hat{B}^\dagger)^{N-1}|0\rangle$$
$$=N\beta_k^*\beta_{k'}$$
$$\langle\Psi_{\rm HB}|\hat{b}_k^\dagger\hat{b}_l^\dagger\hat{b}_{l'}\hat{b}_{k'}|\Psi_{\rm HB}\rangle=\tfrac{1}{N!}\langle0|(\hat{B})^N\hat{b}_k^\dagger\hat{b}_l^\dagger\hat{b}_{l'}\hat{b}_{k'}(\hat{B}^\dagger)^N|0\rangle$$
$$=\beta_k^*\beta_{k'}\tfrac{N^2}{N!}\langle0|(\hat{B})^{N-1}\hat{b}_l^\dagger\hat{b}_{l'}(\hat{B}^\dagger)^{N-1}|0\rangle=N(N{-}1)\beta_k^*\beta_l^*\beta_{k'}\beta_{l'}$$

The energy average (energy functional) in the space of condensate states:

$$\boxed{\langle\Psi_{\rm HB}|\hat{H}|\Psi_{\rm HB}\rangle=N\sum_{k,k'}\varepsilon_{kk'}\beta_k^*\beta_{k'}+\tfrac{N(N-1)}{2}\sum_{\substack{k,k'\\l,l'}}\nu_{klk'l'}\beta_k^*\beta_l^*\beta_{k'}\beta_{l'}\equiv\mathcal{E}(\{\beta_k\})}$$

To find parameters $\{\beta_k\}$ of the condensate state, the function $\mathcal{E}(\{\beta_k\})$ must be **minimized**, respecting the normalization condition $\sum_k|\beta_k|^2=1$.

Alternatively, one can skip the normalization constraint and minimize the expression: $\tilde{\mathcal{E}}(\{\beta\})=\dfrac{\langle\Psi_{\rm HB}|\hat{H}|\Psi_{\rm HB}\rangle}{\langle\Psi_{\rm HB}|\Psi_{\rm HB}\rangle}$

◀ Historical remark

1924-5: A. Einsten & S.N. Bose predict that systems of bosons at $T\to0$ form a condensate state with unusual properties (the first laboratory preparation in 1995)
1938: F. London relates boson condensation to **superfluidity** of some liquids

■ Pairing & BCS method

The Hartree-Fock method does not work well for the fermionic systems whose valence shell (or valence band) of single-particle states is filled up approximately to the middle. Indeed, the existence of a number of partly occupied valence orbits with nearly degenerate spectrum makes the HF method unstable (it has many almost equivalent solutions). In this situation, an attractive short-range type of interaction produces a new effect beyond the mean field — pairing of particles in conjugate states related by the time reversal. It turns out that at low temperatures, the systems with pairing exhibit **superconductivity**, a phenomenon partly analogous to the superfluidity of some Bose systems. The basic many-body theory which takes the fermionic pairing into account is abbreviated after its inventors Bardeen, Cooper, and Schrieffer.

▶ Pairing interaction

Consider a short-range (approximately contact) interaction given by:

$$\boxed{V(\vec{x}_1-\vec{x}_2)\approx -V_0\,\delta(\vec{x}_1-\vec{x}_2)}$$

Matrix element $\langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle \approx$

$$-V_0\sum_{\mu_1,\mu_2}\iint \phi_i^*(\vec{x}_1,\mu_1)\phi_j^*(\vec{x}_2,\mu_2)\delta(\vec{x}_1-\vec{x}_2)\phi_{i'}(\vec{x}_1,\mu_1)\phi_{j'}(\vec{x}_2,\mu_2)\,d\vec{x}_1 d\vec{x}_2$$
$$= -V_0\int\Big[\sum_{\mu_1}\phi_i^*(\vec{x},\mu_1)\phi_{i'}(\vec{x},\mu_1)\Big]\Big[\sum_{\mu_2}\phi_j^*(\vec{x},\mu_2)\phi_{j'}(\vec{x},\mu_2)\Big]d\vec{x}$$

Assuming that:

$$\left.\begin{aligned}\phi_i(\vec{x},\mu)=\phi_j^*(\vec{x},-\mu)\equiv\hat{\mathcal{T}}\phi_j(\vec{x},\mu)\\ \phi_{i'}(\vec{x},\mu)=\phi_{j'}^*(\vec{x},-\mu)\equiv\hat{\mathcal{T}}\phi_{j'}(\vec{x},\mu)\end{aligned}\right\}\Rightarrow\begin{cases}\langle\phi_i\phi_j|\hat{V}|\phi_{i'}\phi_{j'}\rangle\approx\\ \quad -V_0\int\big|\sum_{\mu}\phi_i^*(\vec{x},\mu)\phi_{i'}(\vec{x},\mu)\big|^2 d\vec{x}\\ \text{we get large attractive interaction}\end{cases}$$

We may approximate this situation by assuming that $\hat{V}$ acts *only* between pairs of states $\boxed{\underbrace{|\phi_k\rangle}_{\hat{a}_k^\dagger|0\rangle}\leftrightarrow\underbrace{|\phi_{\bar{k}}\rangle}_{\hat{a}_{\bar{k}}^\dagger|0\rangle}\equiv\hat{\mathcal{T}}|\phi_k\rangle}$ related by the **time reversal** transformation $\hat{\mathcal{T}}$

Examples of such states are:

$|+\vec{p},\uparrow\rangle \leftrightarrow |-\vec{p},\downarrow\rangle$ quasimomentum-spin electron states in metals

$|n,l,j,+m_j\rangle \leftrightarrow |n,l,j,-m_j\rangle$ angular-momentum nucleon states in nuclei

▶ Simplified Hamiltonian

For fermionic systems possessing the time-reversal symmetry the so-called **Kramers theorem** asserts that the Hamiltonian eigenstates $|E_i\rangle$ and $\hat{\mathcal{T}}|E_i\rangle$ with half-integer total angular momentum are orthogonal and have the same energy. This must hold also for the one-body mean-field Hamiltonian given by $\hat{H}_{\rm MF}=\hat{T}+\hat{V}_{\rm HF}=\sum_k\varepsilon_k(\hat{a}_k^\dagger\hat{a}_k+\hat{a}_{\bar{k}}^\dagger\hat{a}_{\bar{k}})$. To this Hamiltonian we now add the pairing interaction $\hat{V}_{\rm pair}$. The above approximation yields a so-called **monopole pairing** interaction:

$$\boxed{\hat{V}_{\rm pair}\approx -G\sum_{k,l}{}'\,\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger\hat{a}_l\hat{a}_{\bar{l}}}$$

G ≡ pairing interaction strength

$\sum_{k,l}'$ ≡ sum over the states close to the **Fermi energy** $\varepsilon_{\rm F}$: $\boxed{|\varepsilon_k-\varepsilon_{\rm F}|<S}$

(with $\varepsilon_{\rm F}$ taken now as the *energy of the highest occupied orbital* in $|\Psi_{\rm HB}\rangle$)

This interaction can be expressed with the aid of the following bifermion operators:

$$\boxed{\hat{V}_{\rm pair}\approx -Gn\,\hat{P}^\dagger\hat{P}}$$

$$\boxed{\hat{P}^\dagger\equiv\tfrac{1}{\sqrt{n}}\sum_k{}'\,\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger}\qquad\boxed{\hat{P}\equiv\tfrac{1}{\sqrt{n}}\sum_l{}'\,\hat{a}_l\hat{a}_{\bar{l}}}$$

where $n\equiv$ number of levels ε_k in the $|\varepsilon_k-\varepsilon_{\rm F}|<S$ interval around $\varepsilon_{\rm F}$

If the $k,\bar{k}$ states correspond to $|n,l,j,\pm m_j\rangle$, the $\hat{P}^\dagger$ operator creates a pair with zero total angular momentum (hence the term "monopole")

Boson-like commutator (see Sec. 14): $\big[\hat{P},\hat{P}^\dagger\big]=1-\frac{1}{n}\sum_k{}'\underbrace{\big(\hat{a}_k^\dagger\hat{a}_k+\hat{a}_{\bar{k}}^\dagger\hat{a}_{\bar{k}}\big)}_{\hat{N}_k\in[0,2]}\in[-1,+1]$

The full Hamiltonian then reads as follows:

$$\hat{H} = \underbrace{\sum_k \varepsilon_k(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}})}_{\hat{T}+\hat{V}_{\rm HF}} \underbrace{-G\sum_{k,l}{}' \hat{a}_{\bar{k}}^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_{\bar{l}}}_{\hat{V}_{\rm pair}} = \sum_k \varepsilon_k \hat{n}_k - Gn\,\hat{P}^\dagger \hat{P}$$

► **The BCS approach**

Splitting of the full Hamiltonian into $\begin{cases} \hat{H}_0 = \hat{T}+\hat{V}_{\rm HF}+\hat{V}'_{\rm pair} & \text{(the main part)} \\ \hat{V}''_{\rm pair} & \text{(the rest)} \end{cases}$

$$\hat{H} = \overbrace{E_0 + \underbrace{\sum_k \varepsilon_k(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}})}_{\hat{T}+\hat{V}_{\rm HF}} \underbrace{-\Delta\sum_k{}' (\hat{a}_{\bar{k}}^\dagger \hat{a}_k^\dagger + \hat{a}_k \hat{a}_{\bar{k}})}_{\hat{V}'_{\rm pair}}}^{\hat{H}_0} \overbrace{+\Delta\sum_k{}' (\hat{a}_{\bar{k}}^\dagger \hat{a}_k^\dagger + \hat{a}_k \hat{a}_{\bar{k}}) - G\sum_{k,l}{}' \hat{a}_{\bar{k}}^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_{\bar{l}} - E_0}^{\hat{V}''_{\rm pair}}$$

$[\hat{H},\hat{N}]=0$
$[\hat{H}_0,\hat{N}]\neq 0\neq[\hat{V}''_{\rm pair},\hat{N}]$

Here, Δ is a so far undetermined parameter called **pairing gap** (see below). It is believed that $\hat{V}'_{\rm pair}$ included in $\hat{H}_0$ represents "a larger part" of the full pairing interaction $\hat{V}_{\rm pair}$, while the rest $\hat{V}''_{\rm pair}$ is "small".

The subsequent procedure consists of **2 steps**:
(1) The ground state of $\hat{H}_0$ found analytically ⇒ wavefunction $|\Psi_{\rm BCS}(\Delta)\rangle$
(2) $|\Psi_{\rm BCS}(\Delta)\rangle$ is used as the ansatz wavefunction for the variational procedure using the full Hamiltonian ⇒ minimization of $\mathcal{E}(\Delta) = \langle\Psi_{\rm BCS}(\Delta)|\hat{H}|\Psi_{\rm BCS}(\Delta)\rangle$ determines the value of parameter Δ.

The **idea behind**:
$$\hat{P}^\dagger\hat{P} = \overbrace{\left[\hat{P}^\dagger - \langle\hat{P}^\dagger\rangle_\Psi\right]\left[\hat{P} - \langle\hat{P}\rangle_\Psi\right]}^{\text{small contribution} \to 0} + \overbrace{\langle\hat{P}\rangle_\Psi \hat{P}^\dagger + \langle\hat{P}^\dagger\rangle_\Psi \hat{P}}^{\text{the main part} \to \hat{V}'_{\rm pair}} - \overbrace{\langle\hat{P}^\dagger\rangle_\Psi\langle\hat{P}\rangle_\Psi}^{\text{const.} \to E_0}$$

The gap can be identified with: $\boxed{G\sqrt{n}\langle\hat{P}^\dagger\rangle_\Psi = G\sqrt{n}\langle\hat{P}\rangle_\Psi \approx \Delta}$

► **Bogolyubov transformation** (a toy form)

Spin states $\begin{cases} |\uparrow\rangle \equiv \hat{a}_\uparrow^\dagger|0\rangle \\ |\downarrow\rangle \equiv \hat{a}_\downarrow^\dagger|0\rangle \end{cases}$

quadraticHamiltonian

$$\boxed{\hat{h}_0 = \varepsilon_0 + \varepsilon\left(\hat{a}_\uparrow^\dagger\hat{a}_\uparrow + \hat{a}_\downarrow^\dagger\hat{a}_\downarrow\right) + \delta\hat{a}_\downarrow\hat{a}_\uparrow + \delta\hat{a}_\uparrow^\dagger\hat{a}_\downarrow^\dagger}$$

Eigenproblem of $\hat{h}_0$ in the 3D Hilbert space (spanned by states $|N_a\rangle$ with particle numbers N_a=0,1,2) can be solved analytically via Bogolyubov transform.:

$$\left.\begin{matrix}\hat{a}_\uparrow, \hat{a}_\uparrow^\dagger \\ \hat{a}_\downarrow, \hat{a}_\downarrow^\dagger\end{matrix}\right\} \mapsto \begin{cases} \hat{\alpha}_\uparrow = u\hat{a}_\uparrow + v\hat{a}_\downarrow^\dagger & \hat{\alpha}_\uparrow^\dagger = u\hat{a}_\uparrow^\dagger + v\hat{a}_\downarrow \\ \hat{\alpha}_\downarrow = u\hat{a}_\downarrow - v\hat{a}_\uparrow^\dagger & \hat{\alpha}_\downarrow^\dagger = u\hat{a}_\downarrow^\dagger - v\hat{a}_\uparrow \end{cases} \quad \begin{matrix} u,v \in \mathbb{R} \\ u^2+v^2=1 \end{matrix}$$

particles **quasiparticles**

Quasiparticles are fermions (the transformation is "canonical"):

$$\{\hat\alpha_\uparrow,\hat\alpha_\uparrow\}=\{\hat\alpha_\uparrow^\dagger,\hat\alpha_\uparrow^\dagger\}=\{\hat\alpha_\downarrow,\hat\alpha_\downarrow\}=\{\hat\alpha_\downarrow^\dagger,\hat\alpha_\downarrow^\dagger\}=\{\hat\alpha_\uparrow,\hat\alpha_\downarrow\}=\{\hat\alpha_\uparrow^\dagger,\hat\alpha_\downarrow^\dagger\}=0$$
$$\{\hat\alpha_\uparrow,\hat\alpha_\downarrow^\dagger\}=\{\hat\alpha_\downarrow,\hat\alpha_\uparrow^\dagger\}=0 \qquad \{\hat\alpha_\uparrow,\hat\alpha_\uparrow^\dagger\}=\{\hat\alpha_\downarrow,\hat\alpha_\downarrow^\dagger\}=u^2+v^2=1$$

Coefficients u,v are determined by the required form of Hamiltonian after the transformation, which is:

$$\boxed{\hat h_0 \mapsto \hat h_0' = e_0 + e\underbrace{(\hat\alpha_\uparrow^\dagger\hat\alpha_\uparrow+\hat\alpha_\downarrow^\dagger\hat\alpha_\downarrow)}_{\hat{\mathscr{N}}_\alpha}}$$

This Hamiltonian is solvable: eigensolutions identified with the states having fixed numbers of quasiparticles: $|\mathscr{N}_\alpha\rangle \equiv |0_\alpha\rangle, |1_\alpha\rangle, |2_\alpha\rangle$
The ground state is the quasiparticle vacuum: $|\psi_0\rangle \equiv |0_\alpha\rangle$

Amplitudes u,v & constants e,e_0 (together 4 real variables) obtained from the condition $\hat h_0' = \hat h_0$, yielding together with the normalization constraint 4 real equations:

$$\hat h_0' = \overbrace{e_0+2ev^2}^{=\varepsilon_0} + \overbrace{e\big(u^2-v^2\big)}^{=\varepsilon}(\hat a_\uparrow^\dagger\hat a_\uparrow+\hat a_\downarrow^\dagger\hat a_\downarrow) + \overbrace{euv}^{=\delta}\,\hat a_\downarrow\hat a_\uparrow + \overbrace{euv}^{=\delta}\,\hat a_\uparrow^\dagger\hat a_\downarrow^\dagger = \hat h_0$$

▶ Solving the main part of the pairing Hamiltonian

The part $\hat H_0$ of the total pairing Hamiltonian is quadratic ⇒ solvable
Bogolyubov transformation (the full form):

$$\boxed{\begin{array}{|cc|cc|}\hline \hat\alpha_k=u_k\hat a_k+v_k\hat a_{\bar k}^\dagger & \hat\alpha_k^\dagger=u_k\hat a_k^\dagger+v_k\hat a_{\bar k} & \hat a_k=u_k\hat\alpha_k-v_k\hat\alpha_{\bar k}^\dagger & \hat a_k^\dagger=u_k\hat\alpha_k^\dagger-v_k\hat\alpha_{\bar k} \\ \hat\alpha_{\bar k}=u_k\hat a_{\bar k}-v_k\hat a_k^\dagger & \hat\alpha_{\bar k}^\dagger=u_k\hat a_{\bar k}^\dagger-v_k\hat a_k & \hat a_{\bar k}=u_k\hat\alpha_{\bar k}+v_k\hat\alpha_k^\dagger & \hat a_{\bar k}^\dagger=u_k\hat\alpha_{\bar k}^\dagger+v_k\hat\alpha_k \\ \hline \end{array}}$$

$u_k, v_k \in \mathbb{R}$
$u_k^2+v_k^2=1$

$\{\hat\alpha_k,\hat\alpha_l\}=0=\{\hat\alpha_k^\dagger,\hat\alpha_l^\dagger\}$ $\quad \{\hat\alpha_k,\hat\alpha_l^\dagger\}=\delta_{kl}$
$\{\hat\alpha_{\bar k},\hat\alpha_{\bar l}\}=0=\{\hat\alpha_{\bar k}^\dagger,\hat\alpha_{\bar l}^\dagger\}$ $\quad \{\hat\alpha_{\bar k},\hat\alpha_{\bar l}^\dagger\}=\delta_{kl}$
$\{\hat\alpha_k,\hat\alpha_{\bar l}\}=0=\{\hat\alpha_k^\dagger,\hat\alpha_{\bar l}^\dagger\}$ $\quad \{\hat\alpha_k,\hat\alpha_{\bar l}^\dagger\}=0=\{\hat\alpha_{\bar k},\hat\alpha_l^\dagger\}$

Remarks:
(a) We assume $(u_k,v_k)=(1,0)$ for levels "far from" the Fermi level: $|\varepsilon_k-\varepsilon_{\rm F}|>S$
(b) Instead of $\hat H_0$ we consider $\hat{\mathscr{H}}_0=\hat H_0-\mu\hat N$, where μ will become a Lagrange multiplier for fixing the average particle number (⇒ chemical potential)
The required form of $\hat{\mathscr{H}}_0$ expressed through the quasiparticles reads as:

$$\hat{\mathscr{H}}_0' = \underbrace{2\sum_k\big[(\varepsilon_k-\mu)v_k^2-\Delta u_kv_k\big]}_{E_0} + \Big(\sum_k \underbrace{\big[2(\varepsilon_k-\mu)u_kv_k-\Delta(u_k^2-v_k^2)\big]}_{0}\hat\alpha_{\bar k}^\dagger\hat\alpha_k + \text{H.c.}\Big) + \sum_k \overbrace{\big[(\varepsilon_k-\mu)(u_k^2-v_k^2)+2\Delta u_kv_k\big]}^{e_k}\overbrace{\big(\hat\alpha_k^\dagger\hat\alpha_k+\hat\alpha_{\bar k}^\dagger\hat\alpha_{\bar k}\big)}^{\hat{\mathscr{N}}_k}$$

Solution of the diagonalization condition:

$$2(\varepsilon_k-\mu)u_kv_k-\Delta(u_k^2-v_k^2)=0 \quad\Rightarrow\quad 2(\varepsilon_k-\mu)u_k\sqrt{1-u_k^2}=\Delta(2u_k^2-1) \quad\Rightarrow$$
$$4\big[\Delta^2+(\varepsilon_k-\mu)^2\big]u_k^4-4\big[\Delta^2+(\varepsilon_k-\mu)^2\big]u_k^2+\Delta^2=0$$

$$\boxed{e_k=\sqrt{\Delta^2+(\varepsilon_k-\mu)^2} \qquad u_k^2=\tfrac12\Big[1+\tfrac{\varepsilon_k-\mu}{\sqrt{\Delta^2+(\varepsilon_k-\mu)^2}}\Big] \qquad v_k^2=\tfrac12\Big[1-\tfrac{\varepsilon_k-\mu}{\sqrt{\Delta^2+(\varepsilon_k-\mu)^2}}\Big]}$$

▶ Ground-state wavefunction

The ground state of $\hat{\mathscr{H}}_0' \equiv$ **vacuum of quasiparticles** ($\Rightarrow \mathscr{N}_k = 0$). Written in terms of creation/annihilation operators of the original particles and their vacuum, this state has the following form:

$$\boxed{|\Psi_{\rm BCS}\rangle = \prod_k \left(u_k + v_k \hat{a}_{\bar{k}}^\dagger \hat{a}_k^\dagger\right)|0\rangle}$$

Proof:

$$\hat{\alpha}_l|\Psi_{\rm BCS}\rangle = \overbrace{\left(u_l\hat{a}_l + v_l\hat{a}_{\bar{l}}^\dagger\right)}^{\hat{\alpha}_l}\prod_k \overbrace{\left(u_k + v_k\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger\right)}^{\hat{\beta}_k}|0\rangle = \left\{\left[\hat{\alpha}_l, \prod_k \hat{\beta}_k\right] + \left(\prod_k \hat{\beta}_k\right)\hat{\alpha}_l\right\}|0\rangle =$$

$$\left\{u_l v_l \underbrace{\left[\hat{a}_l, \hat{a}_{\bar{l}}^\dagger \hat{a}_{\bar{l}}^\dagger\right]}_{-\hat{a}_{\bar{l}}^\dagger} \prod_{k\neq l}\left(u_k + v_k\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger\right) + \prod_{k\neq l}\left(u_k + v_k\hat{a}_{\bar{k}}^\dagger\hat{a}_k^\dagger\right)\underbrace{\left(u_l + v_l\hat{a}_{\bar{l}}^\dagger\hat{a}_l^\dagger\right)\left(u_l\hat{a}_l + v_l\hat{a}_{\bar{l}}^\dagger\right)}_{+u_l v_l \hat{a}_{\bar{l}}^\dagger|0\rangle}\right\}|0\rangle$$

$$\Rightarrow \boxed{\hat{\alpha}_l|\Psi_{\rm BCS}\rangle = 0} \quad \text{similarly:} \quad \boxed{\hat{\alpha}_{\bar{l}}|\Psi_{\rm BCS}\rangle = 0}$$

The solution $|\Psi_{\rm BCS}\rangle$ approximates the **superconducting state** at $T = 0$

▶ Interpretation

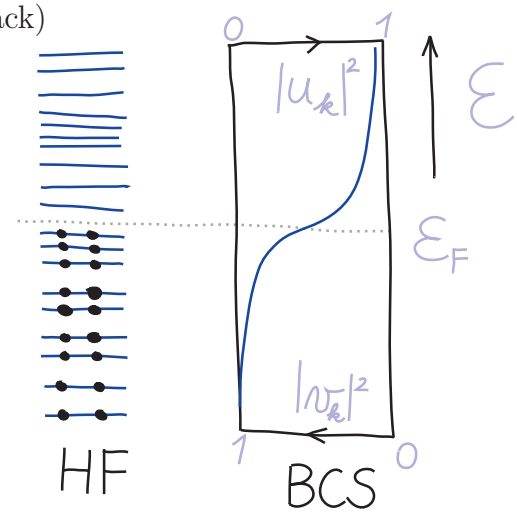
(a) $|\Psi_{\rm BCS}\rangle$ is a state with **undetermined particle number**

(b) The **average** $\boxed{\langle N\rangle_{\rm BCS} = \sum_k \langle\Psi_{\rm BCS}|\underbrace{\left(\hat{a}_k^\dagger\hat{a}_k + \hat{a}_{\bar{k}}^\dagger\hat{a}_{\bar{k}}\right)}_{\hat{n}_k}|\Psi_{\rm BCS}\rangle \stackrel{!}{=} N}$ fixed by μ

(c) The **dispersion** $\langle\!\langle N^2\rangle\!\rangle_{\rm BCS} = \langle N^2\rangle_{\rm BCS} - \langle N\rangle_{\rm BCS}^2$ is beyond the control (for small systems like nuclei this is a drawback)

(d) u_k and v_k represent probability amplitudes for the pair of states $|\phi_k\rangle, |\phi_{\bar{k}}\rangle$ being empty and occupied:

$$\boxed{p_k^{\rm empty} = |u_k|^2 \quad \text{and} \quad p_k^{\rm occup} = |v_k|^2}$$

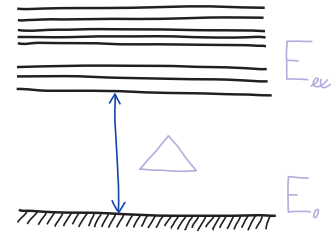


(e) The occupation probability $|v_k|^2$ as a function of ε_k is **smeared** around the value μ. The smearing width $\sim \Delta$. For $\Delta = 0$ we get:

$$|v_k|^2 = 1 - |u_k|^2 = \begin{cases} 1 \text{ for } \varepsilon_k \leq \mu \\ 0 \text{ for } \varepsilon_k > \mu \end{cases}$$

$$\Rightarrow \boxed{\mu \equiv \varepsilon_{\rm F}}$$

(f) Excited states (with $\hat{\mathfrak{n}}_k \geq 1$) have energies $\boxed{E_{\rm exc} \geq {\rm Min}\{e_k\} \geq \Delta}$ $\Rightarrow$ **energy gap** above the ground state in the spectrum is a typical signature of pairing and one of the origins of



the superconducting behavior (the friction is suppressed due to the difficulty to excite the system)

► **Determination of the gap**

(a) Variational approach: $\mathcal{E}'(\Delta) = \langle\Psi_{\rm BCS}(\Delta)|(\hat{H}-\mu\hat{N})|\Psi_{\rm BCS}(\Delta)\rangle =$

$$\underbrace{\langle\Psi_{\rm BCS}|\hat{\mathscr{H}}_0|\Psi_{\rm BCS}\rangle + \Delta\sum_k{}'\langle\Psi_{\rm BCS}|(\hat{a}^\dagger_{\bar{k}}\hat{a}^\dagger_k + \hat{a}_k\hat{a}_{\bar{k}})|\Psi_{\rm BCS}\rangle}_{2\sum_k{}'(\varepsilon_k-\mu)v_k(\Delta)^2} - G\underbrace{\langle\Psi_{\rm BCS}|\sum_{k,l}{}'\hat{a}^\dagger_{\bar{k}}\hat{a}^\dagger_k\hat{a}_l\hat{a}_{\bar{l}}|\Psi_{\rm BCS}\rangle}_{\left[\sum_k{}'u_k(\Delta)v_k(\Delta)\right]^2}$$

Minimization of $\mathcal{E}'(\Delta)$: $\frac{\partial}{\partial\Delta}\{2\sum_k{}'(\varepsilon_k-\mu)v_k(\Delta)^2 - G\big[\sum_k{}'u_k(\Delta)v_k(\Delta)\big]^2\} = 0$

(b) Derivation from **expectation values of pair operators** $\hat{P}$ or $\hat{P}^\dagger$:

$$\Delta = G\sqrt{n}\langle\Psi_{\rm BCS}(\Delta)|\hat{P}|\Psi_{\rm BCS}(\Delta)\rangle =$$

$$= G\langle 0|\prod_{k'}(u_{k'} + v_{k'}\hat{a}_{k'}\hat{a}_{\bar{k}'})\underbrace{\Big(\sum_l{}'\hat{a}_l\hat{a}_{\bar{l}}\Big)\prod_k(u_k + v_k\hat{a}^\dagger_{\bar{k}}\hat{a}^\dagger_k)}_{\sum_l{}'v_l\underbrace{(1-\hat{n}_l)}_{1}\prod_{k\neq l}(u_k+v_k\hat{a}^\dagger_{\bar{k}}\hat{a}^\dagger_k)}|0\rangle = \underbrace{G\sum_l{}'u_l(\Delta)v_l(\Delta)}_{\frac{G}{2}\sum_l{}'\sqrt{1-\frac{(\varepsilon_l-\mu)^2}{\Delta^2+(\varepsilon_l-\mu)^2}}}$$

Both derivations equivalent ⇒ **gap equation**: $\Delta\left(1 - \frac{G}{2}\sum_k{}'\frac{1}{\sqrt{\Delta^2+(\varepsilon_k-\mu)^2}}\right) = 0$

⇒ ∃ a **critical value** $G_{\rm c}$ of pairing strength: $\boxed{\frac{2}{G_{\rm c}} = \sum_k{}'\frac{1}{|\varepsilon_k-\mu|}}$

⇒ Solutions:

(1) $G \le G_{\rm c}$:	$\Delta = 0$	(normal solution)
(2) $G > G_{\rm c}$:	$\frac{2}{G} = \sum_k{}'\frac{1}{\sqrt{\Delta^2+(\varepsilon_k-\mu)^2}} \Rightarrow \Delta \neq 0$	(superconducting solution)

◄ **Historical remark**

1947: N. Bogolyubov introduces the transformation to quasiparticles
1957: J. Bardeen, L.N. Cooper & J.R. Schrieffer formulate the BCS method

■ Quantum gases

At last we turn to systems of non-interacting indistinguishable particles, bosons or fermions, at nonzero temperature. Generalizing the concept of the canonical ensemble (see Sec. 6a), we will point out some crucial differences in thermodynamic properties of Bose and Fermi gases. We will evaluate partition functions of these gases and show how these can be used to calculate various thermodynamic properties and also the energy level densities of these many-body systems. The level density of the Fermi gas will be actually derived and discussed.

▶ Grand-canonical ensemble

Consider a gas of indistinguishable particles at temperature $T{=}(k\beta)^{-1}$ (with $k \equiv$ Boltzmann constant and $\beta \equiv$ inverse temperature) in volume V. Assuming an **exchange** of both **energy** & **particles** between the system and a bath, we *cannot* fix either the total energy E or the actual number of particles N in the system, but only their averages $\langle E\rangle$ and $\langle N\rangle$. The **density operator** describing the most probable state of the system follows from the **maximum entropy** principle. The resulting grand-canonical ensemble generalizes the canonical ensemble (Sec. 6a) by taking into account also the effects of particle exchange.

Hamiltonian $\hat{H}$ commutes with the particle-number operator $\hat{N}$. For each particle number N, the system has a discrete energy spectrum $\{E_{Ni}\}$. The equilibrium density operator $\hat{\rho}$ is diagonal in the common eigenbasis of $\hat{H}, \hat{N} \Rightarrow$ diagonal matrix elements (probabilities) $\boxed{\rho(N, E_{Ni}) \equiv \rho_{Ni}}$

Constraints induced by the normalization and fixed averages:

$$\sum_{N=0}^{\infty}\sum_{i=1}^{\infty}\rho_{Ni} = 1 \qquad \sum_{N=0}^{\infty}\sum_{i=1}^{\infty}\rho_{Ni}N = \langle N\rangle \qquad \sum_{N=0}^{\infty}\sum_{i=1}^{\infty}\rho_{Ni}E_{Ni} = \langle E\rangle$$

Entropy $S = -k\sum_{N,i}\rho_{Ni}\ln\rho_{Ni}$ to be maximized with the above constraints:

$$f = -\sum_{N,i}\rho_{Ni}\ln\rho_{Ni} + (\alpha{+}1)\sum_{N,i}\rho_{Ni} - \beta\sum_{N,i}\rho_{Ni}E_{Ni} + \gamma\sum_{N,i}\rho_{Ni}N$$

$$\frac{\partial f}{\partial\rho_{Ni}} = -\ln\rho_{Ni} - 1 + (\alpha{+}1) - \beta E_{Ni} + \gamma N = 0 \quad \Rightarrow \quad \ln\rho_{Ni} = \alpha - \beta E_{Ni} + \gamma N$$

This leads to the **grand-canonical** form of the density operator, which describes an equilibrium state of a many-particle system exchanging energy & particles with the environment:

$$\boxed{\boxed{\rho_{Ni} = \frac{1}{Z(\beta,\mu)}\,e^{-\beta\left(E_{Ni}-\mu N\right)}}} \quad \text{where} \quad \boxed{\begin{array}{ll}\mu = \frac{\gamma}{\beta} & \textbf{chemical potential}\\ Z(\beta,\mu) = \sum_{N,i} e^{-\beta(E_{Ni}-\mu N)} & \textbf{partition function}\end{array}}$$

▶ Thermodynamic quantities derived from the partition function

(a) Energy & particle number **averages**:

$$\underbrace{\langle E\rangle_{\beta,\mu}}_{\equiv\langle E\rangle_{T,\mu}} = \sum_{N,i}\rho_{N,i}E_{Ni} = \frac{1}{Z(\beta,\mu)}\sum_{N,i}E_{Ni}\,e^{-\beta(E_{Ni}-\mu N)} = -\frac{1}{Z(\beta,\mu)}\frac{\partial Z(\beta,\mu)}{\partial\beta} = -\frac{\partial}{\partial\beta}\ln Z(\beta,\mu)$$

$$\underbrace{\langle N\rangle_{\beta,\mu}}_{\equiv\langle N\rangle_{T,\mu}} = \sum_{N,i}\rho_{N,i}N = \frac{1}{Z(\beta,\mu)}\sum_{N,i}N\,e^{-\beta(E_{Ni}-\mu N)} = \frac{1}{\beta Z(\beta,\mu)}\frac{\partial Z(\beta,\mu)}{\partial\mu} = +\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z(\beta,\mu)$$

Energy & particle number **(b) variances**:

$$\underbrace{\langle\!\langle E^2\rangle\!\rangle_{\beta,\mu}}_{\equiv\langle\!\langle E^2\rangle\!\rangle_{T,\mu}} = +\frac{\partial^2}{\partial\beta^2}\ln Z(\beta,\mu)$$

specific heat $\quad c_V(T,\mu) \equiv \frac{\partial}{\partial T}\langle E\rangle_{T,\mu} = \frac{1}{kT^2}\langle\!\langle E^2\rangle\!\rangle_{T,\mu}$ (Sec. 6a)

$$\underbrace{\langle\langle N^2\rangle\rangle_{\beta,\mu}}_{\equiv\langle\langle N^2\rangle\rangle_{T,\mu}} = \underbrace{\langle N^2\rangle_{\beta,\mu}}_{\frac{1}{Z}\frac{\partial^2}{\beta^2\partial\mu^2}Z} - \langle N\rangle^2_{\beta,\mu} = \frac{1}{\beta^2}\frac{Z(\beta,\mu)\frac{\partial^2}{\partial\mu^2}Z(\beta,\mu) - \left[\frac{\partial}{\partial\mu}Z(\beta,\mu)\right]^2}{Z(\beta,\mu)^2} = +\frac{1}{\beta^2}\frac{\partial^2}{\partial\mu^2}\ln Z(\beta,\mu)$$

$$\frac{\partial}{\partial\mu}\langle N\rangle_{T,\mu} = \frac{1}{kT}\langle\langle N^2\rangle\rangle_{T,\mu}$$

▶ Partition function of the Bose gas

Bose gas is an ensemble of **non-interacting bosons**. We assume single-particle states with discrete energies $\{\varepsilon_k\}$ and occupation numbers $\boxed{n_{ik} = 0, 1, 2, 3, \ldots}$

Index i specifies the state with the total energy: $E_{Ni} = \sum_{k=1}^{\infty} n_{ik}\varepsilon_k$

The total number of particles is: $N = \sum_{k=1}^{\infty} n_{ik}$

$\Rightarrow$ partition function: sum over all sets of occupation numbers

$$Z(\beta,\mu) = \sum_N \sum_i e^{-\beta(E_{Ni}-\mu N)} = \overbrace{\sum_{\{n_{ik}\}}}^{} e^{-\beta\left(\sum_k n_{ik}\varepsilon_k - \mu\sum_k n_{ik}\right)} = \prod_k \underbrace{\sum_{n_{ik}=0}^{\infty} e^{-\beta\left(n_{ik}\varepsilon_k - \mu n_{ik}\right)}}_{\frac{1}{1-e^{-\beta(\varepsilon_k-\mu)}}}$$

$$\boxed{\ln Z(\beta,\mu) = -\sum_k \ln\left[1 - e^{-\beta(\varepsilon_k-\mu)}\right]}$$

For the Bose gas in a finite volume V the sum goes over the elementary phase-space cells, so we change the sum into an integral via the substitutions:

$$\begin{cases} \varepsilon_k & \mapsto & \frac{p^2}{2M} \\ \sum\limits_k & \mapsto & \frac{4\pi V}{(2\pi\hbar)^3}\int\limits_0^\infty p^2 dp \end{cases}$$

▶ Partition function of the Fermi gas

Fermi gas is ensemble of **non-interacting fermions**. We assume discrete single-particle energies $\{\varepsilon_k\}$ and Pauli-restricted occupation numbers $\boxed{n_{ik} = 0, 1}$ for states with total energy $E_{Ni} = \sum_{k=1}^{\infty} n_{ik}\varepsilon_k$ and total particle number $N = \sum_{k=1}^{\infty} n_{ik}$

$\Rightarrow$ partition function: sum over all sets of occupation numbers

$$Z(\beta,\mu) = \sum_N \sum_i e^{-\beta(E_{Ni}-\mu N)} = \overbrace{\sum_{\{n_{ik}\}}}^{} e^{-\beta\left(\sum_k n_{ik}\varepsilon_k - \mu\sum_k n_{ik}\right)} = \prod_k \underbrace{\sum_{n_{ik}=0,1} e^{-\beta\left(n_{ik}\varepsilon_k - \mu n_{ik}\right)}}_{1+e^{-\beta(\varepsilon_k-\mu)}}$$

$$\boxed{\ln Z(\beta,\mu) = +\sum_k \ln\left[1 + e^{-\beta(\varepsilon_k-\mu)}\right]}$$

For the Fermi gas in a finite volume V the sum is replaced by the same phase-space integral as for bosons.

▶ Distributions of occupation numbers

Average total particle number:

$$\langle N\rangle_{\beta,\mu} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z(\beta,\mu) = \begin{cases} \sum\limits_k \frac{e^{-\beta(\varepsilon_k-\mu)}}{1-e^{-\beta(\varepsilon_k-\mu)}} = \sum\limits_k \frac{1}{e^{+\beta(\varepsilon_k-\mu)}-1} & \text{Bose gas} \\ \sum\limits_k \frac{e^{-\beta(\varepsilon_k-\mu)}}{1+e^{-\beta(\varepsilon_k-\mu)}} = \sum\limits_k \frac{1}{e^{+\beta(\varepsilon_k-\mu)}+1} & \text{Fermi gas} \end{cases}$$

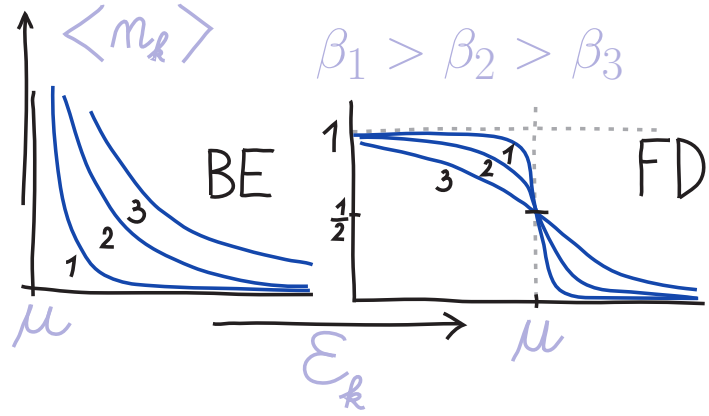
From the expression $\langle N\rangle_{\beta,\mu}=\sum_k\langle n_k\rangle_{\beta,\mu}$ using the average occupation numbers $\langle n_k\rangle_{\beta,\mu}$ we get:

$$\langle n_k\rangle_{\beta,\mu}=\begin{cases}\frac{1}{e^{+\beta(\varepsilon_k-\mu)}-1} & \textbf{Bose–Einstein statistics}\\ \frac{1}{e^{+\beta(\varepsilon_k-\mu)}+1} & \textbf{Fermi–Dirac statistics}\end{cases}$$

Chemical potential μ is determined from a fixed average $\langle N\rangle_{\beta,\mu}$ of the total number of paricles.

For bosons we require: $\boxed{\mu\le\varepsilon_1}$ (the lowest single-particle energy)

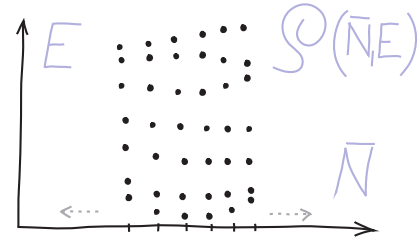
For fermions we identify: $\boxed{\mu\equiv\varepsilon_{\mathrm{F}}}$ **Fermi energy**



► Level density as the Laplace inversion of the partition function

The density of energy levels E_{Ni} for a fixed particle number N on the continuous energy axis E is defined as: $\varrho(N,E)=\sum_i\delta(E-E_{Ni})$

In analogy, the level density in the plane (particle number) × (energy) is defined using a continuous particle-number variable $\bar N$:



$$\boxed{\varrho(\bar N,E)=\sum_N\sum_i\delta(\bar N-N)\delta(E-E_{Ni})}$$

$$\Rightarrow\ \int_{N-\epsilon}^{N+\epsilon}\varrho(\bar N,E)d\bar N=\varrho(N,E)$$

The grand-canonical partition function and the level density are tightly connected:

$$Z(\beta,\mu)=\sum_N\sum_i e^{-\beta(E_{Ni}-\mu N)}\ =\ \iint\varrho(\bar N,E)\,e^{-\beta(E-\mu\bar N)}d\bar N\,dE$$

partition function — 2D Laplace transform. of state density

$$\begin{aligned}\varrho(\bar N,E)\ &=\ \left(\tfrac{1}{2\pi i}\right)^2\iint_{-i\infty}^{+i\infty}Z(\beta,\mu)\,e^{+\beta(E-\mu\bar N)}\beta\,d\mu\,d\beta\\ &=\left(\tfrac{1}{2\pi i}\right)^2\iint_{-i\infty}^{+i\infty}e^{\ln Z(\beta,\mu)+\beta(E-\mu\bar N)}\beta\,d\mu\,d\beta\end{aligned}$$

state density — inverse 2D Laplace transform. of partition function

⇒ The grand-canonical partition function of a many-body system enables one to calculate the density of energy eigenstates for each particle number.

► The saddle-point approximation

To perform the exact Laplace inversion of the partition function is a difficult task even for system as simple as the Bose or Fermi gases. The commonly used method is the saddle-point approximation. We first introduce it for the **canonical** partition function $Z(\beta)=\sum_i e^{-\beta E_i}=\int dE\,\varrho(E)e^{-\beta E}$, for which the Laplace inversion reads: $\varrho(E)=\frac{1}{2\pi i}\int\limits_{\beta_0-i\infty}^{\beta_0+i\infty} d\beta\, Z(\beta)e^{+\beta E}=\frac{1}{2\pi i}\int\limits_{\beta_0-i\infty}^{\beta_0+i\infty} d\beta\, Z(\beta)e^{\ln Z(\beta)+\beta E}$ where $\beta_0\in\mathbb{R}$ is an adjustable constant. The complexified variable β we denote as $\beta=x+iy$ and $\beta_0\equiv x_0$, so:

$$\boxed{\varrho(E)=\tfrac{1}{2\pi i}\int\limits_{-\infty}^{+\infty} i\,dy\,e^{\ln Z(x_0+iy)+(x_0+iy)E}}$$

The function $f(x,y)=\ln Z(x+iy)+(x+iy)E$ in the exponent is generally a fast-varying complex function, so the contributions of the whole exponential have a tendency to cancel each other. Only in a vicinity of a stationary point (x_0,y_0) satisfying $\frac{\partial f}{\partial x}|_{(x_0,y_0)}=\frac{\partial f}{\partial y}|_{(x_0,y_0)}=0$ the contributions add coherently. We find a stationary point on the real axis, $(x_0,y_0)=(x_0,0)$, and associate it with the value β_0. So we can write: $\varrho(E)\approx\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} dy\,e^{\ln Z(x_0+i0)+x_0E+\frac{1}{2}\frac{\partial^2\ln Z}{\partial y^2}|_{x_0+i0}\,y^2}$

We know that $\frac{\partial^2}{\partial x^2}\mathrm{Re}\ln Z+\frac{\partial^2}{\partial y^2}\mathrm{Re}\ln Z=0$ (Cauchy-Riemann condition) and also $\frac{\partial^2}{\partial x^2}\mathrm{Re}\ln Z|_{x_0+i0}=\langle\!\langle E^2\rangle\!\rangle_{\beta_0}\geq 0$. Hence the real part of the quadratic term in the exponential of the above formula is (semi)negative and we can use the familiar Gauss integral, arriving at:

Note that the energy dependence is hidden also in $x_0=\beta_0=\beta_0(E)$.

$$\boxed{\varrho(E)\approx\tfrac{1}{2\pi}\,e^{\ln Z(\beta_0)+\beta_0E}\sqrt{\frac{2\pi}{\left|\frac{\partial^2}{\partial y^2}\ln Z(\beta_0)\right|}}}$$

The Laplace inversion of the **grand-canonical** partition function is evaluated in a similar way (not reviewed here), resulting in an analogous formula:

where we use the Hessian $F(\beta,\gamma)=\begin{pmatrix}\frac{\partial^2\ln Z}{\partial\beta^2},\frac{\partial^2\ln Z}{\partial\beta\partial\gamma}\\ \frac{\partial^2\ln Z}{\partial\gamma\partial\beta},\frac{\partial^2\ln Z}{\partial\gamma^2}\end{pmatrix}$

$$\boxed{\boxed{\varrho(\bar N,E)\approx\tfrac{1}{(2\pi)^2}\,e^{\ln Z(\beta_0,\gamma_0)+\beta_0E-\gamma_0N}\sqrt{\frac{(2\pi)^2}{\left|\mathrm{Det}F(\beta_0,\gamma_0)\right|}}}}$$

► Level density of the Fermi gas

We express the above-derived Fermi-gas partition function as

$$\ln Z(\beta,\mu)=\sum_k\ln\bigl[1+e^{-\beta(\varepsilon_k-\varepsilon_{\rm F})}\bigr]=\int\limits_0^\infty d\varepsilon\,\underbrace{g(\varepsilon)}_{\sum_k\delta(\varepsilon-\varepsilon_k)}\ln\bigl[1+e^{-\beta(\varepsilon-\varepsilon_{\rm F})}\bigr]$$

single-particle level density

$$=\int\limits_0^{\varepsilon_{\rm F}} d\varepsilon\,g(\varepsilon)\ln\bigl[1+e^{-\beta(\varepsilon-\varepsilon_{\rm F})}\bigr]+\int\limits_{\varepsilon_{\rm F}}^{+\infty} d\varepsilon\,g(\varepsilon)\ln\bigl[1+e^{-\beta(\varepsilon-\varepsilon_{\rm F})}\bigr]$$

The first term can be written as: $\ln\Big\{e^{\beta(\varepsilon-\varepsilon_{\rm F})}[1+e^{-\beta(\varepsilon-\varepsilon_{\rm F})}]\Big\}$

$$-\beta\int_0^{\varepsilon_{\rm F}} d\varepsilon\, g(\varepsilon)(\varepsilon-\varepsilon_{\rm F}) + \int_0^{\varepsilon_{\rm F}} d\varepsilon\, g(\varepsilon)\overbrace{\ln\big[1+e^{+\beta(\varepsilon-\varepsilon_{\rm F})}\big]}$$

So we have:

$$\ln Z(\beta,\mu) = -\beta\int_0^{\varepsilon_{\rm F}} d\varepsilon g(\varepsilon)(\varepsilon-\varepsilon_{\rm F}) + \underbrace{\int_0^{\varepsilon_{\rm F}} d\varepsilon g(\varepsilon)\ln\big[1+e^{+\beta(\varepsilon-\varepsilon_{\rm F})}\big] + \int_{\varepsilon_{\rm F}}^{+\infty} d\varepsilon g(\varepsilon)\ln\big[1+e^{-\beta(\varepsilon-\varepsilon_{\rm F})}\big]}_{\int_0^{+\infty} dx[g(\varepsilon_{\rm F}-x)+g(\varepsilon_{\rm F}+x)]\ln[1+e^{-\beta x}] \approx 2g(\varepsilon_{\rm F})\underbrace{\int_0^{+\infty} dx\ln[1+e^{-\beta x}]}_{\frac{\pi^2}{12\beta}}}$$

We obtain an approximation:

$$\boxed{\ln Z(\beta,\mu) \approx -\beta\int_0^{\varepsilon_{\rm F}} d\varepsilon\, g(\varepsilon)(\varepsilon-\varepsilon_{\rm F}) + \frac{\pi^2}{6\beta}\, g(\varepsilon_{\rm F})} = -\beta\int_0^{\gamma/\beta} d\varepsilon\, g(\varepsilon)(\varepsilon-\tfrac{\gamma}{\beta}) + \tfrac{\pi^2}{6\beta}\, g(\tfrac{\gamma}{\beta})$$

This can be used in the above saddle-point formula of the grand-canonical Laplace inverse. First we evaluate all the needed derivatives:

$$\begin{aligned}
\tfrac{\partial}{\partial\beta}\ln Z(\beta,\tfrac{\gamma}{\beta}) &\approx -\int_0^{\gamma/\beta} d\varepsilon\, g(\varepsilon)(\varepsilon-\tfrac{\gamma}{\beta}) - \beta\int_0^{\gamma/\beta} d\varepsilon\, g(\varepsilon)\tfrac{\gamma}{\beta^2} - \tfrac{\pi^2}{6\beta^2}\, g(\tfrac{\gamma}{\beta}) - \overbrace{\tfrac{\pi^2}{6\beta}\, g'(\tfrac{\gamma}{\beta})\tfrac{\gamma}{\beta^2}}^{\approx 0 \text{ (see below)}} \\
&\approx -\int_0^{\gamma/\beta} d\varepsilon\, g(\varepsilon)\varepsilon - \tfrac{\pi^2}{6\beta^2}\, g(\tfrac{\gamma}{\beta}) \\
\tfrac{\partial}{\partial\gamma}\ln Z(\beta,\tfrac{\gamma}{\beta}) &\approx \beta\int_0^{\gamma/\beta} d\varepsilon\, g(\varepsilon)\tfrac{1}{\beta} + \overbrace{\tfrac{\pi^2}{6\beta}\, g'(\tfrac{\gamma}{\beta})\tfrac{1}{\beta}}^{\approx 0 \text{ (see below)}} \qquad \approx \int_0^{\gamma/\beta} d\varepsilon\, g(\varepsilon) \\
\tfrac{\partial^2}{\partial\beta^2}\ln Z(\beta,\tfrac{\gamma}{\beta}) &\approx \tfrac{\gamma}{\beta^2} g(\tfrac{\gamma}{\beta})\tfrac{\gamma}{\beta} + \tfrac{\pi^2}{3\beta^3}\, g(\tfrac{\gamma}{\beta}) + \overbrace{\tfrac{\pi^2}{6\beta^2}\, g'(\tfrac{\gamma}{\beta})\tfrac{\gamma}{\beta^2}}^{\approx 0 \text{ (see below)}} \qquad \approx \big(\tfrac{\gamma^2}{\beta^3} + \tfrac{\pi^2}{3\beta^3}\big)\, g(\tfrac{\gamma}{\beta}) \\
\tfrac{\partial^2}{\partial\gamma^2}\ln Z(\beta,\tfrac{\gamma}{\beta}) &\qquad\qquad\qquad\qquad\qquad\qquad \approx \tfrac{1}{\beta}\, g(\tfrac{\gamma}{\beta}) \\
\tfrac{\partial^2}{\partial\beta\partial\gamma}\ln Z(\beta,\tfrac{\gamma}{\beta}) &= \tfrac{\partial^2}{\partial\gamma\partial\beta}\ln Z(\beta,\mu) \qquad\qquad\qquad\qquad \approx -\tfrac{\gamma}{\beta^2}\, g(\tfrac{\gamma}{\beta})
\end{aligned}$$

$\Rightarrow$ the Hessian determinant: $\mathrm{Det}\, F(\beta,\gamma) \approx \frac{\pi^2}{3\beta^4}\, g(\frac{\gamma}{\beta})^2$

$\Rightarrow$ determination of the stationary point (β_0,γ_0):

$$\tfrac{\partial}{\partial\gamma}\big[\ln Z(\beta,\tfrac{\gamma}{\beta}) + \beta E - \gamma N\big]_{(\beta_0,\gamma_0)} = 0 \quad\Rightarrow\quad -N + \underbrace{\int_0^{\gamma_0/\beta_0} d\varepsilon\, g(\varepsilon)}_{\text{num.of particles with } \varepsilon\in[0,\frac{\gamma_0}{\beta_0}]} = 0 \quad\Rightarrow\quad \boxed{\gamma_0 = \beta_0\varepsilon_{\rm F}}$$

$$\tfrac{\partial}{\partial\beta}\big[\ln Z(\beta,\tfrac{\gamma}{\beta}) + \beta E - \gamma N\big]_{(\beta_0,\gamma_0)} = 0 \quad\Rightarrow\quad E - \underbrace{\int_0^{\varepsilon_{\rm F}} d\varepsilon\, g(\varepsilon)\varepsilon}_{E_0 \equiv \text{the ground-state energy}} - \tfrac{\pi^2}{6\beta^2}\, g(\varepsilon_{\rm F}) \quad\Rightarrow\quad \boxed{\beta_0 = \sqrt{\tfrac{\frac{\pi^2}{6} g(\varepsilon_{\rm F})}{E-E_0}}}$$

The above-assumed neglect of terms with $g'(\varepsilon) \equiv \frac{d}{d\varepsilon} g(\varepsilon)$ is based on a required condition $\boxed{\frac{1}{\beta_0} g'(\varepsilon_{\rm F}) \ll g(\varepsilon_{\rm F})}$ which can be expected to hold for $N \gg 1$.

Putting all partial results together, we arrive at the final expression:

$$\boxed{\boxed{\varrho(\bar N, E) \approx \frac{e^{2\sqrt{\frac{\pi^2}{6} g(\varepsilon_{\rm F})(E-E_0)}}}{\sqrt{48}(E-E_0)}}}$$

Bethe formula { where the dependence on $\bar N$ is hidden in $\boxed{\varepsilon_{\rm F} \equiv \varepsilon_{\rm F}(\bar N)}$

This formula is very close to the one used to approximate the density of discrete energy spectra of atomic nuclei. However, the nuclear Bethe formula is slightly different as it follows from a *two-component* Fermi gas, composed of N neutrons and Z protons. Deviations from the nuclear Bethe formula are of course due to mutual interactions of nucleons, so the formula can only be used with some phenological corrections (e.g., the inclusion of the pairing gap).

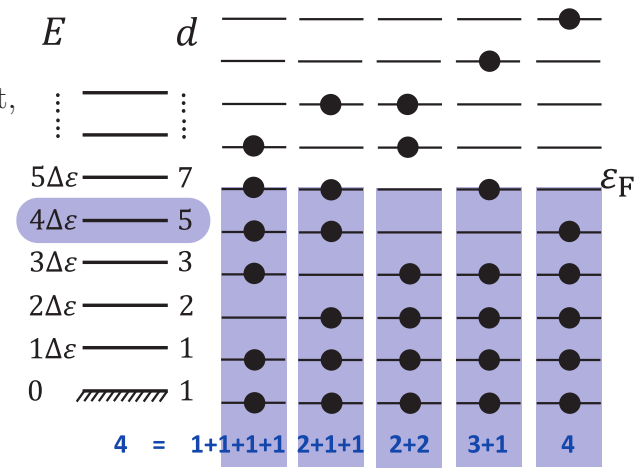
► Bethe and Ramanujan-Hardy formulas

In the number theory, the so-called Ramanujan-Hardy formula estimates the number of partitions $p(n)$ of an integer n to smaller positive integers.
For instance, $p(4)=5$ since $4 = 3+1 = 2+2 = 2+1+1 = 1+1+1+1$.

The Ramanujan-Hardy formula holds for $n \gg 1$ and reads as follows:

$$p(n) = \frac{e^{2\sqrt{\frac{\pi^2}{6}n}}}{\sqrt{48\,n}}$$

This is equivalent to the Bethe formula:
Assume that the single-particle levels ε_k near the Fermi energy ε_F are approximately equidistant, the gap between levels being given by $\Delta\varepsilon = \frac{1}{g(\varepsilon_F)}$. Excitations of the whole system above its ground state are created by lifting individual particles above the Fermi energy. For excited states involving only single-particle excitations in a vicinity of the Fermi energy, the total excitation energy is given by $E - E_0 = n\,\Delta\varepsilon$, where the integer n is the number of energy gaps crossed by one or more fermions. The number of partitions $p(n)$ coincides with the number of ways in which a given total excitation $n\Delta\varepsilon$ can be decomposed to different single-particle excitations, so it determines the degeneracy d of the given excited level. The total level density is therefore given by:



$$\varrho(E) = \frac{p(n=\frac{E-E_0}{\Delta\varepsilon})}{\Delta\varepsilon} = g(\varepsilon_F)\frac{e^{2\sqrt{\frac{\pi^2}{6}g(\varepsilon_F)(E-E_0)}}}{\sqrt{48\,g(\varepsilon_F)(E-E_0)}} = \text{Bethe formula}$$

◄ Historical remark

1878: J.W. Gibbs introduces the notion of statistical ensembles
1918: S. Ramanujan & G.H. Hardy derive the asymptotic partition-number formula
1924-5: S. Bose & A. Einstein derive the statistical distribution for bosons
1926: E. Fermi and P. Dirac derive the statistical distribution for fermions
1937: H. Bethe presents the Fermi-gas level-density formula and applies it to nuclei

CONCLUDING WORDS

It's time to close. There is no doubt that we could continue for long, gathering more and more results and explanations. So this is really a random place to stop. But, at the same time, perhaps it is not so bad place as the last example gives us a very important lesson on physics in general, which we may see as a kind of climax. It shows that physics is like a garden where the paths do not diverge but converge. Taking any of the many different paths, one may reach the same point with the same result. Physics, unlike many other human endeavors, is consistent.

In 2025, when I am writing these lines, quantum physics is celebrating its 100th birthday. Indeed, the first proper form of quantum theory, the so-called matrix mechanics, was created by Werner Heisenberg in 1925 on the North-Sea island Helgoland. What have we learned in the first century of studying matter at the subatomic level? First of all, we have learned that the world down there — even though everything around us grows out of it — is completely different from the world of our common experience. People are still quite confused when they try to define what the word "reality" actually means in the quantum realm. We have nevertheless found that the elusive quantum world is governed by rather simple laws, which are formulated in an elegant, though highly abstract mathematical language. Perhaps the most surprising finding is that despite its apparent strangeness, we can understand this language perfectly. The fact that behind the physical phenomena around us there is a beautiful and still comprehensible for us mathematical order is probably the most amazing message that science brings.

The first quantum century also taught us a more practical lesson. We have learned that understanding quantum processes can multiply our technological possibilities. Quantum physics turned out essential in the development of tools such as the transistor, laser, superconductor, electron microscope, atomic clock and others. But now it seems that a new era of quantum technologies is downing. Quantum physics promises to produce new materials with incredible properties, to construct measuring devices with extremely high sensitivity, and to establish quantum information procedures transcending classical limitations. All of this can be of crucial importance in solving the challenging problems facing humanity. I hope that some of you, the readers of this book, will actively participate in this ongoing adventure.

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