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A Condensed Course of Quantum Mechanics

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

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Contents

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:* $\boxed{\text{important}}$ $\boxed{\boxed{\text{essential 1}}}$ $\boxed{\text{essential 2}}$ $\boxed{\boxed{\text{crucial}}}$

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 $\equiv$ 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
$\Psi(\boldsymbol{\xi}_1\ldots\boldsymbol{\xi}_N)$	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 ($n\equiv$princ.q.num., $l\equiv$orb.ang.mom., $k\equiv$|wave vec.|)
$C_{j_1m_1j_2m_2}^{jm}\equiv\langle j_1j_2jm\|j_1m_1j_2m_2\rangle$	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
$\hat{\dot{A}}$	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 $\mathcal{H}_{\pm}^{(N)}$
$\hat{P}_a,\hat{\Pi}_a,\hat{\boldsymbol{\Pi}}_{(a_1,a_2)}$	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 $t_0 \xrightarrow{t} t_1$
$\hat{G}^{\pm}(t,t_0)$, $G^{+}(\vec{x}t\vert\vec{x}_0t_0)$	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)
$\mathfrak{a}_{ji}(t), \mathfrak{p}_{ji}(t), \mathcal{R}_{ji}(t), \mathcal{R}_{\mathrm{X}}$	$\vert\phi_i\rangle \xrightarrow{t} \vert\phi_j\rangle$ 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}, $\bar{\lambda}_{\mathrm{C}}$, λ_{B}, $\bar{\lambda}_{\mathrm{B}}$, 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
$j_l, n_l, h^{\pm}_l(kr)$	Bessel, Neumann & Hankel functions
$L^j_i(\rho)$, $H_n(\xi)$	associated or generalized Laguerre polynomials & Hermite polynomials
$P_{lm}(\cos\vartheta)$,$Y_{lm}(\vartheta,\varphi)$	associated Legendre polynomial, spherical harmonics (ϑ,$\varphi\equiv$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, $\mathrm{Sup}\{X_i\}_i$	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.

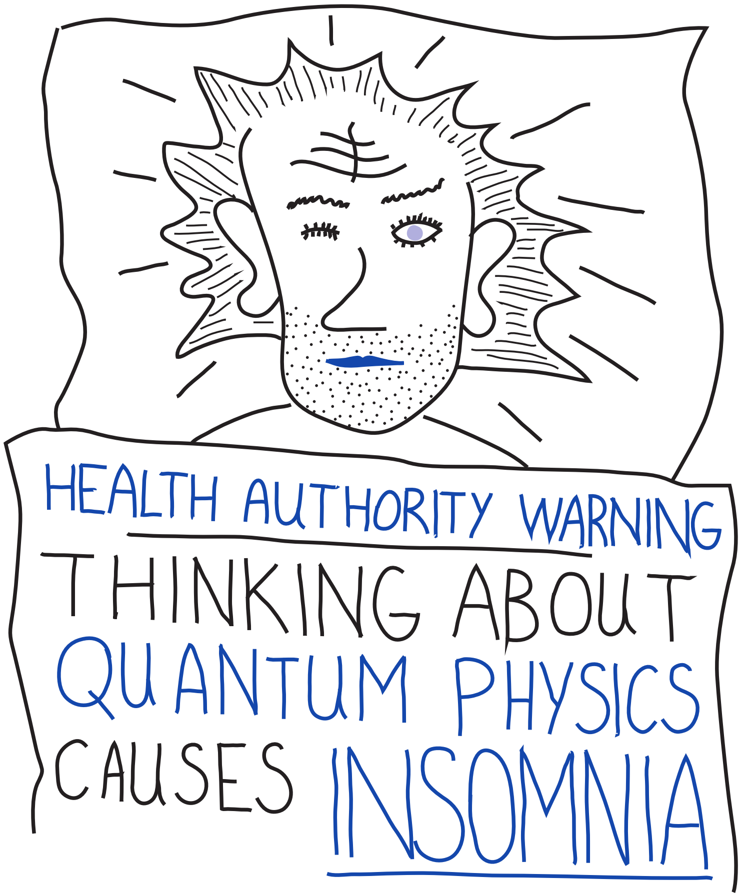
Linearity: Underlying the dynamics of quantum probabilities, there is a rather simple linear theory which makes use of so-called quantum amplitudes. An amplitude $\mathfrak{a}=|\mathfrak{a}|e^{i\varphi}$ of a certain physical event is a number inside the unit circle of the $\mathbb{C}$ plane such that 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**.

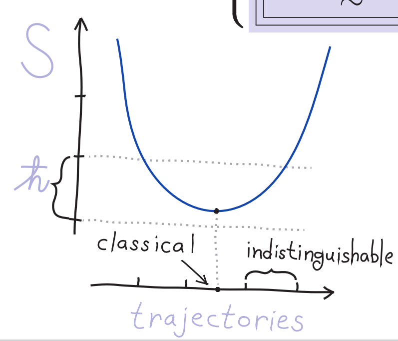
▶ Planck constant

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:

$$\left.\begin{array}{l}\textbf{Classical mechanics}\\ \textbf{Quantum mechanics}\end{array}\right\}\ \text{applies if the difference satisfies}\ \left\{\boxed{\begin{array}{c}\Delta S \gg \hbar\\ \Delta S \lesssim \hbar\end{array}}\right.$$

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

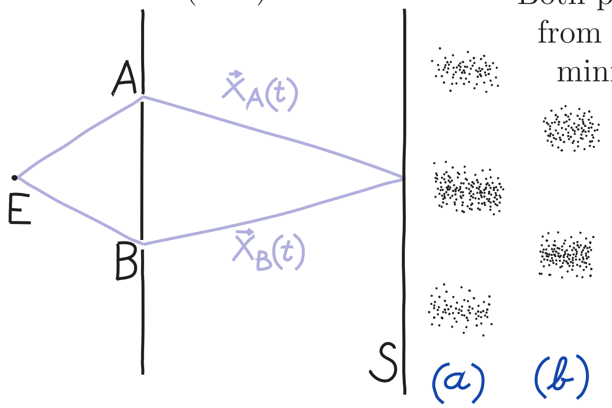
1900: Max Planck introduced $\hbar$ along with the quanta of electromagnetic radiation to explain the blackbody radiation law
1905: Albert Einstein confirmed elmag. quanta in the explanation of photoeffect
1913: Niels Bohr introduces a quantum model of atoms (“old quantum mechanics”)

■ Double-slit experiment

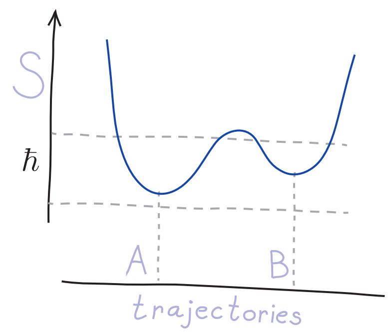
According to Richard Feynman and many others, this is the most crucial quantum experiment that allows one to realize how unusual the quantum world is. There exist numerous variations and improvements of this experiment.

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



▶ Regimes and results of measurements

(a) Interference setup: position of the particle is measured only at the screen $\Rightarrow$ 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 $\Rightarrow$ 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.

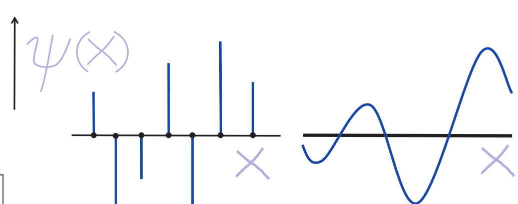
■ Wavefunction and superposition principle

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 $\psi_{\rm A}(\vec{x},t)$ and $\psi_{\rm B}(\vec{x},t)$:

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

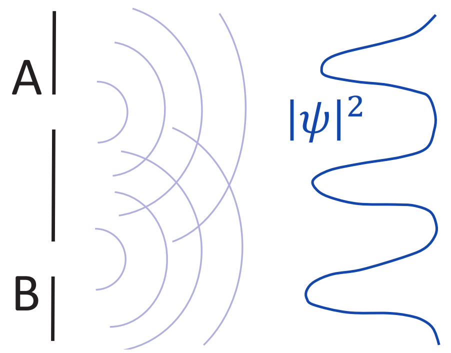
$\Rightarrow$ any linear combination of normalizable wavefunctions is a normalizable wavefunction $\Rightarrow$ these functions form a linear vector space $\mathcal{L}^2(\mathbb{R}^3)$

▶ 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 $\int|\alpha\psi_{\rm A}+\beta\psi_{\rm B}|^2\,d\vec{x}=1$ with both $\psi_{\rm A}$ and $\psi_{\rm B}$ normalized ($\int|\psi_\bullet|^2\,d\vec{x}=1$)

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

▶ 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

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

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:

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

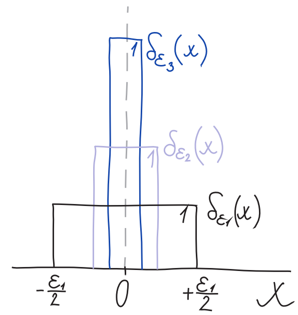
Thus the probability distribution on the screen shows the interference pattern.

▶ 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:

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

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) $\boxed{\delta_\epsilon(x) = \frac{1}{\pi} \frac{\sin(x\epsilon^{-1})}{x} = \frac{1}{2\pi} \int\limits_{-\epsilon^{-1}}^{+\epsilon^{-1}} e^{iqx} dq}$ (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.

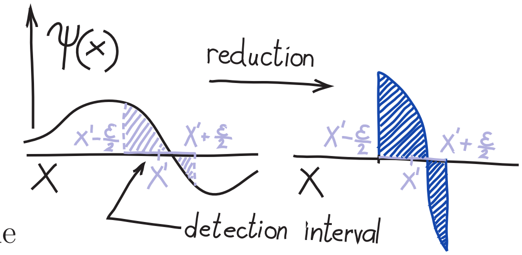
▶ **Change of wavefunction in measurement**

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 $\vec{x}'$:

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



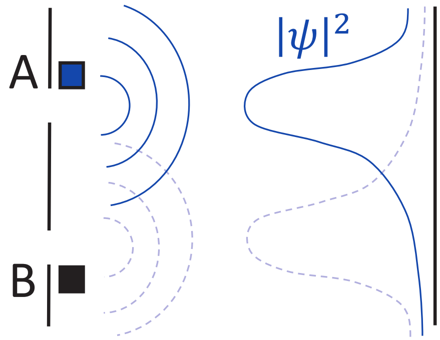
After the position measurement, the wavefunction evolves from a localized one

▶ **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:

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

(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

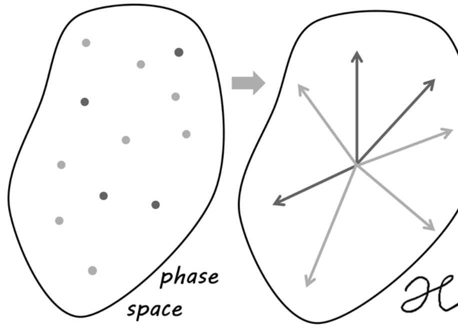
1a. SPACE OF QUANTUM STATES

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).

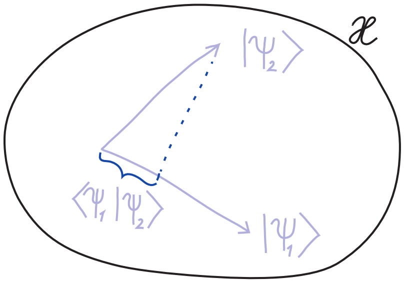
Distance of 2 vectors: $d^2(\psi_1, \psi_2) \equiv ||\psi_1 - \psi_2||^2 = \langle\psi_1|\psi_1\rangle + \langle\psi_2|\psi_2\rangle - 2\mathrm{Re}\langle\psi_1|\psi_2\rangle$

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:



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

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 $\boxed{\langle\phi_i|\phi_j\rangle = \delta_{ij}}$

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

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

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

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 $\boldsymbol{\ell^2}$** 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

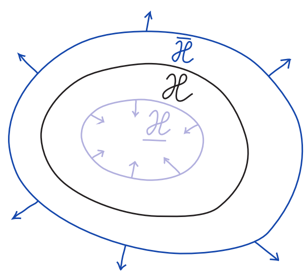
$\overline{\mathcal{H}}$ (conjugate space to $\underline{\mathcal{H}}$) is a space of sequences $\{\alpha'_i\}_{i=1}^{\infty} \equiv |\psi'\rangle$ satisfying $\langle\psi|\psi'\rangle < \infty$ for any $|\psi\rangle \in \underline{\mathcal{H}}$. This set contains ℓ^2 as a subset.

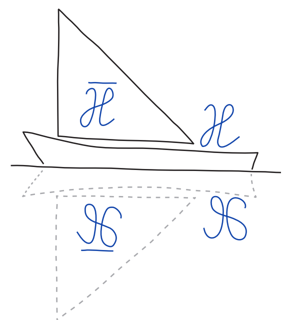
$$\langle\psi|\psi'\rangle \equiv \sum_i \alpha_i^* \alpha'_i < \infty \quad \Rightarrow \sum_i |\alpha'_i|^2 \tfrac{1}{i^m} < \infty \quad \Rightarrow |\alpha'_i|^2 \text{ may polynomially diverge}$$

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

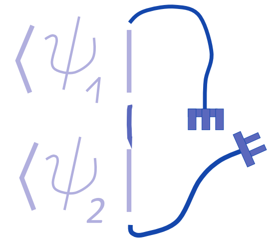
For any vector $|\psi\rangle \in \mathcal{H}$, called **ket**, there exists a linear functional $F_\psi \equiv \langle\psi|$, called **bra**, such that the value assigned by F_ψ to $|\phi\rangle \in \mathcal{H}$ is $\boxed{F_\psi(\phi) \equiv \langle\psi|\phi\rangle}$ (the words following from "bra-c-ket")

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



▶ 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:

$$\boxed{\sum_{i=1}^{d_\mathcal{H}} |\phi_i\rangle\langle\phi_i| = \hat{I}} \quad \overset{\{|\phi_i\rangle\} \xrightarrow{\hat{I}} \{|\phi_i\rangle\}}{\equiv \textbf{unit operator}} \Rightarrow \quad \boxed{\underbrace{\hat{O}}_{\hat{I}\hat{O}\hat{I}} = \sum_{i=1}^{d_\mathcal{H}} \sum_{j=1}^{d_\mathcal{H}} \underbrace{\langle\phi_j|\hat{O}\phi_i\rangle}_{\langle\phi_j|\hat{O}|\phi_i\rangle \equiv O_{ji}} |\phi_j\rangle\langle\phi_i|}$$

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

▶ Projectors

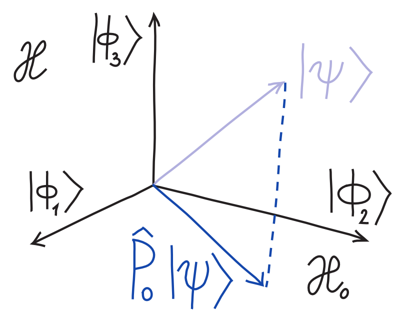
Projection operators (projectors) are linear operators satisfying $\boxed{\hat{P}^2 = \hat{P}}$

(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 $|\psi_k\rangle \in \mathcal{H}_k$ $(k=1,2)$

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

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 $\begin{cases} |\psi_k\rangle = \hat{P}_k|\Psi\rangle \\ |\psi_k'\rangle = \hat{P}_k|\Psi'\rangle \end{cases}$