Pavel Cejnar

A Condensed Course of Quantum Mechanics

KAROLINUM

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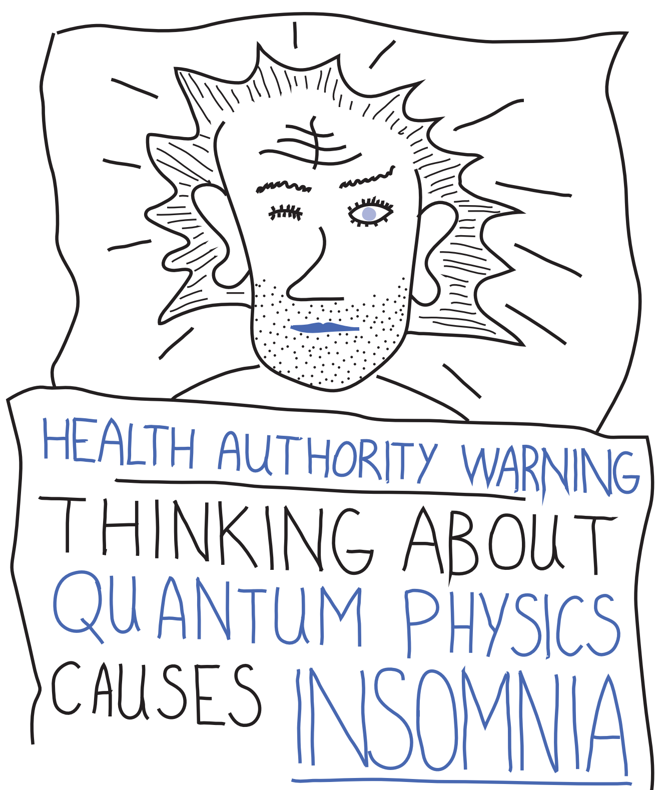


HEALTH AUTHORITY WARNING
THINKING ABOUT
QUANTUM PHYSICS
CAUSES INSOMNIA

Preface

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 [1–8].

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 [9]. 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

Recommended textbooks:

[1] J.J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, 1985, 1994)
A modified edition of the same book:
[2] J.J. Sakurai, J.J. Napolitano, *Modern Quantum Mechanics* (Addison-Wesley, 2011)
[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)

Further reading:

[9] J.S. Bell, *Speakable and Unspeakable in Quantum Mechanics* (Cambridge University Press, 1987)

Rough guide to notation (succinct and incomplete)

symbol	meaning
	Spaces, state vectors & wavefunctions
$\underline{\mathcal{H}}$, $\mathcal{H}$, $\overline{\mathcal{H}}$	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
$\vert\psi\rangle$, $\langle\psi'\vert$; $\langle\psi'\vert\psi\rangle$	"ket" & "bra" forms of state vectors; scalar product
$\vert\vert\psi\vert\vert=\sqrt{\langle\psi\vert\psi\rangle}$	vector norm
$\alpha\vert\psi\rangle+\beta\vert\psi'\rangle$	superposition ≡ linear combination of state vectors ($\alpha,\beta\in\mathbb{C}$)
$\vert\phi_i\rangle$,$\vert\Phi_{ij}\rangle\equiv\vert\phi_{1i}\rangle_1\vert\phi_{2j}\rangle_2$	general basis vector in $\mathcal{H}$; separable basis vector in $\mathcal{H}_1\otimes\mathcal{H}_2$
$\vert\psi\rangle_1\vert\psi'\rangle_2$	general separable vector in $\mathcal{H}_1\otimes\mathcal{H}_2$
$\vert a\rangle$, $\vert a_i\rangle$, $\vert a_i^{(k)}\rangle$	eigenvector of $\hat{A}$ with eigenvalue a or a_i (degeneracy index k)
$\vert E_i\rangle$, $\vert E\rangle$	energy eigenvectors
$\vert\uparrow\rangle$, $\vert\downarrow\rangle$	up & down projection states of spin $s{=}\frac{1}{2}$
$^{\vert lm_l\rangle}_{\vert sm_s\rangle}$, $\vert jm_j\rangle$	states with ($^{\text{orbital}}_{\text{spin}}$,total) ang. momentum ($^{l}_{s}$, j), projection $m_\bullet$
$\psi(\underbrace{\vec{x},m_s}_{\boldsymbol{\xi}})\equiv\boldsymbol{\Psi}(\vec{x})$	single-particle wavefunction in single/multicomponent forms
$\Psi(\boldsymbol{\xi}_1\ldots\boldsymbol{\xi}_N)$	N-particle wavefunction
$R_{nl}(r)=\frac{u_{nl}(r)}{r}$	radial wavefunction
Span$\{\vert\psi_1\rangle...\vert\psi_n\rangle\}$	linear space spanned by the given vectors
$\mathcal{N}$, $d_{\mathcal{H}}$	normalization coefficient & dimension of space $\mathcal{H}$
	Observables & operators
$\hat{O}$, $\hat{O}^\dagger$, $\hat{O}^{-1}$	operator, its Hermitian conjugate & inverse
$\hat{I}$, $\hat{U}$	identity operator & unitary operator
$\hat{P}_a$, $\hat{\mathbf{\Pi}}_{(a_1,a_2)}$	projectors to discrete & continuous eigenvalue subspaces
$\vert\vert\hat{A}\vert\vert$	operator norm
$\hat{A}_1\otimes\hat{A}_2$	tensor product of operators acting in $\mathcal{H}_1\otimes\mathcal{H}_2$
$\hat{H}$, $\hat{T}$, $\hat{V}$; $\hat{H}'$	Hamiltonian, its kinetic & potential terms; perturbation
$\vec{\nabla}$, Δ	gradient & Laplace operator (or also an interval, gap...)
$\hat{\vec{x}}$, $\hat{\vec{p}}$, $\hat{P}$	coordinate, momentum vectors & spatial parity operator
$\hat{\vec{L}}$, $\hat{\vec{S}}$; $\hat{\vec{J}}$, $\hat{J}_\pm$	orbital, spin & total angular momentum, shift operators for $\hat{J}_3$
$\hat{\vec{\sigma}}$	the triplet of Pauli matrices
$\hat{T}_{\Delta o}$	$\vert o\rangle\to\vert o{+}\Delta o\rangle$ eigenvector shift operator for general operator $\hat{O}$
$\hat{G}_i$, $\hat{C}_{\mathcal{G}}$	generator & Casimir operator of a group $\mathcal{G}$
$\hat{b},\hat{b}^\dagger$; $\hat{a},\hat{a}^\dagger$; $\hat{c},\hat{c}^\dagger$	annihilation, creation operators for bosons, fermions, or both
$\hat{N}$, $\hat{N}_k$	total number of particles & number of particles in k^{th}state
$\hat{R}_{\vec{n}\phi}$, $\mathbf{R}(\alpha\beta\gamma)$	rotation operator in $\mathcal{H}$ & rotation matrix in 3D (Euler angles)
$\hat{U}(t)$, $\hat{U}(t_1,t_0)$	evolution operator for times $t_0\xrightarrow{t}t_1$
$\hat{\mathcal{T}}$, $\mathfrak{T}$	time reversal operator & time ordering of operator product
$\hat{G}(t)$, $G(\vec{x}t\vert\vec{x}_0t_0)$	Green operator & propagator

$\hat{O}_{\rm S}$, $\hat{O}_{\rm H}(t)$, $\hat{O}_{\rm D}(t)$	Schrödinger, Heisenberg, Dirac representations of operator
$[\hat{A}^{\lambda_1}\times\hat{B}^{\lambda_1}]^{\lambda}_{\mu}$	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 A, B
${\rm Tr}\,\hat{O}$, ${\rm Tr}_1\hat{O}$	trace of operator/matrix, partial trace over $\mathcal{H}_1$ in $\mathcal{H}_1\otimes\mathcal{H}_2$
${\rm Det}\,\hat{O}$, ${\rm Def}(\hat{O})$	determinant of matrix/operator, definition domain of operator
	Statistics, probabilities & densities
$p_{\psi}(a)$	probability to measure value a of observable A in state $\|\psi\rangle$
$\langle A\rangle_{\psi}$, $\langle a\rangle_c$	average of A-distribution in $\|\psi\rangle$, average of a for a parameter c
$\langle\langle A^2\rangle\rangle_{\psi}\equiv\Delta^2_{\psi}A$	dispersion of A-distribution in $\|\psi\rangle\equiv$ squared uncertainty
$p_c(a\|b)$	conditional probability of a given b (depending on parameter c)
$\rho(\vec{x},t)$, $\vec{j}(\vec{x},t)$	probability density & flow at point $\vec{x}$, time t
$\hat{\rho}$, $W_{\rho}(\vec{x},\vec{p})$, S_{ρ}	density operator/matrix, Wigner distribution function, entropy
$\varrho(E)$	density of energy eigenstates
	Functions
$j_l, n_l, h^{\pm}_l(kr)$	Bessel, Neumann & Hankel functions
$L^j_i(\rho)$, $H_n(\xi)$	$\left\{{\rm associated \atop generalized}\right\}$ Laguerre polynomials & Hermite polynomials
$P_{lm}(\cos\vartheta)$,$Y_{lm}(\vartheta,\varphi)$	associated Legendre polynomial, spherical harmonics (sph.angles)
$D^j_{m'm}(\alpha\beta\gamma)$	Wigner matrix function $\equiv D^j_{m'm}(\mathbf{R})$ (Euler angles of rotation $\mathbf{R}$)
$\delta(x)$, $\delta_{\epsilon}(x)$; $\Theta(x)$	Dirac δ-function, sequence of functions $\stackrel{\epsilon\to 0}{\longrightarrow}\delta$; step function
$Z(\beta), Z(\beta,\mu)$	(grand)canonical partition funcs. (inv.temperature,chem.potential)
$\left\{{S[\vec{x}(t)] \atop S(\vec{x},t)}\right\}$, $\mathcal{L}(\vec{x},\dot{\vec{x}})$	classical action (functional & function forms), Lagrangian
$V(\vec{x})$, $\vec{A}(\vec{x})$	scalar & vector potentials
$S_{ji}, P_{ji}, W_{ji}(t)$	$j\to i$ transition amplitude, probability & rate (time)
F_l, S_l, $\delta_l(k)$	partial wave amplitude, S-matrix & phase shift (|wavevector|)
$f_{\vec{k}}(\vec{k}\,')\equiv f_{\vec{k}}(\vartheta,\varphi)$	scattering amplitude (direction/angles)
$\frac{d\sigma}{d\Omega}(\vartheta,\varphi)$	differential cross section ($\sigma\equiv$ integral cross section)
	Miscellaneous
$(1,2,3)\equiv(x,y,z)$	indices of Cartesian components
$\vec{n}$, $\left\{{(\vec{n}_x,\vec{n}_y,\vec{n}_z) \atop (\vec{n}_r,\vec{n}_{\vartheta},\vec{n}_{\varphi})}\right\}$	unit vector, $\left\{{\rm Cartesian \atop spherical}\right\}$ orthonormal coordinate vectors
δ_{ij}, ε_{ijk}	Kronecker & Levi-Civita symbols
$C^{jm}_{j_1m_1j_2m_2}$	Clebsch-Gordan coefficient $\equiv\langle j_1j_2jm\|j_1m_1j_2m_2\rangle$
$\hbar, c, e$	Planck constant, speed of light, elementary charge
$M, \mathcal{M}$; q	particle mass & two-particle reduced mass; particle charge
$\vec{k}$, ω, λ	wavevector, frequency, wavelength (or perturbation parameter)
ε_k, n_k	energies & occupation numbers of single-particle states
$\{X_i\}_{i\in\mathcal{D}}$,$\{X(c)\}_{c\in\mathcal{C}}$	discrete/continuous set of objects
Min,Max,Sup$\{X_i\}_i$	minimum, maximum, supremum of a set of numbers
$\bullet$; *iff*	blind index denoting objects from a given set; if and only if

INTRODUCTION

Before sailing out, we encourage the crew to get ready for adventures. Quantum mechanics deals with phenomena, which are rather unusual from 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**.

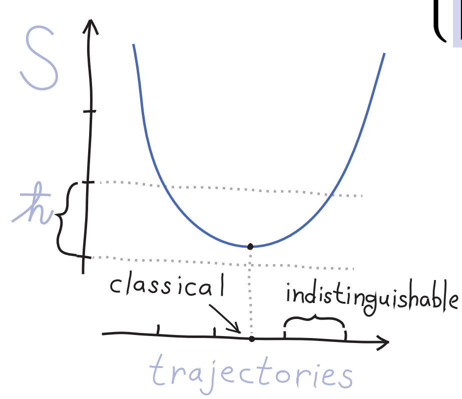
▶ Planck constant

The domain of applicability of quantum mechanics determined with the aid of a new constant: $\boxed{\hbar \doteq 1.05 \cdot 10^{-34}\,\mathrm{J\cdot s} \doteq 0.66\,\mathrm{eV\cdot fs}}$ (units of action)

▶ Consider 2 classical trajectories $\mathbf{q}_1(t)$ & $\mathbf{q}_2(t)$ (in a general multidimensional configuration space) which (in the given experimental situation) are on the limit of distinguishability. The difference of actions: $\Delta S = |S[\mathbf{q}_1(t)] - S[\mathbf{q}_2(t)]|$

Classical mechanics / **Quantum mechanics** applies if the relevant actions satisfy $\Delta S \gg \hbar$ / $\Delta S \lesssim \hbar$

In particular, if the minimum of action measured with resolution $\sim \hbar$ is wide with respect to distinguishable trajectories, quantum description is 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

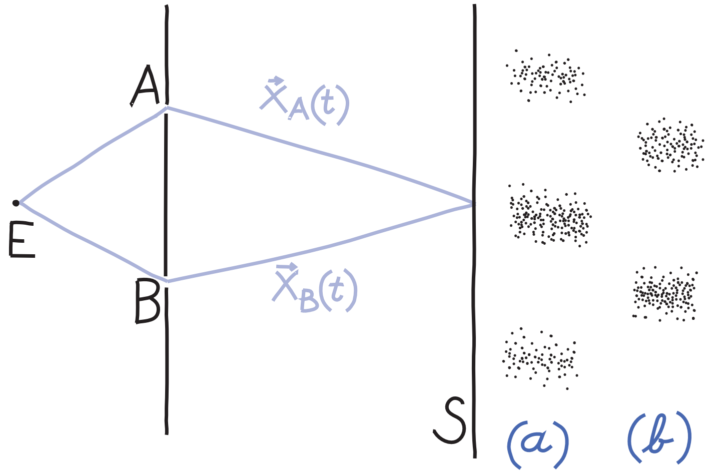
According to Richard Feynman & some others, this is the most crucial quantum experiment that allows one to realize how unusual the quantum world is.

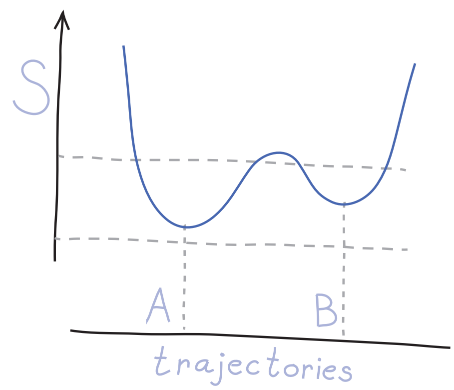
▶ Arrangement

Emitter E of *individual* particles, shield with slits A and B, screen S

Both trajectories $\vec{x}_{\mathrm{A}}(t)$ and $\vec{x}_{\mathrm{B}}(t)$ from $\vec{x}_{\mathrm{E}}$ to $\vec{x}_{\mathrm{S}}$ minimize the action

Suppose $\boxed{|S_\mathrm{A} - S_\mathrm{B}| \lesssim \hbar}$





▶ **Regimes of measurement**

(a) **Interference setup**: particle position measured only at the screen
$\Rightarrow$ interference pattern with individual particle hits

(b) **Which-path setup**: prior the screen measurement, the particle position measured immediately after the slits $\Rightarrow$ no interference pattern

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

Paradox: The outcome of the interference setup indicates a wave-like behavior of particles (passage through both slits simultaneously). The outcome of the which-path setup shows a corpuscular behavior (passage through one slit only). The outcome of the delayed-choice experiment invalidates the possibility that the particle "changes clothes" according to the setup selected.

◀ **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 & superposition principle

To explain the outcome of the interference setup of the double-slit experiment, one has to assume that particles possess some wave properties.

▶ Particle attributed by a wavefunction: $\boxed{\psi(\vec{x},t) \equiv \sqrt{\rho(\vec{x},t)}\; e^{i\varphi(\vec{x},t)}} \in \mathbb{C}$

Squared modulus $|\psi(\vec{x},t)|^2 = \rho(\vec{x},t) \geq 0$ is the **probability density** to detect the particle at position $\vec{x}$. Normalization: $\boxed{\int |\psi(\vec{x},t)|^2\, d\vec{x} = 1}$ $\forall t$

Phase $\varphi(\vec{x},t) \in \mathbb{R}$ has **no "classical" interpretation**

$\psi(\vec{x},t) \equiv$ instantaneous density of the **probability amplitude** for finding the particle at various places (**particle** is inherently a **delocalized object!**)

▶ **Superposition of wavefunctions**

The outcome of the interference setup depends on the fact that waves can be summed up. Consider 2 wavefunctions $\psi_{\rm A}(\vec{x},t)$ & $\psi_{\rm B}(\vec{x},t)$

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

$\Rightarrow$ 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 $\left\{ \begin{smallmatrix} \alpha=|\alpha|e^{i\varphi_\alpha} \\ \beta=|\beta|e^{i\varphi_\beta} \end{smallmatrix} \right\}$ such that $\int \left|\alpha\psi_{\rm A}+\beta\psi_{\rm B}\right|^2 d\vec{x} = 1$ (with $\left\{ \begin{smallmatrix} \psi_{\rm A} \\ \psi_{\rm B} \end{smallmatrix} \right\}$ normalized)

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

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

1) Initial wavefunction between emission ($t{=}0$) and slits ($t{=}t_{\rm AB}$): $\psi(\vec{x},t)$

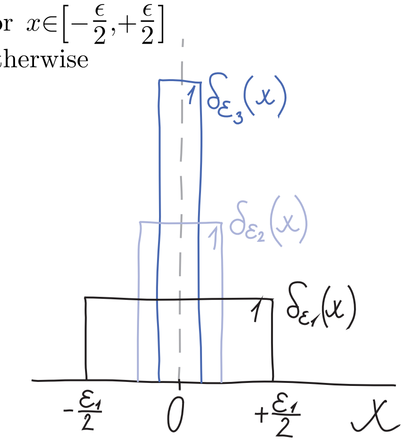
2) Wf. at $t \gtrsim t_{\rm AB}$ (right after the slits): $\psi(\vec{x},t^+_{\rm AB}) \approx \alpha\delta_{\rm A}(\vec{x}-\vec{x}_{\rm A}) + \beta\delta_{\rm B}(\vec{x}-\vec{x}_{\rm B})$ with $\delta_\bullet(\vec{x}-\vec{x}_\bullet) \equiv$ wf. localized on the respective slit ($\delta_\bullet{=}0$ away from the slit) and $\alpha,\beta \equiv$ coefficients depending on the "experimental details"

3) Wf. at $t_{\rm S}{=}t_{\rm AB}{+}\Delta t$ (just before screen): $\psi(\vec{x},t_{\rm S}) \approx \alpha\psi_{\rm A}(\vec{x},\Delta t) + \beta\psi_{\rm B}(\vec{x},\Delta t)$ with $\psi_\bullet(\vec{x},\Delta t) \equiv$ the wf. developed from $\delta_\bullet(\vec{x}-\vec{x}_\bullet)$ in time Δt

$\Rightarrow$ Distribution on screen: $\boxed{\rho(\vec{x}_{\rm S}) \approx \left|\alpha\psi_{\rm A}(\vec{x}_{\rm S},\Delta t) + \beta\psi_{\rm B}(\vec{x}_{\rm S},\Delta t)\right|^2}$

▶ **Dirac delta function** (mathematical intermezzo)

$\delta(x) \equiv$ a generalized function (distribution) $\equiv$ limit of a series of ordinary functions: $\boxed{\delta(x) = \lim_{\epsilon\to 0} \delta_\epsilon(x)}$ with, e.g.: $\delta_\epsilon(x) \equiv \left\{ \begin{array}{ll} \frac{1}{\epsilon} & \text{for } x\in[-\frac{\epsilon}{2},+\frac{\epsilon}{2}] \\ 0 & \text{otherwise} \end{array} \right.$



$$\Rightarrow \boxed{\text{Support}\,[\delta(x)] \equiv \{x{=}0\} \quad \& \quad \int_{-\infty}^{+\infty} \delta(x)\, dx = 1}$$

Other limiting realizations of δ-function:

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

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

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

In 3D space:

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

Defining property 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: $$\boxed{\overbrace{\psi(\vec{x},t)}^{|\psi(t)\rangle} = \int \psi(\vec{x}\,',t)\,\overbrace{\delta(\vec{x}-\vec{x}\,')}^{|\vec{x}\,'\rangle}\,d\vec{x}\,'}$$

$\Rightarrow$ general state $|\psi(t)\rangle \equiv$ **superposition of localized states** $|\vec{x}\,'\rangle \equiv \delta(\vec{x}-\vec{x}\,')$ with coefficients equal to the respective wavefunction values $\psi(\vec{x}\,',t)$

But note that $\delta(\vec{x}-\vec{x}\,') \notin \mathcal{L}^2(\mathbb{R}^3) \quad \Leftarrow \quad$ no sense of $|\delta(\vec{x}-\vec{x}\,')|^2$

◀ 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
1940's-60's: L. Schwarz, I.M. Gelfand, N.Y. Vilenkin work out proper mathematical background for the generalized functions (distribution theory, rigged Hilbert spaces)

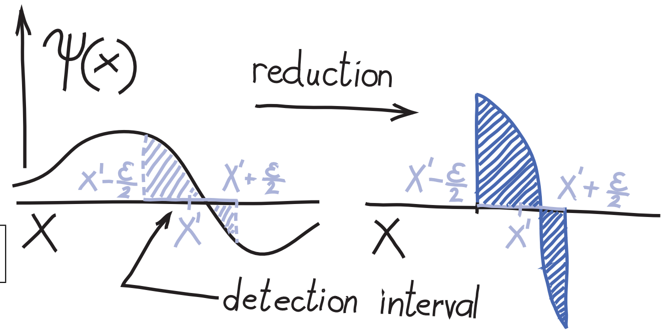
■ Quantum measurement

To explain the outcome of the which-path setup of the interference experiment, one has to assume that in quantum mechanics the measurement has a dramatic effect on the system: "**reduction**","**collapse**" of its wavefunction

▶ Change of the 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 changed:

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



In an *ideal* $(\epsilon\to 0)$ measurement:

$\boxed{\psi(\vec{x},t) \to \delta(\vec{x}-\vec{x}')}$ or $\boxed{|\psi(t)\rangle \to |\vec{x}'\rangle}$

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

1) Initial wavefunction: $\psi(\vec{x},t)$

2) After the slits: $\psi(\vec{x},t^{+}_{\rm AB})\approx\alpha\delta_{\rm A}(\vec{x}-\vec{x}_{\rm A})+\beta\delta_{\rm B}(\vec{x}-\vec{x}_{\rm B})$

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

4) Before screen: $\psi(\vec{x},t_{\rm S})\approx\begin{cases}\psi_{\rm A}(\vec{x},\Delta t) & \text{probability } \approx|\alpha|^2\\ \psi_{\rm B}(\vec{x},\Delta t) & \text{probability } \approx|\beta|^2\end{cases}$

⇒ Distribution on screen: $\boxed{\rho(\vec{x}_{\rm S})\approx|\alpha|^2|\psi_{\rm A}(\vec{x}_{\rm S},\Delta t)|^2+|\beta|^2|\psi_{\rm B}(\vec{x}_{\rm S},\Delta t)|^2}$

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

◀ **Historical remark**
1927: the first explicit note of wavefunction collapse by Werner Heisenberg
1932: inclusion of collapse into the math. formulation of QM by John von Neumann
1930's-present: discussions about physical meaning of the collapse

■ Some general consequences

Already at this initial stage, we can foresee some general features of the "quantum world", which seem counterintuitive in the classical context.

▶ **Contextuality**
Particles show either wave or corpuscular properties, in accord with the specific experimental arrangement. One may say—in more sweeping manner—that the observed "reality" emerges during the act of observation. The actual result depends on a wider "context" of the physical process that is investigated.

▶ **Quantum logic**
An attempt 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":

$$\left.\begin{array}{l}A\equiv\ \text{passage through slit A}\\ B\equiv\ \text{passage through slit B}\end{array}\right\}\rightarrow S\equiv\text{detection at given place of screen}$$

Different outcomes of interference & which-path setups indicate the inequality:

$$\boxed{\underbrace{(A\vee B)\wedge S}_{\textbf{interference setup}}\neq\underbrace{(A\wedge S)\vee(B\wedge S)}_{\textbf{which-path setup}}}\quad\Rightarrow\text{violation of a common logic axiom}$$

▶ Rule for **general branching processes** with alternative paths A & B:

Probability that the system passed through the branching (real or "logical") while its path has not been detected depends on whether the paths can/cannot, *in principle*, be distinguished (e.g., by a delayed or more detailed measurement):

Indistinguishable paths ⇒ sum of amplitudes $\boxed{\psi_{\mathrm{A}\vee\mathrm{B}} \propto \psi_{\mathrm{A}} + \psi_{B}}$

Distinguishable paths ⇒ sum of probabilities (densities) $\boxed{\rho_{\mathrm{A}\vee\mathrm{B}} \propto \rho_{\mathrm{A}} + \rho_{B}}$

◀ **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)
1936: Garrett Birkhoff and John von Neumann formally introduce quantum logic
1920's-present: Neverending discussions on the interpretation of quantum physics

1. FORMALISM ⇝ 2. SIMPLE SYSTEMS

Quantum mechanics has rather deep mathematical foundations. Such that the interpretation of abstract formalism in terms of "common sense" becomes a nontrivial issue. This may lead some of us to philosophical meditations about the link of physical theory to reality. Here we focus mostly on mastering the theory on a technical level. Elements of the abstract formalism are outlined in Chapter 1, while their simple concrete applications are sketched in Chapter 2. To keep a link between the *Geist* and *Substanz*, we present these chapters in an alternating, entangled way.

1.1 Space of quantum states

Any theory starts from identification of the relevant attributes of the system under study which are necessary for its unique characterization. In physical theories, these attributes represent specific mathematical entities which fill in some spaces.

■ Hilbert space

The formalism of quantum theory is based on mathematics matured at the beginning of 20th century. The essential idea turned out to be the following: to capture quantum uncertainty, distinct states of a system cannot be always perfectly distinguishable. The states must show some "overlaps". This is exactly the property of vectors in linear spaces.

▶ **State of a physical system**

State ≡ a "complete" set of parameters characterizing the physical system. The set does not have to be exhaustive (determining all aspects of the given system), but it has to be *complete* in the sense of *autonomous determinism*: the knowledge of state at a single time (t=0) suffices to uniquely determine the state at any time ($t \gtrless 0$).
Let $|\psi\rangle$ denote a *mathematical entity* describing an arbitrary physical state ψ of a given quantum system (shortcut: $|\psi\rangle \equiv$ "a state"). Let $\mathcal{H}$ be a system-specific *space* of all such entities.

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

$|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{C} \Rightarrow$ $$\boxed{|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle \quad \in \mathcal{H}}$$

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

Scaling $|\psi'\rangle = \alpha|\psi\rangle$ has no physical consequences: states = rays of vectors

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

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

Norm: $||\psi||^2 \equiv \langle\psi|\psi\rangle$

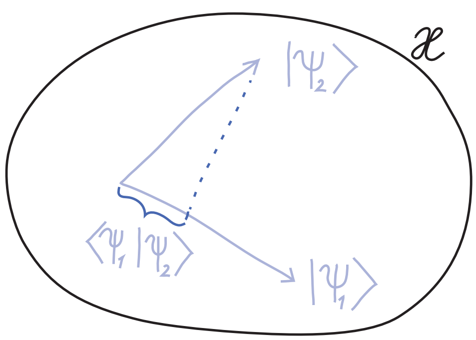
$\Rightarrow$ Distance: $d^2(\psi_1, \psi_2) \equiv ||\psi_1 - \psi_2||^2 = \langle\psi_1|\psi_1\rangle + \langle\psi_2|\psi_2\rangle - 2\text{Re}\langle\psi_1|\psi_2\rangle$

$\Rightarrow$ Normalized state vector: $\langle\psi|\psi\rangle = 1$

Schwarz inequality: $|\langle\psi_1|\psi_2\rangle|^2 \leq \underbrace{\langle\psi_1|\psi_1\rangle}_{1}\underbrace{\langle\psi_2|\psi_2\rangle}_{1}$

Why we need scalar product:
Outcomes of measurements on a quantum system are in general **indeterministic** (described in the probabilistic way, see Sec. 1.2). A single measurement does not allow one to uniquely determine the state. Quantum **amplitude** & **probability** to identify state $|\psi_2\rangle$ with $|\psi_1\rangle$ or vice versa (for $||\psi_1||=||\psi_2||=1$) in an "optimal" single measurement:

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



Consequence: States $|\psi_1\rangle, |\psi_2\rangle$ are perfectly distinguishable *iff* orthogonal

General QM terminology:

amplitude $A \in \mathbb{C}$

probability $|A|^2 \equiv P \in [0, 1]$

▶ **Requirement 3**: $\mathcal{H}$ is *complete* (for "security" reasons)

$\forall$ converging sequence of vectors the limit $\in \mathcal{H}$

▶ 1)+2)+3)$\Rightarrow$ **Postulate**: space of physical states $\mathcal{H}$ = **Hilbert space**

▶ $\mathcal{H}$ is **separable** if $\exists$ countable (sometimes finite) basis of vectors

Systems with finite particle numbers, subspaces of selected degrees of freedom

$\{|\phi_i\rangle\}_i \equiv$ an orthonormal basis $\langle\phi_i|\phi_j\rangle = \delta_{ij}$ $\Rightarrow$
Each state $|\psi\rangle$ can be expressed as a complex superposition of an enumerable set of basis states $|\phi_i\rangle$

$$\boxed{|\psi\rangle = \sum_i \underbrace{\langle\phi_i|\psi\rangle}_{\alpha_i} |\phi_i\rangle}$$

▶ $\mathcal{H}$ is **nonseparable** if it has *no countable basis*

Systems with unbounded particle numbers, quantum fields, continuum

▶ **Any separable $\mathcal{H}$ is isomorphic with ℓ^2**

Definition of the ℓ^2 **space**: infinite "columns" $|\psi\rangle \equiv \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix}$ with $\sum_{i=1}^{\infty} |\alpha_i|^2 < \infty$

Mapping $\mathcal{H} \to \ell^2$: components α_i associated with expansion coefficients $\langle\phi_i|\psi\rangle$ of $|\psi\rangle$ in a given basis

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: $\langle\psi|\psi'\rangle \equiv \sum_i \alpha_i^* \alpha'_i = (\alpha_1^*, \alpha_2^*, \ldots) \begin{pmatrix} \alpha'_1 \\ \alpha'_2 \\ \vdots \end{pmatrix}$

◀ **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 (Sec. 2.1) that its suitable extension is very helpful.

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

$\underline{\mathcal{H}} \equiv$ sequences $|\psi\rangle$ with $\sum_i |\alpha_i|^2 i^m < \infty$ for $m = 0, 1, 2, \ldots$ (dense subset of ℓ^2)

$\overline{\mathcal{H}}$ (conjugate space to $\underline{\mathcal{H}}$) $\equiv$ sequences $|\psi\rangle$ for which $\langle\psi'|\psi\rangle < \infty \; \forall |\psi'\rangle \in \underline{\mathcal{H}}$

$\Rightarrow \sum_i \alpha_i'^* \alpha_i < \infty \Rightarrow \sum_i |\alpha_i|^2 \frac{1}{i^m} < \infty \Rightarrow |\alpha_i|^2$ may polynomially diverge

These are linear vector spaces but not Hilbert spaces:

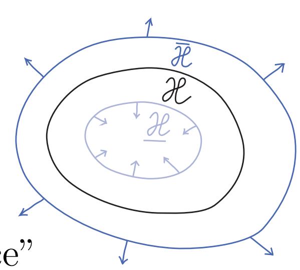
$\underline{\mathcal{H}}$ is not complete

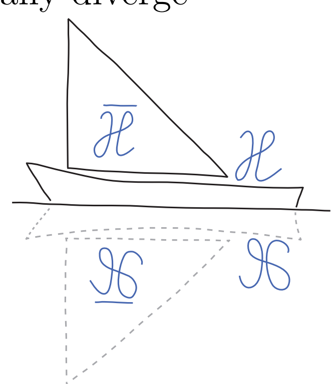
$\overline{\mathcal{H}}$ does not have scalar product

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

▶ **Gelfand triplet** ("sandwich")

$\boxed{\underline{\mathcal{H}} \subset \mathcal{H} \subset \overline{\mathcal{H}}}$ $\equiv$ "rigged Hilbert space"





It turns out that solutions of some basic quantum problems $\notin \mathcal{H}$ but $\in \overline{\mathcal{H}}$, while the definition domain of some quantum operators is not $\mathcal{H}$ but $\underline{\mathcal{H}}$

■ 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.