Second Edition

THE PICTURE BOOK OF QUANTUM MECHANICS

图解量子力学

第 2 版

S. Brandt
H. D. Dahmen

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To Renate Brandt
and Ute Dahmen

Foreword to the Second Edition

In the present edition aim and style of the *Picture Book* were left unchanged. It is our aim to explain and exemplify the concepts and results of quantum mechanics by visualization through computer graphics and, in parallel, by the discussion of the relevant physical laws and mathematical formulae. The scope of the book, however, was widened appreciably.

The most important extension is the chapter about *spin* and *magnetic resonance*. In three-dimensional quantum mechanics the presentation of *wave-packet motion on elliptical and hyperbolic Kepler orbits* should help to establish the correspondence and the differences between the classical and the quantum-mechanical description of planetary motion.

Maybe the best known quantum-mechanical concept is that of uncertainty introduced by Heisenberg who formulated the celebrated uncertainty relation $\Delta x \Delta p \geq \hbar/2$ for the product of the uncertainties of a particle in position and in momentum. Also in classical mechanics position and momentum of a particle may be known only up to some uncertainty so that a probability density in phase space (spanned by position x and momentum p) is needed to describe the particle. For many physical situations we present and compare the time development of this *classical phase-space probability density* with the probability density of quantum mechanics.

An additional tool we use is the *analyzing amplitude* introduced in Appendix C. It allows the definition of a directional distribution which is very helpful in visualizing angular momentum and spin wave functions.

To generate the computer graphics of the first edition of the *Picture Book* we developed an interactive program on quantum mechanics. A modernized version which we call INTERQUANTA (abbreviated **IQ**) together with an accompanying text has been published by Springer-Verlag in various editions.[1–4] It is a pleasure to acknowledge the generous help provided by IBM Germany in the development of **IQ**. In particular we want to thank Dr. U. Groh for his competent help in the early phase of the work. At various stages of the project we were helped considerably by friends and students in Siegen. We would particularly like to thank Tilo Stroh for his many valuable contributions.

All computer-drawn figures in the present edition were produced using the published version of **IQ** or recent extensions realized with the help of Sergei Boris, Anli Shundi, and Tilo Stroh. The computer typesetting and the layout of the text were done by Ute Bender and Anli Shundi. We would like to thank them for their excellent work.

Last but not least, we thank Drs. H.-U. Daniel, T. von Foerster, and H. J. Kölsch of Springer-Verlag for their constant interest and support.

Siegen, May 1994

Siegmund Brandt
Hans Dieter Dahmen

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[1] S. Brandt and H. D. Dahmen, *Quantum Mechanics on the Personal Computer*, 3rd ed., Springer-Verlag, Berlin, Heidelberg, New York, 1994.

[2] S. Brandt and H. D. Dahmen, *Quantum Mechanics on the Macintosh*, Springer-Verlag, New York, Berlin, Heidelberg, 1991.

[3] S. Brandt and H. D. Dahmen, *Pasocon de Manebu Ryoushi Nikigacu*, Springer-Verlag, Tokyo, 1992.

[4] S. Brandt and H. D. Dahmen, *Quantenmechanik auf dem Personalcomputer*, Springer-Verlag, Berlin, Heidelberg, New York, 1993.

Preface

Students of classical mechanics can rely on a wealth of experience from everyday life to help them understand and apply mechanical concepts. Even though a stone is not a mass point, the experience of throwing stones certainly helps them to understand and analyze the trajectory of a mass point in a gravitational field. Moreover, students can solve many mechanical problems on the basis of Newton's laws and, in doing so, gain additional experience. When studying wave optics, they find that their knowledge of water waves, as well as experiments in a ripple tank, are very helpful in forming an intuition about the typical wave phenomena of interference and diffraction.

In quantum mechanics, however, beginners are without any intuition. Because quantum-mechanical phenomena happen on an atomic or a subatomic scale, we have no experience of them in daily life. The experiments in atomic physics involve more or less complicated apparatus and are by no means simple to interpret. Even if students are able to take Schrödinger's equation for granted, as many students do Newton's laws, it is not easy for them to acquire experience in quantum mechanics through the solution of problems. Only very few problems can be treated without a computer. Moreover, when solutions in closed form are known, their complicated structure and the special mathematical functions, which students are usually encountering for the first time, constitute severe obstacles to developing a heuristic comprehension. The most difficult hurdle, however, is the formulation of a problem in quantum-mechanical language, for the concepts are completely different from those of classical mechanics. In fact, the concepts and equations of quantum mechanics in Schrödinger's formulation are much closer to those of optics than to those of mechanics. Moreover, the quantities that we are interested in – such as transition probabilities, cross sections, and so on – usually have nothing to do with mechanical concepts such as the position, momentum, or trajectory of a particle. Nevertheless, actual insight into a process is a prerequisite for understanding its quantum-mechanical description and interpreting basic properties in quantum mechanics like position, linear and angular momentum, as well as cross sections, lifetimes, and so on.

Actually, students must develop an intuition of how the concepts of classical mechanics are altered and supplemented by the arguments of optics in order to acquire a roughly correct picture of quantum mechanics. In particular, the time evolution of microscopic physical systems has to be studied to establish how it corresponds to classical mechanics. Here computers and computer graphics offer incredible help, for they produce a large number of examples which are very detailed and which can be looked at in any phase of their time development. For instance, the study of wave packets in motion, which is practically impossible without the help of a computer, reveals the limited validity of intuition drawn from classical mechanics and gives us insight into phenomena like the tunnel effect and resonances, which, because of the importance of interference, can be understood only through optical analogies. A variety of systems in different situations can be simulated on the computer and made accessible by different types of computer graphics.

Some of the topics covered are

- scattering of wave packets and stationary waves in one dimension,
- the tunnel effect,
- decay of metastable states,
- bound states in various potentials,
- energy bands,
- distinguishable and indistinguishable particles,
- angular momentum,
- three-dimensional scattering,
- cross sections and scattering amplitudes,
- eigenstates in three-dimensional potentials, for example, in the hydrogen atom, partial waves and resonances,
- motion of wave packets in three dimensions,
- spin and magnetic resonance.

As conceptual tools bridging between classical and quantum concepts serve

- the phase-space probability density of statistical mechanics,
- the Wigner phase-space distribution,

- the absolute square of the analyzing amplitude as probability or probability density.

The graphical aids comprise

- time evolutions of wave functions for one-dimensional problems,
- parameter dependences for studying, for example, the scattering over a range of energies,
- three-dimensional surface plots for presenting two-particle wave functions or functions of two variables,
- polar (antenna) diagrams in two and three dimensions,
- plots of contour lines or contour surfaces, i.e., constant function values, in two and three dimensions,
- ripple-tank pictures to illustrate three-dimensional scattering.

Whenever possible, how particles of a system would behave according to classical mechanics has been indicated by their positions or trajectories. In passing, the special functions typical for quantum mechanics, such as Legendre, Hermite, and Laguerre polynomials, spherical harmonics, and spherical Bessel functions, are also shown in sets of pictures.

The text presents the principal ideas of wave mechanics. The introductory Chapter 1 lays the groundwork by discussing the particle aspect of light, using the fundamental experimental findings of the photoelectric and Compton effects and the wave aspect of particles as it is demonstrated by the diffraction of electrons. The theoretical ideas abstracted from these experiments are introduced in Chapter 2 by studying the behavior of wave packets of light as they propagate through space and as they are reflected or refracted by glass plates. The photon is introduced as a wave packet of light containing a quantum of energy.

To indicate how material particles are analogous to the photon, Chapter 3 introduces them as wave packets of de Broglie waves. The ability of de Broglie waves to describe the mechanics of a particle is explained through a detailed discussion of group velocity, Heisenberg's uncertainty principle, and Born's probability interpretation. The Schrödinger equation is found to be the equation of motion.

Chapters 4 through 8 are devoted to the one-dimensional quantum-mechanical systems. Study of the scattering of a particle by a potential helps us understand how it moves under the influence of a force and how the probability interpretation operates to explain the simultaneous effects of transmission and reflection. We study the tunnel effect of a particle and the excitation and decay of a metastable state. A careful transition to a stationary bound state is carried out. Quasi-classical motion of wave packets confined to the potential range is also examined.

Chapters 7 and 8 cover two-particle systems. Coupled harmonic oscillators are used to illustrate the concept of indistinguishable particles. The striking differences between systems composed of different particles, systems of identical bosons, and systems of identical fermions obeying the Pauli principle are demonstrated.

Three-dimensional quantum mechanics is the subject of Chapters 9 through 14. We begin with a detailed study of angular momentum and discuss methods of solving the Schrödinger equation. The scattering of plane waves is investigated by introducing partial-wave decomposition and the concepts of differential cross sections, scattering amplitudes, and phase shifts. Resonance scattering, which is the subject of many fields of physics research, is studied in detail in Chapter 13. Bound states in three dimensions are dealt with in Chapter 12. The hydrogen atom and the motion of wave packets under the action of a harmonic force as well as the Kepler motion on elliptical orbits are among the topics covered. Chapter 14 is devoted to Coulomb scattering in terms of stationary wave functions as well as wave-packet motion on hyperbolical orbits.

Spin is treated in Chapter 15. After the introduction of spin states and operators the Pauli equation is used for the description of the precession of a magnetic moment in a homogeneous magnetic field. The discussion of Rabi's magnetic resonance concludes this chapter.

The last chapter is devoted to results obtained through experiments in atomic, molecular, solid-state, nuclear, and particle physics. They can be qualitatively understood with the help of the pictures and the discussion in the body of the book. Thus examples for

- typical scattering phenomena,
- spectra of bound states and their classifications with the help of models,
- resonance phenomena in total cross sections,
- phase-shift analyses of scattering and Regge classification of resonances,
- radioactivity as decay of metastable states,
- magnetic resonance phenomena,

taken from the fields of atomic and subatomic physics, are presented. Comparing these experimental results with the computer-drawn pictures of the book and their interpretation gives the reader a glimpse of the vast fields of science that can be understood only on the basis of quantum mechanics.

In Appendix A the simplest aspects of the structure of quantum mechanics are discussed and the matrix formulation in an infinite-dimensional vector space is juxtaposed to the more conventional formulation in terms of wave functions and differential operators. Appendix B gives a short account of two-level systems which is helpful for the discussion of spin. In Appendix C we introduce the analyzing amplitude using as examples the free particle and the harmonic oscillator. Appendix D discusses Wigner's phase-space distribution. Appendixes E through G give short accounts of the gamma, Bessel, and Airy functions, as well as the Poisson distribution.

There are more than a hundred problems at the ends of the chapters. Many are designed to help students extract the physics from the pictures. Others will give them practice in handling the theoretical concepts. On the endpapers of the book are a list of frequently used symbols, a short list of physical constants, and a brief table converting SI units to particle-physics units. The constants and units will make numerical calculations easier.

We are particularly grateful to Professor Eugen Merzbacher for his kind interest in our project and for many valuable suggestions he gave before the publication of the first edition and which helped to improve the book.

Siegmund Brandt
Hans Dieter Dahmen

Frequently Used Symbols

a	Bohr radius
$a(x_0, p_0, x_S, p_S)$	analyzing amplitude
$A_I, A_{II}, \ldots$ $B_I, B_{II}, \ldots$	amplitude factors in regions I, II, ... of space
$\mathbf{B}$	magnetic-induction field
c	speed of light
c	correlation coefficient
$d^\ell_{mm'}$	Wigner function
$D^\ell_{mm'}$	Wigner function
$\mathrm{d}\sigma/\mathrm{d}\Omega$	differential scattering cross section
e	elementary charge
E_c	complex electric field strength
E	energy
E_n	energy eigenvalue
E_{kin}	kinetic energy
$\mathbf{E}$	electric field strength
$f(k)$	spectral function with respect to wave number
$f(p)$	spectral function with respect to momentum
$f(\vartheta)$	scattering amplitude
f_ℓ	partial scattering amplitude
$f_{\ell m}(\Theta, \Phi)$	directional distribution
g	gyromagnetic factor
h $\hbar = h/(2\pi)$	Planck's constant
$h_\ell^{(+)}(\rho)$	spherical Hankel function of the first kind
$h_\ell^{(-)}(\rho)$	spherical Hankel function of the second kind
H	Hamiltonian
j	probability current density
$j_\ell(\rho)$	spherical Bessel function
k	wave number
ℓ	angular-momentum quantum number
L_n^α	Laguerre polynomials
$\mathbf{L}$	angular momentum
$\hat{\mathbf{L}}$	angular-momentum operator
m	quantum number of z component of angular momentum
$m,\ M$	mass
$M(x,t)$	amplitude function
$\mathbf{M}$	magnetization
n	refractive index
n	principal quantum number
$n_\ell(\rho)$	spherical Neumann function
$\mathbf{n}$	unit vector
p	momentum
$\hat{p}$	momentum operator
$\langle p \rangle$	momentum expectation value
$\mathbf{p}$	momentum vector
$\hat{\mathbf{p}}$	vector operator of momentum
P_ℓ	Legendre polynomial
P_ℓ^m	associated Legendre function
r	relative coordinate
r	radial distance
$\mathbf{r}$	position vector
R	center-of-mass coordinate

$R(r)$, $R_\ell(k,r)$	radial wave function
$R_{n\ell}$	radial eigenfunction
s	spin quantum number
$\mathbf{S} = (\mathrm{S}_1, \mathrm{S}_2, \mathrm{S}_3)$	spin-vector operator
S_ℓ	scattering-matrix element
t	time
T	oscillation period
T	transmission coefficient
T	kinetic energy
T_T, T_R	transition-matrix elements
U	voltage
v_0	group velocity
v_p	phase velocity
V	potential (energy)
V_ℓ^eff	effective potential
w	average energy density
W	Wigner distribution
W	energy
W_ℓ, $W_{\ell m}$	coefficients in the angular decomposition of a wave packet
x	position
$\langle x\rangle$	position expectation value
$Y_{\ell m}$	spherical harmonic
Z	atomic number
α	fine-structure constant
δ_ℓ	scattering phase shift
Δk	wave-number uncertainty
Δp	momentum uncertainty
Δx	position uncertainty
ε_0	vacuum permittivity
η_1, η_{-1}	spin $\frac{1}{2}$ base states
$\eta_\mathbf{k}(\mathbf{r})$	scattered wave
$\eta_\ell(\mathbf{r})$	scattered partial wave
ϑ, Θ	polar angle
ϑ	scattering angle
λ	wavelength
μ_0	vacuum permeability
μ	reduced mass
$\boldsymbol{\mu}$	magnetic moment
ρ	probability density
ρ^cl	classical phase-space probability density
σ_0	width of ground state of harmonic oscillator
σ_1, σ_2, σ_3	Pauli matrices
σ_k	width in wave number
σ_ℓ	partial cross section
σ_p	width in momentum
σ_x	width in position
σ_tot	total cross section
$\varphi(x)$	stationary wave function
$\varphi_\mathbf{p}(\mathbf{r})$	stationary harmonic wave function
$\boldsymbol{\varphi}$	state vector of stationary state
ϕ, Φ	azimuthal angle
χ	magnetic susceptibility
$\boldsymbol{\chi}$	general spin state
$\psi(x,t)$	time-dependent wave function
$\psi_\mathbf{p}(\mathbf{r},t)$	harmonic wave function
$\boldsymbol{\psi}$	state vector
ω	angular frequency
Ω	solid angle
∇	nabla (or del) operator
∇^2	Laplace operator

Basic Equations

de Broglie wave	$\psi_{\mathbf{p}}(\mathbf{r},t) = \frac{1}{(2\pi\hbar)^{3/2}} \exp\left(-\frac{\mathrm{i}}{\hbar}Et\right) \exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)$
time-dependent Schrödinger equation	$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r},t)$
stationary Schrödinger equation	$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r})\right]\varphi_E(\mathbf{r}) = E\varphi_E(\mathbf{r})$
momentum operators	$\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) = \frac{\hbar}{\mathrm{i}}\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = \frac{\hbar}{\mathrm{i}}\nabla$
angular-momentum operators	$\hat{\mathbf{L}} = \mathbf{r}\times\hat{\mathbf{p}} = \frac{\hbar}{\mathrm{i}}\mathbf{r}\times\nabla$
radial Schrödinger equation for spherically symmetric potential	$-\frac{\hbar^2}{2M}\left[\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r - \frac{\ell(\ell+1)}{r^2} - \frac{2M}{\hbar^2}V(r)\right]R_\ell(k,r) = ER_\ell(k,r)$
stationary scattering wave	$\varphi_{\mathbf{k}}^{(+)}(\mathbf{r}) \xrightarrow[kr \gg 1]{} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} + f(\vartheta)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}$
scattering amplitude	$f(\vartheta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\vartheta)$
differential, partial, and total cross sections	$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \lvert f(\vartheta)\rvert^2\,, \quad \sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\lvert f_\ell(k)\rvert^2\,, \quad \sigma_{\mathrm{tot}} = \sum_{\ell=0}^{\infty}\sigma_\ell$

Physical Constants

Planck's constant	$h = 4.136 \cdot 10^{-15}\,\mathrm{eV \cdot s} = 6.626 \cdot 10^{-34}\,\mathrm{J \cdot s}$ $\hbar = h/(2\pi) = 6.582 \cdot 10^{-16}\,\mathrm{eV \cdot s}$ $= 1.055 \cdot 10^{-34}\,\mathrm{J \cdot s}$
speed of light	$c = 2.998 \cdot 10^{8}\,\mathrm{ms^{-1}}$
elementary charge	$e = 1.602 \cdot 10^{-19}\,\mathrm{C}$
fine-structure constant	$\alpha = \dfrac{e^2}{4\pi\epsilon_0 \hbar c} = \dfrac{1}{137.036}$
electron mass	$m_e = 0.5110\,\mathrm{MeV}/c^2 = 9.110 \cdot 10^{-31}\,\mathrm{kg}$
proton mass	$m_p = 938.3\,\mathrm{MeV}/c^2 = 1.673 \cdot 10^{-27}\,\mathrm{kg}$
neutron mass	$m_n = 939.6\,\mathrm{MeV}/c^2 = 1.675 \cdot 10^{-27}\,\mathrm{kg}$

Conversion Factors

mass	$1\,\mathrm{kg} = 5.609 \cdot 10^{35}\,\mathrm{eV}/c^2$,	$1\,\mathrm{eV}/c^2 = 1.783 \cdot 10^{-36}\,\mathrm{kg}$
energy	$1\,\mathrm{J} = 6.241 \cdot 10^{18}\,\mathrm{eV}$,	$1\,\mathrm{eV} = 1.602 \cdot 10^{-19}\,\mathrm{J}$
momentum	$1\,\mathrm{kg \cdot ms^{-1}} = 1.871 \cdot 10^{27}\,\mathrm{eV}/c$,	$1\,\mathrm{eV}/c = 5.345 \cdot 10^{-28}\,\mathrm{kg \cdot ms^{-1}}$

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