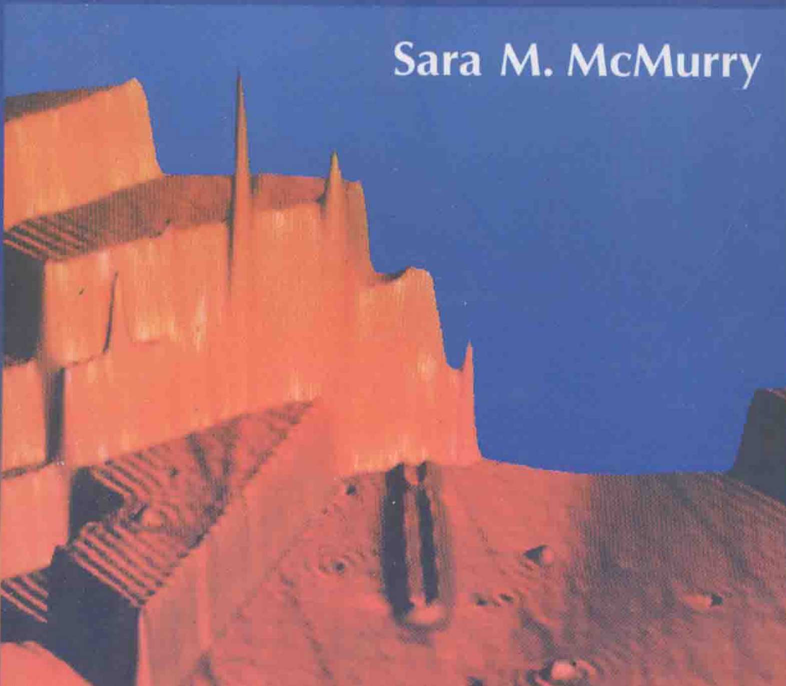
# QUANTUM MECHANICS

# 量子力学

Sara M. McMurry



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书　　名：Quantum Mechanics
作　　者：S.M.McMurry
中 译 名：量子力学
出 版 者：世界图书出版公司北京公司
印 刷 者：北京世图印刷厂
发　　行：世界图书出版公司北京公司（北京朝阳门内大街 137 号　100010）
开　　本：大 32 开　850 × 1168　印　张：12.25
版　　次：1998 年 8 月第 1 版　1998 年 8 月第 1 次印刷
书　　号：7-5062-3826-8/ O•236
版权登记：图字 01-98-0646
定　　价：68.00 元

Cover designed by Designers & Partners, Oxford
and printed by The Riverside Printing Co. (Reading) Ltd.
Typeset by Keytec Typesetting, Bridport, Dorset.
Printed and bound in Great Britain by T.J. Press (Padstow) Ltd, Cornwall.

First printed 1993

ISBN 0-201-54439-3

**British Library Cataloguing-in-Publication Data**
A catalogue record for this book is available from the British Library.

**Library of Congress Cataloging-in-Publication Data is available**

This edition of **Quantum Mechanics, First edition** is published by arrangement with Addison Wesley Longman Limited, London

# Preface

Perhaps the best way for students of experimental physics to meet quantum theory for the first time is through a course in quantum physics, in which the emphasis is on a description of quantum phenomena and the general ideas (such as the uncertainty principle) that are essential for explaining them. The aim of such a course would be to give the students some feeling for the experimental phenomena described by quantum theory, and an understanding of how classical mechanics fails to explain them. They are then ready for a more mathematical presentation of quantum mechanics in the final two years of their undergraduate course. This text is intended to cover a course of the latter type, and the first chapter is a rapid overview of the important ideas that I assume students will have already met in an introductory course.

## Maths and quantum physics

A course in quantum mechanics inevitably introduces some mathematics that is unfamiliar to most students. The reader of this text is expected to have a good knowledge of elementary calculus (including integration by parts), vectors and the solution of simple differential equations – that is, those of first order, and of second order with constant coefficients. Chapter 9 uses the expansion of a function in a Fourier series to introduce the superposition principle, and in Chapter 10 some elementary knowledge of matrix algebra is assumed. Appropriate references are provided for those not familiar with these last two topics. Concepts associated with the use of linear operators, their commutation relations and eigenvalue equations are introduced in the text, assuming no prior knowledge on the part of the reader.

It is important that students should try to come to grips with the basic mathematical ideas that are necessary for a proper understanding of quantum theory. However, this does not mean that they need to become experts at actually performing complex mathematical operations. In practice almost all quantum calculations on real systems can only be performed numerically, using a computer. What is necessary, therefore, is that the student should acquire an understanding of the overall strategy of solving the mathematical problems that arise in quantum mechanics – he or she should understand the nature of the predictions that it is possible to make about a given physical system, the type of mathematical calculation that is entailed, the way physical restrictions on the system are translated into mathematics, and what sort of results to expect.

## Content and organization

It is traditional in textbooks on quantum mechanics to collect the basic mathematical ideas together in one chapter, with a title that is some variation of 'Mathematical foundations of quantum mechanics'. Although this is logical and concise, I feel that it is not the best approach for the student meeting the formal theory for the first time. In contrast I have spread the mathematical ideas throughout the text, using and expanding on one concept before introducing the next.

The fundamental assumptions on which quantum mechanics is based are encapsulated in four postulates, to be found in Chapters 2, 3, 9 and 12. Chapter 2 concerns the wave function and its probability interpretation, and Chapter 3 introduces the operator representation of dynamical variables, and the idea of an eigenvalue equation, in particular the time-independent Schrödinger equation. Chapters 4–8 continue the discussion of solutions of eigenvalue equations, in particular those for energy (the time-independent Schrödinger equation) and angular momentum. Commutators are introduced in Chapter 4, and are used throughout the book as an important tool, not only mathematically (as in Chapters 5 and 6, where they are applied in the solution of eigenvalue problems by algebraic methods) but also as an indication of the physical characteristics of a system (as in Chapter 7, where they are used to investigate the state of a particle in a central potential).

The description of an arbitrary state of a particle through the superposition principle is introduced in Chapter 9, and this mathematical formalism is necessary, to a greater or lesser extent, for developments in the last five chapters. It is impossible to cover all aspects of non-relativistic quantum mechanics in a single book. Important topics that are discussed briefly include the matrix formulation of the theory (Chapter 10), approximate methods for solving the Schrödinger equation (Chapter 11), time-dependent problems (Chapter 12), and the idea of a joint probability distribution for a system of many non-interacting particles (Chapter 13). Quantum scattering theory is omitted, but it would be artificial to avoid all mention of scattering experiments, since they provide such an important means of investigating quantum systems. Consequently scattering from a potential step and from a square well is discussed in Chapter 3, and the Born approximation is derived as an example of the application of time-dependent perturbation theory in Chapter 12. The final chapter is not intended to be part of an examined course, but aims to clarify the concepts of indeterminacy and non-locality that underlie quantum mechanics.

## Examples

The physical examples used in the text have been chosen to reflect the enormously wide range of phenomena explained by quantum mechanics, and include some (in particular the scanning tunnelling microscope and quantum well structures) that are of importance in modern technology. Restrictions in the time allotted to a lecture course would usually make it impossible to cover all the examples mentioned, but many would be encountered in parallel physics courses – on spectroscopy or condensed matter physics, for example.

## Problems

Problems are provided at the end of each chapter, some of which are fairly simple elaborations on the text, while others extend the theory that has been presented to different systems. Some problems (indicated by an asterisk) refer to programs on the accompanying computer disk, and provide detailed suggestions for using them. Briefly, the interactive programs allow students to solve energy eigenvalue equations for a range of systems and plot the associated wave functions and probability distributions, to examine the transmission of a plane wave through a one-dimensional square well or barrier, to watch the scattering of a Gaussian wave packet by a square barrier, and to construct wave packets for a particle in an infinitely deep one-dimensional square well or a one-dimensional simple harmonic oscillator and observe how they evolve with time.

The programs on the disk are described in detail in Appendix C. The full menu is as follows:

(1) The one-dimensional Schrödinger equation
  (a) Infinite square well
  (b) Finite square well
  (c) Harmonic oscillator
  (d) Anharmonic oscillator
  (e) Triangular well
(2) The Kronig–Penney model
(3) The Schrödinger equation: central potentials
  (a) Coulomb potential
  (b) Harmonic oscillator (three-dimensional)
(4) Orbital angular momentum
(5) Transmission
  (a) Plane wave, one-dimensional square well
  (b) Plane wave, one-dimensional square barrier
  (c) Gaussian wave packet, one-dimensional square barrier
(6) Wave packets (one-dimensional)
  (a) Infinite square well
  (b) Harmonic oscillator

The disk will run on any IBM-compatible pc, with at least a VGA monitor, though some of the programs will be rather slow on machines without a maths co-processor.

It should be noted that the software on the disk is free to qualified adopters only.

## Acknowledgements

I should like to thank all my colleagues for useful discussions, advice, and technical information, and in particular Professor D.L. Weaire and Dr E.C. Finch for critical reading of the whole manuscript. I also wish to thank Andrew McMurry for writing the computer programs on the accompanying disc, and Fergal Toomey for the program demonstrating the scattering of a Gaussian wave packet. Finally, I am indebted to all those students on whom I have experimented with methods of teaching quantum mechanics over the last 25 years!

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# List of Symbols and Physical Constants

## Physical constants

| | | |
|---|---|---|
| $\alpha$ | $7.297 \times 10^{-3} = 1/137.04$ | fine structure constant |
| $c$ | $2.998 \times 10^{8}\ \mathrm{m\,s^{-1}}$ | speed of light in vacuum |
| $E_{\mathrm{R}}$ | $13.61\ \mathrm{eV}$ | Rydberg energy |
| $e$ | $1.602 \times 10^{-19}\ \mathrm{C}$ | magnitude of electron charge |
| $\varepsilon_0$ | $8.854 \times 10^{-12}\ \mathrm{F\,m^{-1}}$ | permittivity of free space |
| $h$ | $6.626 \times 10^{-34}\ \mathrm{J\,s}$ | Planck's constant |
| $\hbar$ | $1.055 \times 10^{-34}\ \mathrm{J\,s}$ | |
| $k_{\mathrm{B}}$ | $1.381 \times 10^{-23}\ \mathrm{J\,K^{-1}}$ | Boltzmann's constant |
| $m_{\mathrm{e}}$ | $9.11 \times 10^{-31}\ \mathrm{kg}$ | electron rest mass |
| $m_{\mathrm{p}}$ | $1.673 \times 10^{-27}\ \mathrm{kg}$ | proton rest mass |
| $\mu_{\mathrm{B}}$ | $9.274 \times 10^{-24}\ \mathrm{J\,T^{-1}}$ | Bohr magneton |
| $N_{\mathrm{A}}$ | $6.022 \times 10^{23}\ \mathrm{mol^{-1}}$ | Avogadro's constant |
| $R_{\mathrm{H}}$ | $1.0968 \times 10^{7}\ \mathrm{m^{-1}}$ | Rydberg constant for hydrogen |
| $r_{\mathrm{B}}$ | $5.292 \times 10^{-11}\ \mathrm{m}$ | Bohr radius |

## List of symbols

| | |
|---|---|
| $A$ | atomic mass number |
| $A_n$ | Fourier expansion coefficient |
| $\hat{A}$, $\hat{A}^{\dagger}$ | ladder operators |
| $\hat{A}$, $\hat{B}$, ... | linear Hermitian operators |
| $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$ | matrices |
| $A_{ij}$, $\hat{A}_{ij}$ | matrix elements |
| $\boldsymbol{A}^{\mathrm{T}}$ | transpose of matrix |

# List of symbols and physical constants

| | |
|---|---|
| $\boldsymbol{A}^*$ | complex conjugate of matrix |
| $\boldsymbol{A}^\dagger$ | Hermitian conjugate of matrix |
| $\det(\boldsymbol{A})$ | determinant of matrix |
| $\mathcal{A}, \mathcal{A}_x, \mathcal{A}_y, \mathcal{A}_z$ | electromagnetic vector potential and its components |
| $\mathbb{A}$ | area |
| $\hat{a}, \hat{a}^\dagger$ | annihilation and creation operators |
| $a_n, a$ | eigenvalues of $\hat{A}$ |
| $\mathcal{B}, \mathcal{B}_x, \mathcal{B}_y, \mathcal{B}_z$ | magnetic induction and its components |
| $\boldsymbol{b}, \boldsymbol{b}_n$ | state vector and its components |
| $\boldsymbol{b}^\dagger$ | Hermitian conjugate of state vector |
| $C(j, j_z; l, m_l, s, m_s)$ | Clebsch–Gordan coefficient |
| $c_s$ | velocity of sound in a crystal lattice |
| $c_v$ | specific heat |
| $\mathcal{D}$ | electric dipole moment |
| $\hat{\mathcal{D}}$ | electric dipole moment operator |
| $\dfrac{d\sigma}{d\Omega}$ | differential cross-section |
| $d\Omega$ | element of solid angle |
| $E, E_{tot}$ | total energy |
| $E_D$ | dissociation energy of diatomic molecule |
| $E_F$ | Fermi energy |
| $E_G$ | energy gap |
| $E_G$ | ground state energy |
| $E_R$ | Rydberg energy |
| $\hat{E}_{tot}$ | total energy operator |
| $\mathbb{E}$ | correlation function |
| $\mathcal{E}, \mathcal{E}_x, \mathcal{E}_y, \mathcal{E}_z$ | electric field strength and its components |
| $\mathscr{E}$ | electromagnetic energy density |
| $\mathcal{F}$ | force |
| $g$ | electron $g$-factor |
| $g(E)$ | density of states |
| $\boldsymbol{g}$ | reciprocal lattice vector |
| $H_n$ | Hermite polynomial |
| $\hat{H}$ | Hamiltonian operator |
| $\mathscr{I}$ | electric current |
| $\mathcal{I}$ | moment of inertia |
| $J$ | total angular momentum quantum number |
| $\hat{\boldsymbol{J}}, \hat{J}_x, \hat{J}_y, \hat{J}_z$ | angular momentum operator and its components |
| $\mathscr{J}_x, \mathscr{J}_y, \mathscr{J}_z$ | components of the electric current density |
| $j, j_z$ | angular momentum quantum numbers |
| $\boldsymbol{j}$ | probability current density |
| $k, \boldsymbol{k}$ | crystal momentum |
| $\boldsymbol{k}, k_x, k_y, k_z$ | wave vector and its components |
| $L$ | orbital angular momentum quantum number |

| | |
|---|---|
| $L_k^q(x)$ | Laguerre polynomials |
| $\hat{\boldsymbol{L}}, \hat{L}_x, \hat{L}_y, \hat{L}_z$ | orbital angular momentum operator and its components |
| $\mathbb{L}$ | length |
| $l$ | orbital angular momentum quantum number |
| $M_J, M_L, M_S$ | total, orbital and spin angular momentum quantum numbers |
| $\boldsymbol{M}$ | classical angular momentum vector |
| $m$ | mass |
| $m^*$ | effective mass |
| $m_l, m_s$ | orbital and spin angular momentum quantum numbers |
| $\hat{N}$ | number operator |
| $N$ | number of unit cells |
| $N$ | number density |
| $N$ | number of events |
| $n$ | principal quantum number |
| $n_c$ | density of conduction electrons |
| $\boldsymbol{n}$ | unit vector |
| $\hat{P}_r$ | radial momentum operator |
| $P_l(\cos\theta)$ | Legendre polynomial |
| $P_l^{m_l}(\cos\theta)$ | associated Legendre function |
| $\hat{\boldsymbol{P}}, \hat{P}_x, \hat{P}_y, \hat{P}_z$ | momentum operator and its components |
| $\mathbb{P}$ | probability |
| $p_r$ | radial momentum |
| $\boldsymbol{p}$ | linear momentum |
| $q$ | electric charge |
| $R(r), R_{nl}$ | radial wave function |
| $R_H$ | Rydberg constant for hydrogen |
| $R_H$ | Hall coefficient |
| $\hat{\boldsymbol{R}}, \hat{X}, \hat{Y}, \hat{Z}$ | position operator and its components |
| $\boldsymbol{R}_{\mathbb{L}}$ | lattice vector |
| $\mathbb{R}$ | radius |
| $\mathbb{R}$ | reflection coefficient |
| $\boldsymbol{r}, x, y, z$ | position vector and its components |
| $r$ | radial distance |
| $S$ | spin quantum number |
| $\hat{\boldsymbol{S}}, \hat{S}_x, \hat{S}_y, \hat{S}_z$ | spin operator and its components |
| $s$ | spin quantum number |
| $\hat{T}$ | transformation matrix |
| $T$ | temperature in kelvin |
| $\hat{T}_{\mathbb{L}}$ | translation operator |
| $T_{max}$ | maximum kinetic energy |
| $\mathbb{T}$ | transmission coefficient |
| $t$ | time |
| $u_k(x)$ | periodic part of Bloch function |

| | |
|---|---|
| $V(x)$, $V(r)$ | potential energy function |
| $\hat{V}_{\text{mag}}$ | magnetic dipole interaction operator |
| $V_{\text{so}}$ | spin–orbit coupling potential |
| $\mathcal{V}$ | electromagnetic scalar potential |
| $\mathbb{V}$ | volume |
| $\boldsymbol{v}$, $v$ | velocity, speed |
| $\boldsymbol{x}$, $\boldsymbol{y}$, $\boldsymbol{z}$ | unit vectors along Cartesian axes |
| $Y_{lm_l}(\theta, \phi)$ | spherical harmonic |
| $Z$ | atomic number |
| $\alpha$, $\beta$ | eigenvalues |
| $\gamma$ | constant phase |
| $\Delta x$ | uncertainty in $x$ |
| $\delta(x - x')$ | Dirac delta function |
| $\epsilon$ | dimensionless energy eigenvalue |
| $\theta$ | angle |
| $\lambda$ | wavelength |
| $\lambda$, $\lambda_{\pm}$ | eigenvalue of matrix |
| $\lambda$ | variational parameter |
| $\boldsymbol{\mu}$ | magnetic dipole moment |
| $\hat{\boldsymbol{\mu}}_l$, $\hat{\boldsymbol{\mu}}_s$ | magnetic moment operators |
| $\nu$ | frequency |
| $\xi$ | dimensionless position variable |
| $\hat{\Pi}$ | parity operator |
| $\rho$ | dimensionless position variable |
| $\rho'(\lambda, T)$ | spectral energy density as a function of wavelength |
| $\rho(\nu, T)$ | spectral energy density as a function of frequency |
| $\rho_{xx}$, $\rho_{xy}$ | resistivity |
| $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ | Pauli matrices |
| $\sigma$ | total cross-section |
| $\sigma$ | width of Gaussian |
| $\Phi$ | magnetic flux |
| $\Phi$ | wave function |
| $\phi(p, t)$ | momentum space wave function |
| $\phi$ | work function |
| $\phi$ | azimuthal angle |
| $\mathcal{X}$, $\chi$ | angular momentum eigenspinors |
| $\Psi$, $\psi$ | wave function |
| $\omega$ | angular frequency |
| $\omega_{\text{c}}$ | cyclotron frequency |
| $\omega_{\text{L}}$ | Larmor frequency |

# Contents