Quantum mechanics forms the foundation of all modern physics, including atomic, nuclear, and molecular physics, the physics of the elementary particles, condensed matter physics. Modern astrophysics also relies heavily on quantum mechanics. Quantum theory is needed to understand the basis for new materials, new devices, the nature of light coming from stars, the laws which govern the atomic nucleus, and the physics of biological systems. As a result the subject of this book is a required course for most physics graduate students.

While there are many books on the subject, this book targets specifically graduate students and it is written with modern advances in various fields in mind. Many examples treated in the various chapters as well as the emphasis of the presentation in the book are designed from the perspective of such problems. For example, the book begins by putting the Schrödinger equation on a spatial discrete lattice and the continuum limit is also discussed, inspired by Hamiltonian lattice gauge theories. The latter and advances in quantum simulations motivated the inclusion of the path integral formulation. This formulation is applied to the imaginary-time evolution operator to project the exact ground state of the harmonic oscillator as is done in quantum simulations. As an example of how to take advantage of symmetry in quantum mechanics, one-dimensional periodic potentials are discussed, inspired by condensed matter physics. Atoms and molecules are discussed within mean-field like treatment (Hartree-Fock) and how to go beyond it. Motivated by the recent intense activity in condensed matter and atomic physics to study the Hubbard model, the electron correlations in the hydrogen molecule are taken into account by solving the two-site Hubbard model analytically. Using the canonical Hamiltonian quantization of quantum electrodynamics, the photons emerge as the quanta of the normal modes, in the same way as the phonons emerge in the treatment of the normal modes of the coupled array of atoms. This is used later to treat the interaction of radiation with atomic matter.

Efstratios Manousakis is Donald Robson Professor of Physics at Florida State University, USA.

'The book teaches students how to approach and solve the types of quantum mechanical problems they will encounter throughout their careers. It will serve as an excellent text for a graduate level course.'

C. Stephen Hellberg, Naval Research Laboratory

Cover image: Russell Kightley/ Science Photo Library

OXFORD UNIVERSITY PRESS

ISBN 978-0-19-874934-9 9 780198 749349

www.oup.com

1	Schrödinger equation on a lattice	1
	1.1 Discretizing the spatial continuum	1
	1.2 The Schrödinger equation in a matrix form	$\frac{1}{2}$
	1.3 Problems	4
2	2 Dirac notation	
Ĩ	2.1 The bit and the q-bit	6
	2.2 Dirac notation	6
	2.3 Outer product	7
	2.4 Matrices and matrix elements	8
	2.5 Quantum gates	9
	2.6 Rotation	9
	2.7 Functions of operators	10
	2.8 Generator of planar rotations	11 12
	2.9 Problems	12
3	Back to the Schrödinger equation	12
	Back to the Schrödinger equation on a lattice 3.1 Lattice states	15
	3.2 Transformation of basis: momentum states	15
	3.3 Continuum limit of space	15
	3.4 Continuum limit of k-space	17
	3.5 Generalization in d-dimensions	19
	3.6 Problems	21 22
4	Operator mechanics	
î	4.1 Operators and observables	23
	4.2 Representation of operators	23
	4.3 The Hamiltonian operator	25
	4.4 Problems	26
5	Time evalution and	27
	Time evolution and wavepackets 5.1 Time-independent Hamiltonian	28
	5.2 An example of time evolution	28
	5.3 Wavepackets	29
	5.4 Time-dependent Hamiltonian	30
	5.5 Problems	31
3	Simultaneous about 11	34
,	Simultaneous observables 6.1 Uncertainty principle	36
	principio	36
	6.2 Commuting operators 6.3 Symmetries of the Hamiltonian	37
	old Symmetries of the Hamiltonian	39

	6.4 Problems	42	
7	Continuity equation and wavefunction properties 7.1 Continuity equation 7.2 Conditions on the wavefunction and its derivative 7.3 Non-negative kinetic energy expectation value 7.4 Variational theorem 7.5 Practical use of the variational theorem 7.6 Problems	44 44 46 47 48 49 52	
8	Bound states in one dimension 8.1 Square-well potential 8.2 Delta function potential 8.3 Problems	54 54 58 60	
9	Scattering in one dimension 9.1 Step barrier potential 9.2 Tunneling 9.3 Attractive square-well potential 9.4 Poles of $S(E)$ 9.5 Resonances 9.6 Analytic structure of $S(E)$ 9.7 Meaning of the resonance 9.8 Problems	68 68 70 72 74 75 79 79	
10	Periodic potentials 10.1 Bloch's theorem 10.2 The Kronig-Penney model 10.3 Problems	83 83 85 89	
11	The harmonic oscillator 11.1 Why is it useful? 11.2 One-dimensional harmonic oscillator 11.3 Eigenstates 11.4 Problems	91 91 92 95 96	
12	2 WKB approximation 12.1 The approximation 12.2 Region of validity of WKB 12.3 Exact solution near a turning point 12.4 Matching of WKB and exact solution: right turning point 12.5 Two turning points: bound states 12.6 Tunneling within the WKB approximation 12.7 Problems		
13	3 Quantum mechanics and path integrals 13.1 Derivation of the path integral in 1D 13.2 Classical mechanics as limit of quantum mechanics		

		Contents	xiii
	13.3 WKB from path integrals 13.4 Further reading		116 117
14			118 118 120 122 124 125 126
15	Angular momentum 15.1 Angular momentum operators 15.2 The spectrum of angular momentum operators 15.3 Eigenstates of angular momentum 15.4 Legendre polynomials and spherical harmonics 15.5 Problems		127 127 129 132 134 135
16	Bound states in spherically symmetric potentials 16.1 Spherical Bessel functions 16.2 Relation to ordinary Bessel equation 16.3 Spherical Bessel functions and Legendre polynomials 16.4 Bound states in a spherical well 16.5 Expansion of a plane wave 16.6 Problems		139 140 145 146 147 148 149
17	The hydrogen-like atom 17.1 The general two-body problem 17.2 The relative motion 17.3 Wavefunctions 17.4 Associated Laguerre polynomials 17.5 Problems		153 153 155 158 159 160
18	Angular momentum and spherical symmetry 18.1 Generators of infinitesimal rotations 18.2 Invariant subspaces and tensor operators 18.3 Wigner–Eckart theorem for scalar operators 18.4 Wigner–Eckart theorem: general case 18.5 Problems		161 162 164 165 166
19	Scattering in three dimensions 19.1 Scattering cross section 19.2 Quantum mechanical scattering 19.3 Scattering amplitude and differential cross section 19.4 Born series expansion 19.5 Partial wave expansion 19.6 Examples: phase shift calculation 19.7 Problems		167 168 171 173 174 177 182

20	Time-independent perturbation expansion 20.1 Statement of the problem 20.2 Non-degenerate case	184 184
		185
	20.3 Degenerate perturbation theory	188
	20.4 Quasi-degenerate perturbation theory	191
	20.5 Problems	192
21	Applications of perturbation theory	195
	21.1 Stark effect	195
	21.2 Origin of the Van der Walls interaction	197
	21.3 Electrons in a weak periodic potential	201
	21.4 Problems	205
00		200
22	Time-dependent Hamiltonian	207
	22.1 Time-dependent perturbation theory	207
	22.2 Adiabatic processes	214
	22.3 Problems	218
23	Spin angular momentum	990
	23.1 Spin and orbital angular momentum	220
	23.2 Spin-1/2	220
	23.3 Coupling of spin to a uniform magnetic field	222
	23.4 Rotations in spin space	223
	23.5 Problems	224
		225
24	Adding angular momenta	227
	24.1 Coupling between angular momenta	227
	24.2 Spin-orbit coupling	228
	24.3 The angular momentum coupling	229
	24.4 Problems	235
25	Identical particles	020
	25.1 Symmetry under particle permutations	236
	25.2 Second quantization	236
	25.3 Hilbert space for identical particles	238
	25.4 Operators	239
	25.5 Creation and annihilation operators	241
	25.6 Problems	242
		245
26	Elementary atomic physics	246
	26.1 Helium atom	246
	26.2 Hartree and Hartree–Fock approximation	249
	26.3 Hartree equations	253
	26.4 Hartree–Fock and non-locality	254
	26.5 Beyond mean-field theory	255
	26.6 Characterization of atomic states	257
	26.7 Spin-orbit interaction in multi-electron atoms	260
	26.8 Problems	263

			7	Contents	XV
27	Molecule	28	//		005
	27.1 H_2^+ and the Born–Oppenheimer approximation				$\frac{265}{265}$
	27.2 Hyb	ridization			268
	27.3 Tigh	t-binding approxim	nation		269
	27.4 The	hydrogen molecule			274
	27.5 Prob	olems			278
28	The elast	ticity field			280
		oatomic chain			280
		omic chain			284
	28.3 Prob	lems			289
29	Quantiza	tion of the free	electromagnetic field		292
	29.1 Class	sical treatment			292
	29.2 Quar				295
	29.3 Prob	lems			297
30	Interaction	on of radiation w	with charged particles		299
		total Hamiltonian			299
		erption and emission	n processes		301
	30.3 Prob				304
31	Elementa	ry relativistic qu	uantum mechanics		306
		-Gordon equation			306
		inuity equation	1		308
		ions of Klein–Gord -order Klein–Gordo			308
9.50		Dirac equation	on equation		309
		tional invariance			310 312
			the Dirac equation		312
		relativistic limit			314
		orbit coupling			315
		ariant form		3	317
	31.11 Cou	oling to external ele	ectromagnetic fields .		318
		tinuity equation pretation of the Di	iron equation		318
	31.14 Prob		nac equation		319
					320
App	A.1 Probl	Review of the	Dirac delta function		323
				3	324
App	pendix B	Normalization	integral of spherical harmonics	3	325
App	pendix C	Legendre equat	tion	3	327
App	pendix D	Expression for	the spherical Bessel function	3	329
Inde	ex			3	330