

# Contents

## I. The Basic Approach

### 1. Foundations

1.1 The Premise	2
An absolute truth, difficult to believe	
1.2 Schroedinger's Equation	3
Packets, the average position, matching velocities, operators, inventing the equation.	
1.3 Light waves	9
The vector potential, Maxwell's Equations	
1.4 New Meaning for Potentials	10
Aharanov and Bohm	
1.5 Measurement	12
Average values, consistent scenarios	
1.6 Eigenstates	13
Eigenvalues, normalization, energy levels	
1.7 Boundary conditions	16
Vanishing and periodic	
1.8 Sound Waves	17
Boundary conditions, modes, speed	

### 2. Simple Cases

2.1 Free Electrons in One Dimension	19
Effect of boundary conditions, $\pi$ -states in benzene	
2.2 Free Electron in Three Dimensions	21
Product wavefunctions, the one-electron approximation, Fermi surfaces, density of states, surface energies	
2.3 Quantum Slabs, Wires, and Dots	24
Giant Magnetoresistance, quantized conductance	
2.4 Circularly and Spherically-Symmetric Systems	31
Cylindrical and spherical systems, spherical harmonics, quantum wells, shallow wells	

2.5 The Harmonic Oscillator	39
Harmonic oscillator wavefunctions, ladder of energies, oscillators in three dimensions	
<b>3. Hamiltonian Mechanics</b>	
3.1 The Lagrangian	45
Lagrange's Equations, canonical momentum	
3.2 Hamilton's Equations	46
The equations, angular coordinates and angular momentum, restating the premise of quantum theory	
3.3 Including the Vector Potential	48
Fields from the vector potential, field energies, forces on charged particles, the Schroedinger Equation with fields	
<b>II. Electronic Structure</b>	
<b>4. Atoms</b>	
4.1 The Hydrogen Atom	53
The ground state, excited states	
4.2 Many-Electron Atoms	56
The two-electron wavefunction, variational calculations, the one-electron, the Hartree and Hartree-Fock Approximations, a table of atomic energy levels	
4.3 Pseudopotentials	62
The Periodic Table of the Elements, pseudowavefunctions, and weak pseudopotentials	
4.4 Nuclear Structure	65
The liquid-drop model, the shell model, structure of the nucleus, nuclear moments, beta and gamma rays, fission, the Standard Model	
<b>5. Molecules</b>	
5.1. The Li <sub>2</sub> Molecule	69
LCAO or tight-binding states, bonding and antibonding states, Dirac notation	
5.2 The Variational Method	73
Lowest-energy state, Lagrange multipliers, the variational equations	
5.3 Molecular Orbitals	68
Polar bonds, nonorthogonality and the overlap repulsion	
5.4 Perturbation Theory	79
First and second order, repulsion of levels	
5.5 N <sub>2</sub> , CO, and CO <sub>2</sub>	81
Cohesion, $\pi$ -bonds, sp-hybrids and $\sigma$ -bonds, multicenter bonds	
<b>6. Crystals</b>	
6.1 The Linear Chain	88
s-bands, the Brillouin Zone, benzene $\pi$ -bands, the finite chain	

6.2 Free-Electron Bands and Tight-Binding Parameters	92
Matching the limits, universal coupling parameters, p-state coupling	
6.3 Metallic, Ionic, and Covalent Solids	98
The Periodic Table and solids, metals and nonmetals, covalent semiconductors, ionic insulators, d- and f-shell metals and compounds	

### III. Time Dependence

#### 7. Transitions

7.1 A Pair of Coupled States	105
The need for a continuum	
7.2 Fermi's Golden Rule	106
Derivation and interpretation	
7.3 Scattering in One and Three Dimensions	109
Scattering by impurities	

#### 8. Tunneling

8.1 Transmission in a 1-D Chain	112
Exact result, scattering and the high-transmission limit, tunneling and the low-transmission limit	
8.2 More General Barriers	115
Three dimensions, working through the barrier, free-electron formula, continuity equation and current operator, general matching conditions	
8.3 Tunneling Systems	120
Tunneling as a quantum transition, metal-oxide-metal systems, the scanning tunneling microscope	
8.4 Tunneling Resonance	121
Decay of states, $\alpha$ -ray emission by nuclei, scattering resonances, resonant states and Coulomb blockades	

#### 9. Transition Rates

9.1 Second-Order Coupling	125
First-order states and second-order matrix elements, resonant tunneling, tunneling through impurity states	
9.2 Carrier Emission and Capture	128
Emission rate from the Golden Rule, capture from detailed balance, sequential tunneling compared with resonant tunneling	
9.3 Time-Dependent Perturbations	128
Fourier expansion of time dependence, energy loss and gain	
9.4 Optical Transitions	130
The interaction with light, selection rules, photon spin, the ionization of an atom	
9.5 Beta-Ray Emission from Nuclei	135
The neutrino, Fermi's theory, and weak interactions	

## IV. Statistical Physics

<b>10. Statistical Mechanics</b>	<b>140</b>
10.1 Distribution Functions	140
Excitations of a harmonic oscillator, distribution of excitations and average excitation	
10.2 Phonon and Photon Statistics	145
Thermal distribution, lattice specific heat, the Planck distribution	
10.3 Bosons	147
The chemical potential, Bose-Einstein condensation	
10.4 Symmetry Under Interchange	149
Two-particle wavefunction, limitation on $O^{16}_2$ tumbling, ortho- and parahydrogen	
10.5 Fermions	153
Antisymmetry, the Pauli Principle, Fermi-Dirac distribution, classical limit	
<b>11. Transport Theory</b>	
11.1 Time-Dependent Distributions	158
Rate equations, detailed balance, steady state	
11.2 The Boltzmann Equation	159
Linearization, relaxation-time approximation	
11.3 Conductivity, etc.	162
Finding the distribution function, evaluating the current, general transport properties	
<b>12. Noise</b>	
12.1 Classical Noise	164
Thermal or Johnson noise, fluctuations and dissipation	
12.2 Quantum Noise and van-der-Waals Interaction	165
Coupled dipole oscillators, correlated zero-point motion, many-body interaction	
12.3 Shot Noise	167
Shot noise in a classical gas, quantum suppression, enhancement, and concentration	
12.4 Other Sources	170
Partition noise, $1/f$ noise	
 <b>V. Electrons and Phonons</b> 	
<b>13. Energy Bands</b>	
13.1 The Empty-Core Pseudopotential	174
Form factors, structure factors	
13.2 A Band Calculation	178
Lattice wavenumbers, Brillouin Zones, diagonalizing the Hamiltonian matrix, free-electron bands	
13.3 Diffraction	184
Finite pseudopotentials, Fermi surfaces	

13.4 Scattering by Impurities	185
Total rates, momentum relaxation time	
13.5 Semiconductor Energy Bands	186
From pseudopotentials, a tight-binding representation	
<b>14. Electron Dynamics</b>	
14.1 Dynamics of Packets	189
Hamilton's Equations, motion in a magnetic field, level crossing	
14.2 Effective Masses and Donor States	192
Effective-mass equations, anisotropic masses, a hydrogenic donor state	
14.3 The Dynamics of Holes	194
Behavior as a positive-charge, positive-mass particle, binding electrons to form excitons, acceleration by fields and by elastic distortions	
<b>15. Lattice Vibrations</b>	
15.1 The Spectrum	197
One-dimensional chain, three-dimensional crystal	
15.2 The Classical-Vibration Hamiltonian	201
Normal coordinates, canonical momentum, the Hamiltonian	
15.3 The Electron-Phonon Interaction	203
Structure factors, electron-phonon matrix elements, Debye-Waller factor	
<b>VI. Quantum Optics</b>	
<b>16. Operators</b>	
16.1 Annihilation and Creation Operators for Electrons	207
Many-particle states, commutation relations, operators for kinetic and potential energies, electron-electron interactions	
16.2 Stepping Operators	212
Guessing a form for the harmonic oscillator, commutation relations, the number operator, normalization, excitation of the oscillator	
16.3 Angular Momentum	216
Raising and lowering operators, commutation relations, selection rules	
<b>17. Phonons</b>	
17.1 Annihilation and Creation Operators for Phonons	220
The Hamiltonian, commutation relations, the electron-phonon interaction	
17.2 Phonon Emission and Absorption	223
Using the Golden Rule, eliminating operators, absorption, spontaneous emission, stimulated emission	
17.3 Polaron Self-Energy	225
Eliminating operators, the polar coupling, the polaron energy	

17.4	Electron-Electron and Nucleon-Nucleon Interactions	228
	Interactions for superconductivity, semiconductors and exchange of virtual phonons, exchange of pions and the interaction between nucleons	
<b>18.</b>	<b>Photons</b>	
18.1	Photons and the Electron-Photon Interaction	232
	Normal coordinates, conjugate momentum, the photon Hamiltonian, annihilation and creation operators, commutation relations, electron-photon interaction	
18.2	Excitation of Atoms	235
	The matrix element, transition rates, equilibrium, saturating a transition	
18.3	The Three-Level Laser	239
	Levels in helium, pumping, laser action	
18.4	Interband Transitions	241
	Optical matrix elements, vertical transitions, light-emitting diodes, solid-state lasers, strain layers	
<b>19.</b>	<b>Coherent States</b>	
19.1	Coherence in a Harmonic Oscillator	247
	Mixed excitation levels, coherent phases	
19.2	A Driven Classical Oscillator	249
	Polarizability, real and imaginary parts	
19.3	A Driven Quantum Oscillator	251
	Dressed states, polarizability, energy loss	
19.4	Coherent Light	254
	Coherence in a single mode, laser radiation	
19.5	Electromagnetically-Induced Transparency	256
	The degenerate case, coupling and probe fields, the nondegenerate case, dynamic states and the Rabi frequency	
<b>VII. Many-Body Effects</b>		
<b>20.</b>	<b>Coulomb Effects</b>	
20.1	Coulomb Shifts	260
	Second ionization potentials, electron affinities, Madelung contributions, band-gap enhancements	
20.2	Screening	263
	Fermi-Thomas approximation, the dielectric function, quantum screening, plasma oscillations, speed of sound in metals	
<b>21.</b>	<b>Cooperative Phenomena</b>	
21.1	Localization and Symmetry Breaking	270
	The Coulomb $U$ and spin segregation, Unrestricted Hartree-Fock, first-order phase transitions	

21.2	The Hubbard Hamiltonian	275
	The half-filled band, antiferromagnetic insulator, spin-density waves, second-order phase transitions, higher dimensions, special points	
21.3	Peierls Distortions	281
	Pairing of atoms, charge-density wave, off-diagonal long-range order	
21.4	Superconductivity	282
	Cooper pairs, the BCS ground state, energy-gap parameter, persistent current	
<b>22.</b>	<b>Magnetism</b>	
22.1	Free Electrons in a Magnetic Field	287
	The Landau gauge, Landau levels, de Haas-van Alphen effect, Quantum Hall Effect	
22.2	Magnetism of Atoms	292
	The Hamiltonian, Zeeman splitting, the Bohr magneton and spin, spin resonance, Nuclear Magnetic Resonance (NMR)	
22.3	Magnetic Susceptibility	295
	Pauli paramagnetism of free electrons, comparison with the diamagnetic term, diamagnetism in atoms and molecules, molecular paramagnetism	
22.4	Ferromagnetism	298
	Criterion for instability of a free-electron gas, the Wigner crystal, the atomic view of magnetic properties	
22.5	Spin-Orbit Coupling	301
	The spin-orbit Hamiltonian, total angular momentum, fine structure for atoms, spin-split bands, anticrossings	
<b>23.</b>	<b>Shake-Off Excitations</b>	
23.1	Adiabatic and Sudden Approximations	306
	Time-dependent boundaries, transition probabilities, a criterion for fast or slow	
23.2	Vibrational Excitations	309
	A model system, a criterion, transition and tunneling times, the Franck-Condon Principle, polaron tunneling, phonon-assisted transitions, the Mössbauer Effect	
23.3	Electronic and Auger processes	315
	Beta-decay, donor states, atoms, shake-off in metals	
23.4	Inelastic Processes	316
	Loss in an intermediate state, interference, random phases or collapse of wavefunctions, cloud-chamber tracks, qubits and quantum computing, quantum cryptography	

xvi Contents

<b>Epilogue</b>	322
<b>Exercises</b>	323
<b>References</b>	343
<b>Subject Index</b>	345