

Contents

Part I Electronic Structure

1	Crystal Lattices in Real and Reciprocal Space	3
1.1	Introduction	3
1.2	Crystalline Lattices: Real Space	4
1.2.1	Bravais Lattices	4
1.2.2	Unit Cells	5
1.3	Lattices in Reciprocal Space	6
1.3.1	Crystal Planes and Miller Indices	6
1.3.2	Reciprocal Lattice Vectors	7
1.4	The Brillouin Zone	8
1.4.1	Graphene and Boron Nitride	8
1.4.2	Diamond and Zinc Blende Lattices	9
	Problems	11
2	Electronic Properties of Solids	13
2.1	Introduction	13
2.2	Hamiltonian of the System	13
2.3	The Electronic Problem	14
2.3.1	The Hartree Method	14
2.3.2	Hartree–Fock (HF) Method	15
2.3.3	Density Functional Theory	16
2.4	Plane Wave and Localized Basis Sets	19
2.5	Hamiltonian Matrix Elements	21
2.6	Bloch Functions	23
2.7	The Slater–Koster Approach	25
	References	26
3	Weak and Tight Binding Approximations for Simple Solid State Models	29
3.1	Introduction	29
3.2	One Electron $E(K)$ in Solids	29

- 3.2.1 Weak Binding or the Nearly Free Electron Approximation 29
- 3.2.2 Tight Binding Approximation 37
- 3.2.3 Comparison of Weak and Tight Binding Approximations 46
- 3.2.4 Tight Binding Approximation with 2 Atoms/Unit Cell 47
- Problems 52
- Suggested Reading 54
- 4 Examples of Energy Bands in Solids 55**
 - 4.1 Introduction 55
 - 4.2 Metals 57
 - 4.2.1 Alkali Metals—e.g., Sodium 57
 - 4.2.2 Noble Metals 58
 - 4.2.3 Polyvalent Metals 62
 - 4.3 Semiconductors 64
 - 4.3.1 PbTe 64
 - 4.3.2 Germanium 66
 - 4.3.3 Silicon 69
 - 4.3.4 III–V Compound Semiconductors 70
 - 4.3.5 Zero Gap Semiconductors – Gray Tin 72
 - 4.3.6 Transition Metal Dichalcogenides, Such as MoS₂ and WS₂ 73
 - 4.3.7 Molecular Semiconductors – Fullerenes 73
 - 4.4 Semimetals 75
 - 4.4.1 Graphene 75
 - 4.4.2 Bismuth 76
 - 4.5 Insulators 77
 - 4.5.1 Rare Gas and Ionic Crystals 77
 - 4.5.2 Boron Nitride 79
 - 4.5.3 Wide Bandgap Semiconductors 79
 - Problems 81
 - Suggested Readings 87
 - Reference 87
- 5 Effective Mass Theory 89**
 - 5.1 Introduction 89
 - 5.2 Wavepackets in Crystals and the Group Velocity of Electrons in Solids 89
 - 5.3 The Effective Mass Theorem 92
 - 5.4 Application of the Effective Mass Theorem to Donor Impurity Levels in a Semiconductor 95
 - 5.5 Quasi-classical Electron Dynamics 98

5.6	Quasi-classical Theory of Electrical Conductivity – Ohm's Law	99
	Problems	102
	Suggested Readings	104
6	Lattice Vibrations	105
6.1	Introduction	105
6.2	Quantum Harmonic Oscillators	105
6.3	Phonons in 1D Solids	108
	6.3.1 A Monoatomic Chain	108
	6.3.2 Diatomic Linear Chain	111
6.4	Phonons in 3D Crystals	113
6.5	Electron-Phonon Interaction	115
	Problems	118
	Reference	121
 Part II Transport Properties		
7	Basic Transport Phenomena	125
7.1	Introduction	125
7.2	The Boltzmann Equation	126
7.3	Electrical Conductivity	128
7.4	Electrical Conductivity of Metals	130
7.5	Electrical Conductivity of Semiconductors	131
	7.5.1 Ellipsoidal Carrier Pockets	134
7.6	Electrons and Holes in Intrinsic Semiconductors	136
7.7	Donor and Acceptor Doping of Semiconductors	140
7.8	Characterization of Semiconductors	144
	Problems	148
	Suggested Readings	153
8	Thermal Transport	155
8.1	Introduction	155
8.2	Thermal Conductivity	155
	8.2.1 General Considerations	155
	8.2.2 Thermal Conductivity for Metals	159
	8.2.3 Thermal Conductivity for Semiconductors	161
	8.2.4 Thermal Conductivity for Insulators	163
8.3	Thermoelectric Phenomena	164
	8.3.1 Thermoelectric Phenomena in Metals	168
	8.3.2 Thermopower for Intrinsic Semiconductors	170
	8.3.3 Effect of Thermoelectricity on the Thermal Conductivity	173

8.4	Thermoelectric Measurements	174
8.4.1	Seebeck Effect (Thermopower)	174
8.4.2	Peltier Effect	175
8.4.3	Thomson Effect	176
8.4.4	The Kelvin Relations	177
8.4.5	The Thermoelectric Figure of Merit	178
8.5	The Phonon Drag Effect	179
	Problems	180
	Suggested Readings	183
	References	183
9	Electron and Phonon Scattering	185
9.1	Electron Scattering	185
9.2	Scattering Processes in Semiconductors	188
9.2.1	Electron-Phonon Scattering in Semiconductors	188
9.2.2	Ionized Impurity Scattering	192
9.2.3	Other Scattering Mechanisms	193
9.2.4	Screening Effects in Semiconductors	194
9.3	Electron Scattering in Metals	197
9.3.1	Electron-Phonon Scattering in Metals	197
9.3.2	Other Scattering Mechanisms in Metals	201
9.4	Phonon Scattering	202
9.4.1	Phonon-Phonon Scattering	202
9.4.2	Phonon-Boundary Scattering	204
9.4.3	Defect-Phonon Scattering	205
9.4.4	Electron-Phonon Scattering	205
9.5	Temperature Dependence of the Electrical and Thermal Conductivity	205
	Problems	207
	Suggested Readings	209
10	Magneto-Transport Phenomena	211
10.1	Introduction	211
10.2	Magneto-Transport in the Classical Regime ($\omega_c \tau < 1$)	211
10.2.1	Classical Magneto-Transport Equations	212
10.2.2	Magneto-resistance	213
10.3	The Hall Effect	214
10.4	Derivation of the Magneto-Transport Equations from the Boltzmann Equation	216
10.5	Two Carrier Model	218
10.6	Cyclotron Effective Mass	220
10.7	Effective Masses for Ellipsoidal Fermi Surfaces	222
10.8	Dynamics of Electrons in a Magnetic Field	222
	Problems	226
	Suggested Readings	230

11	Transport in Low Dimensional Systems	231
11.1	Introduction	231
11.2	Observation of Quantum Effects in Reduced Dimensions	231
11.3	Density of States in Low Dimensional Systems	233
11.3.1	Quantum Dots	234
11.4	Ballistic Transport and the Landauer Formula	235
11.4.1	Relationship Between the Mean Free Path and the Transmission Coefficient	237
11.4.2	Relationship to the Boltzmann Transport	239
11.4.3	Relationship to Mobility Calculations	239
11.4.4	Dependence of the Fermi Energy on Gate Voltage	241
11.4.5	Ballistic Phonon Transport	241
11.5	Quantum Point Contacts (QPC) Effects	242
11.6	Coulomb Blockade and Single Electron Transistors (SETs)	243
	Problems	244
	References	246
12	Two Dimensional Electron Gas, Quantum Wells and Semiconductor Superlattices	247
12.1	Two-Dimensional Electronic Systems	247
12.2	MOSFETS	247
12.3	Two-Dimensional Behavior	251
12.3.1	Quantum Wells and Superlattices	253
12.4	Bound Electronic States	256
12.5	Review of Tunneling Through a Potential Barrier	257
12.6	Quantum Wells of Different Shape and the WKB Approximation	258
12.7	The Kronig–Penney Model	261
12.8	3D Motion Within a 1–D Rectangular Well	263
12.9	Resonant Tunneling in Quantum Wells	265
	Problems	271
	Suggested Readings	274
13	Magneto-Oscillatory and Other Effects Associated with Landau Levels	275
13.1	Introduction to Landau Levels	275
13.2	Quantized Magnetic Energy Levels in 3D	275
13.2.1	Degeneracy of the Magnetic Energy Levels in k_x	277
13.2.2	Dispersion of the Magnetic Energy Levels Along the Magnetic Field	278
13.2.3	Band Parameters Describing the Magnetic Energy Levels	281
13.3	Overview of Landau Level Effects	282
13.4	Quantum Oscillatory Magnetic Phenomena	285

13.5	Selection Rules for Landau Level Transitions	289
13.6	Landau Level Quantization for Large Quantum Numbers	290
	Problems	291
	Suggested Readings	294
14	The Quantum Hall Effect (QHE)	295
14.1	Introduction to the Quantum Hall Effect	295
14.2	Basic Relations for 2D Hall Resistance	297
14.3	The 2D Electron Gas and the Quantum Hall Effect	299
14.4	Effect of Edge Channels and the Quantum Field Effect	304
14.5	Precision of the Quantized Hall Effect and Applications	307
14.6	Fractional Quantum Hall Effect (FQHE)	308
	Problems	312
	Suggested Reading	313
Part III Optical Properties		
15	Review of Fundamental Relations for Optical Phenomena	317
15.1	Introductory Remarks on Optical Probes	317
15.2	The Complex Dielectric Function and the Complex Optical Conductivity	317
15.2.1	Propagating Waves	319
15.3	Relation of the Complex Dielectric Function to Observables	321
15.4	Units for Frequency Measurements	325
	Problems	325
	Suggested Reading	327
16	Drude Theory—Free Carrier Contribution to the Optical Properties	329
16.1	The Free Carrier Contribution	329
16.2	Low Frequency Response: $\omega\tau \ll 1$	332
16.3	High Frequency Response: $\omega\tau \gg 1$	333
16.4	The Plasma Frequency	333
16.5	Plasmon Resonant Nanoparticles	337
16.6	Surface Plasmon Polaritons in Graphene	338
	Problems	341
	Suggested Readings	344
17	Interband Transitions	345
17.1	The Interband Transition Process	345
17.2	Hamiltonian for a Charge in an Electromagnetic Field	348
17.3	Relation Between Momentum Matrix Elements and the Effective Mass	350
17.4	The Joint Density of States	352

17.5	Connecting Optical Properties and the Joint Density of States	353
17.6	Critical Points	356
17.7	Critical Points in Low Dimensional Materials	360
	Problems	361
	Suggested Readings	364
	References	364
18	Absorption of Light in Solids	365
18.1	The Absorption Coefficient	365
18.2	Free Carrier Absorption in Semiconductors	366
18.3	Free Carrier Absorption in Metals	369
18.4	Direct Interband Transitions	370
18.4.1	Temperature Dependence of E_g	374
18.4.2	Dependence of the Absorption Edge on Fermi Energy	374
18.4.3	Dependence of the Absorption Edge on Applied Electric Field	376
18.4.4	Dependence of the Absorption Edge on Applied Magnetic Field	377
18.5	Conservation of Crystal Momentum in Direct Optical Transitions	379
18.6	Indirect Interband Transitions	380
	Problems	386
	Suggested Readings	388
19	Optical Properties of Solids over a Wide Frequency Range	391
19.1	Kramers–Kronig Relations	391
19.2	Optical Properties and Band Structure	397
19.3	Modulated Reflectivity Experiments	398
19.4	Ellipsometry and Measurement of the Optical Constants	403
19.5	Kramers-Kronig Relations in 2D Materials	406
19.6	Summary	407
	Problems	407
	Suggested Readings	409
	References	410
20	Impurities and Excitons	411
20.1	Impurity Level Spectroscopy	411
20.2	Shallow Impurity Levels	412
20.3	Departures from the Hydrogenic Model	416
20.4	Vacancies, Color Centers and Interstitials	416
20.4.1	Schottky Defects	418

20.5	The Concept and Spectroscopy of Excitons	420
20.5.1	Exciton Effects in Bulk Materials	424
20.5.2	Classification of Excitons	426
20.5.3	Optical Transitions in 2D Systems: Quantum Well Structures	430
20.5.4	Excitons in 0D and 1D Systems: Fullerene C ₆₀ and Carbon Nanotubes	435
20.5.5	Excitons and Trions in Transition Metal Dichalcogenides	437
20.5.6	Excitons in Transition Metal Dichalcogenide Heterojunctions	438
	Problems	439
	Suggested Readings	441
	References	441
21	Luminescence and Photoconductivity	443
21.1	Classification of Luminescence Processes	443
21.2	Emission and Absorption	445
21.3	Photoconductivity	451
21.4	Photoluminescence in 2D Materials	454
	Suggested Reading	455
	References	455
22	Optical Study of Lattice Vibrations	457
22.1	Lattice Vibrations in Semiconductors	457
22.1.1	General Considerations	457
22.2	Dielectric Constant and Polarizability	460
22.3	Polariton Dispersion Relations	461
22.4	Light Scattering	471
22.5	Feynman Diagrams for Light Scattering	475
22.6	Raman Spectra in Quantum Wells and Superlattices	478
22.7	Raman Spectroscopy of Nanoscale Materials	480
	Problems	483
	Suggested Readings	488
	References	488
	Appendix A: Time-Independent Perturbation Theory	489
	Appendix B: Time-Dependent Perturbation Theory	499
	Index	507