

The Oxford Solid State Basics

Steven H. Simon

University of Oxford

OXFORD
UNIVERSITY PRESS

Contents

1	About Condensed Matter Physics	1
1.1	What Is Condensed Matter Physics	1
1.2	Why Do We Study Condensed Matter Physics?	1
1.3	Why Solid State Physics?	3
I	Physics of Solids without Considering Microscopic Structure: The Early Days of Solid State	5
2	Specific Heat of Solids: Boltzmann, Einstein, and Debye	7
2.1	Einstein's Calculation	8
2.2	Debye's Calculation	9
2.2.1	Periodic (Born–von Karman) Boundary Conditions	10
2.2.2	Debye's Calculation Following Planck	11
2.2.3	Debye's "Interpolation"	13
2.2.4	Some Shortcomings of the Debye Theory	14
2.3	Appendix to this Chapter: $\zeta(4)$	16
	Exercises	17
3	Electrons in Metals: Drude Theory	19
3.1	Electrons in Fields	20
3.1.1	Electrons in an Electric Field	20
3.1.2	Electrons in Electric and Magnetic Fields	21
3.2	Thermal Transport	22
	Exercises	25
4	More Electrons in Metals: Sommerfeld (Free Electron) Theory	27
4.1	Basic Fermi–Dirac Statistics	27
4.2	Electronic Heat Capacity	29
4.3	Magnetic Spin Susceptibility (Pauli Paramagnetism)	32
4.4	Why Drude Theory Works So Well	34
4.5	Shortcomings of the Free Electron Model	35
	Exercises	37
II	Structure of Materials	39
5	The Periodic Table	41

5.1	Chemistry, Atoms, and the Schroedinger Equation	41
5.2	Structure of the Periodic Table	42
5.3	Periodic Trends	43
5.3.1	Effective Nuclear Charge	45
	Exercises	46
6	What Holds Solids Together: Chemical Bonding	49
6.1	Ionic Bonds	49
6.2	Covalent Bond	52
6.2.1	Particle in a Box Picture	52
6.2.2	Molecular Orbital or Tight Binding Theory	53
6.3	Van der Waals, Fluctuating Dipole Forces, or Molecular Bonding	57
6.4	Metallic Bonding	59
6.5	Hydrogen Bonds	59
	Exercises	61
7	Types of Matter	65
III	Toy Models of Solids in One Dimension	69
8	One-Dimensional Model of Compressibility, Sound, and Thermal Expansion	71
	Exercises	74
9	Vibrations of a One-Dimensional Monatomic Chain	77
9.1	First Exposure to the Reciprocal Lattice	79
9.2	Properties of the Dispersion of the One-Dimensional Chain	80
9.3	Quantum Modes: Phonons	82
9.4	Crystal Momentum	84
	Exercises	86
10	Vibrations of a One-Dimensional Diatomic Chain	89
10.1	Diatomic Crystal Structure: Some Useful Definitions	89
10.2	Normal Modes of the Diatomic Solid	90
	Exercises	96
11	Tight Binding Chain (Interlude and Preview)	99
11.1	Tight Binding Model in One Dimension	99
11.2	Solution of the Tight Binding Chain	101
11.3	Introduction to Electrons Filling Bands	104
11.4	Multiple Bands	105
	Exercises	107
IV	Geometry of Solids	111
12	Crystal Structure	113

12.1	Lattices and Unit Cells	113
12.2	Lattices in Three Dimensions	117
12.2.1	The Body-Centered Cubic (bcc) Lattice	118
12.2.2	The Face-Centered Cubic (fcc) Lattice	120
12.2.3	Sphere Packing	121
12.2.4	Other Lattices in Three Dimensions	122
12.2.5	Some Real Crystals	123
	Exercises	125
13	Reciprocal Lattice, Brillouin Zone, Waves in Crystals	127
13.1	The Reciprocal Lattice in Three Dimensions	127
13.1.1	Review of One Dimension	127
13.1.2	Reciprocal Lattice Definition	128
13.1.3	The Reciprocal Lattice as a Fourier Transform	129
13.1.4	Reciprocal Lattice Points as Families of Lattice Planes	130
13.1.5	Lattice Planes and Miller Indices	132
13.2	Brillouin Zones	134
13.2.1	Review of One-Dimensional Dispersions and Brillouin Zones	134
13.2.2	General Brillouin Zone Construction	134
13.3	Electronic and Vibrational Waves in Crystals in Three Dimensions	136
	Exercises	137
V	Neutron and X-Ray Diffraction	139
14	Wave Scattering by Crystals	141
14.1	The Laue and Bragg Conditions	141
14.1.1	Fermi's Golden Rule Approach	141
14.1.2	Diffraction Approach	142
14.1.3	Equivalence of Laue and Bragg conditions	143
14.2	Scattering Amplitudes	144
14.2.1	Simple Example	146
14.2.2	Systematic Absences and More Examples	147
14.2.3	Geometric Interpretation of Selection Rules	149
14.3	Methods of Scattering Experiments	150
14.3.1	Advanced Methods	150
14.3.2	Powder Diffraction	151
14.4	Still More About Scattering	156
14.4.1	Scattering in Liquids and Amorphous Solids	156
14.4.2	Variant: Inelastic Scattering	156
14.4.3	Experimental Apparatus	157
	Exercises	159

VI	Electrons in Solids	161
15	Electrons in a Periodic Potential	163
15.1	Nearly Free Electron Model	163
15.1.1	Degenerate Perturbation Theory	165
15.2	Bloch's Theorem	169
	Exercises	171
16	Insulator, Semiconductor, or Metal	173
16.1	Energy Bands in One Dimension	173
16.2	Energy Bands in Two and Three Dimensions	175
16.3	Tight Binding	177
16.4	Failures of the Band-Structure Picture of Metals and Insulators	177
16.5	Band Structure and Optical Properties	179
16.5.1	Optical Properties of Insulators and Semiconductors	179
16.5.2	Direct and Indirect Transitions	179
16.5.3	Optical Properties of Metals	180
16.5.4	Optical Effects of Impurities	181
	Exercises	182
17	Semiconductor Physics	183
17.1	Electrons and Holes	183
17.1.1	Drude Transport: Redux	186
17.2	Adding Electrons or Holes with Impurities: Doping	187
17.2.1	Impurity States	188
17.3	Statistical Mechanics of Semiconductors	191
	Exercises	195
18	Semiconductor Devices	197
18.1	Band Structure Engineering	197
18.1.1	Designing Band Gaps	197
18.1.2	Non-Homogeneous Band Gaps	198
18.2	p - n Junction	199
18.3	The Transistor	203
	Exercises	205
VII	Magnetism and Mean Field Theories	207
19	Magnetic Properties of Atoms: Para- and Dia-Magnetism	209
19.1	Basic Definitions of Types of Magnetism	209
19.2	Atomic Physics: Hund's Rules	211
19.2.1	Why Moments Align	212
19.3	Coupling of Electrons in Atoms to an External Field	214
19.4	Free Spin (Curie or Langevin) Paramagnetism	215
19.5	Larmor Diamagnetism	217

19.6 Atoms in Solids	218
19.6.1 Pauli Paramagnetism in Metals	219
19.6.2 Diamagnetism in Solids	219
19.6.3 Curie Paramagnetism in Solids	220
Exercises	222
20 Spontaneous Magnetic Order: Ferro-, Antiferro-, and Ferri-Magnetism	225
20.1 (Spontaneous) Magnetic Order	226
20.1.1 Ferromagnets	226
20.1.2 Antiferromagnets	226
20.1.3 Ferrimagnets	227
20.2 Breaking Symmetry	228
20.2.1 Ising Model	228
Exercises	229
21 Domains and Hysteresis	233
21.1 Macroscopic Effects in Ferromagnets: Domains	233
21.1.1 Domain Wall Structure and the Bloch/Néel Wall	234
21.2 Hysteresis in Ferromagnets	236
21.2.1 Disorder Pinning	236
21.2.2 Single-Domain Crystallites	236
21.2.3 Domain Pinning and Hysteresis	238
Exercises	240
22 Mean Field Theory	243
22.1 Mean Field Equations for the Ferromagnetic Ising Model	243
22.2 Solution of Self-Consistency Equation	245
22.2.1 Paramagnetic Susceptibility	246
22.2.2 Further Thoughts	247
Exercises	248
23 Magnetism from Interactions: The Hubbard Model	251
23.1 Itinerant Ferromagnetism	252
23.1.1 Hubbard Ferromagnetism Mean Field Theory	252
23.1.2 Stoner Criterion	253
23.2 Mott Antiferromagnetism	255
23.3 Appendix: Hubbard Model for the Hydrogen Molecule	257
Exercises	259
A Sample Exam and Solutions	261
B List of Other Good Books	275
Indices	279
Index of People	280
Index of Topics	283