

SOLID STATE THEORY

Walter A. Harrison

Professor of Applied Physics
Stanford University

Dover Publications, Inc.
New York

CONTENTS

<i>Preface</i>	ix
I SOLID TYPES AND SYMMETRY	1
1 Crystal Structures	1
2 Symmetry of Crystals	9
3 Physical Tensors	13
4 Symmetry Arguments and Group Theory	16
4.1 Groups	19
4.2 Representations	23
4.3 Equivalent representations	24
4.4 Symmetry degeneracies	26
4.5 Orthogonality relation	29
4.6 Characters	31
4.7 Reduction of representations	32
	xiii

5	<i>Applications of Group Theory</i>	33
5.1	Lowering of symmetry	33
5.2	Vibrational states	36
5.3	The translation group—one dimension	46
II	ELECTRON STATES	56
1	<i>The Structure of the Bands</i>	56
2	<i>Electron Dynamics</i>	64
3	<i>The Self-Consistent-Field Approximation</i>	71
3.1	The Hartree approximation	73
3.2	The Hartree-Fock approximation	74
3.3	Free-electron exchange	75
3.4	Koopman's theorem	76
3.5	The crystal potential	78
4	<i>Energy-Band Calculations</i>	81
4.1	The cellular method	82
4.2	The plane-wave method	82
4.3	The orthogonalized-plane-wave method	84
4.4	The augmented-plane-wave method	86
4.5	The symmetry of the energy bands	87
4.6	Calculated energy bands	89
5	<i>Simple Metals and Pseudopotential Theory</i>	96
5.1	The pseudopotential	97
5.2	The model-potential method	105
5.3	Free-electron bands	108
5.4	The diffraction approximation	110
5.5	One-OPW Fermi surfaces	110
5.6	Experimental studies of Fermi surfaces	116
5.7	Multiple-OPW Fermi surfaces	131
6	<i>Semiconductor and Semimetal Bands</i>	138
6.1	$\mathbf{k} \cdot \mathbf{p}$ method and effective-mass theory	140
6.2	Dynamics of electrons and holes in semiconductors	145
6.3	Semimetals	150
7	<i>Insulator Bands</i>	150
7.1	The tight-binding approximation	151
7.2	Bands and binding in ionic crystals	157
7.3	Polarons and self-trapped electrons	159
7.4	The Mott transition and molecular solids	161

7.5	Excitons	163
7.6	Wannier functions	166
8	<i>Impurity States</i>	168
8.1	Tight-binding description	169
8.2	Donor and acceptor levels in semiconductors	170
8.3	Quantum theory of surface states and impurity states	173
8.4	Phase-shift analysis	176
8.5	Scattering resonances	187
8.6	Electron scattering by impurities	194
9	<i>Transition-Metal Bands</i>	200
9.1	Transition-metal pseudopotentials	200
9.2	The energy bands	204
9.3	Perturbation theory and properties	207
10	<i>Electronic Structure of Liquids</i>	212
10.1	Simple metals	212
10.2	Insulators and semiconductors	215
10.3	Description in terms of one-electron Green's functions	216
	<i>Appendix on Green's functions</i>	224
10.4	Resistivity in liquid metals	225
III	ELECTRONIC PROPERTIES	237
1	<i>Thermodynamic Properties</i>	237
1.1	The electronic specific heat	239
1.2	The diamagnetic susceptibility of free electrons	246
1.3	Pauli paramagnetism	250
2	<i>Transport Properties</i>	252
2.1	The Boltzmann equation	253
2.2	Electrical conductivity	255
2.3	The Hall effect	257
2.4	Thermal and thermoelectric effects	261
2.5	Electron tunneling	264
3	<i>Semiconductor Systems</i>	270
3.1	The <i>p-n</i> junction	271
3.2	The tunnel diode	276
3.3	The Gunn effect	278
4	<i>Screening</i>	280
4.1	Classical theory of simple metals	283
4.2	Limits and applications of the dielectric function	285

4.3	Quantum theory of screening	290
4.4	Screening of pseudopotentials and of hybridization	301
4.5	The inclusion of exchange and correlation	309
5	<i>Optical Properties</i>	315
5.1	The penetration of light in a metal	315
5.2	The optical conductivity	317
5.3	Simple metals	321
5.4	Interband absorption	323
5.5	Photoelectric emission	332
5.6	Color centers and the Franck-Condon principle	332
5.7	X-ray spectroscopy	340
5.8	Many-body effects	347
5.9	Lasers	350
6	<i>Landau Theory of Fermi Liquids</i>	353
7	<i>Amorphous Semiconductors</i>	358
IV	LATTICE VIBRATIONS AND ATOMIC PROPERTIES	365
1	<i>Calculation with Force Constants</i>	366
1.1	Application to the simple cubic structure	368
1.2	Two atoms per primitive cell	372
2	<i>Phonons and the Lattice Specific Heat</i>	377
3	<i>Localized Modes</i>	381
4	<i>Electron-Phonon Interactions</i>	389
4.1	Classical theory	390
	<i>Ionic crystals</i>	390
	<i>Semiconductors</i>	391
	<i>Simple metals</i>	394
4.2	Second quantization	397
	<i>Electron states</i>	399
	<i>Phonon states</i>	407
	<i>Phase coherence and off-diagonal long-range order</i>	410
	<i>The interaction</i>	413
4.3	Applications	414
	<i>Electron scattering</i>	414
	<i>Electron self-energy</i>	418
	<i>The electron-electron interaction</i>	421
4.4	The Mössbauer effect	423

5	<i>Pseudopotentials and Phonon Dispersion</i>	427
5.1	The total energy	427
5.2	Calculation of vibration spectra	431
5.3	The Bohm-Staver formula	433
5.4	Kohn anomalies	434
6	<i>Interatomic Forces and Atomic Properties</i>	436
6.1	Stability of metallic structures	437
6.2	The effective interaction between ions	440
6.3	Atomic properties of insulators and semiconductors	443
6.4	Dislocations	448
V	COOPERATIVE PHENOMENA	459
A	MAGNETISM	459
1	<i>Exchange</i>	460
2	<i>Band Ferromagnetism</i>	461
3	<i>Spin Operators</i>	465
4	<i>Heisenberg Exchange</i>	467
5	<i>The Molecular-Field Approximation and the Ferromagnetic Transition</i>	470
6	<i>Inhomogeneities</i>	475
6.1	Bloch walls	475
6.2	Spin waves	476
7	<i>Local Moments</i>	479
7.1	The formation of local moments	480
7.2	The Ruderman-Kittel Interaction	486
	<i>The s-d interaction</i>	486
	<i>Interaction between moments</i>	487
7.3	The Kondo effect	490
B	SUPERCONDUCTIVITY	494
8	<i>Cooper Pairs</i>	495
9	<i>Bardeen-Cooper-Schrieffer (BCS) Theory</i>	499
9.1	The ground state	501
9.2	Excited states	506
9.3	Experimental consequences	507

<i>Persistent currents</i>	507
<i>Giaever tunneling</i>	509
<i>Thermodynamic properties</i>	512
9.4 The superconducting wavefunction or order parameter	513
9.5 The Josephson effect	516
10 <i>The Ginsburg-Landau Theory</i>	521
10.1 Evaluation of the free energy	523
10.2 The Ginsburg-Landau equations	525
10.3 Applications of the Ginsburg-Landau theory	527
<i>Zero-field solutions</i>	528
<i>Nonuniform systems</i>	529
<i>Applied magnetic fields</i>	530
10.4 Flux quantization	531
10.5 Fluctuations in superconductors	533
<i>Index</i>	541