

S. V. Vonsovsky M. I. Katsnelson

Quantum Solid-State Physics

With 151 Figures

Springer-Verlag Berlin Heidelberg New York
London Paris Tokyo HongKong

Contents

1. Introduction. General Properties of the Solid State of Matter	1
1.1 General Thermodynamic Description of the Solid State	1
1.2 Crystal Structure of Solids	6
1.3 Reciprocal Lattice	26
1.4 Examples of Simple Crystal Structures	29
1.5 Experimental Techniques for Determining the Periodic Atomic Structure of Solids	32
1.6 Qualitative Concepts of the Electronic and Nuclear Crystal Structure	43
1.7 Fundamental Concepts of the Chemical Bonding in Solids	48
1.7.1 Interaction Between Atoms (Ions) with Filled Electron Shells	49
1.7.2 Molecular Orbitals	55
1.7.3 The Heitler-London Method	60
1.7.4 Covalent Bond	65
1.7.5 Electrostatic Bonding Energy of Ionic Crystals	69
1.8 Types of Crystalline Solids	72
1.8.1 Ionic Crystals	73
1.8.2 Covalent Crystals and Semiconductors	74
1.8.3 Metals, Their Alloys, and Compounds	76
1.8.4 Molecular Crystals	78
1.8.5 Hydrogen-Bonded Crystals	78
1.8.6 Quasi-One-Dimensional and Quasi-Two-Dimensional Crystals	79
1.8.7 Quantum Crystals	80
1.9 Formulation of the General Quantum-Mechanical Problem of the Crystal	85
1.10 Properties of Disordered Condensed Systems	90
1.10.1 General Remarks	90
1.10.2 Metallic Glasses (Example of Amorphous Solids)	92
2. Dynamic Properties of the Crystal Lattice	97
2.1 The Dynamics of the Ionic Lattice	97
2.1.1 A Linear Monatomic Array	97
2.1.2 A Linear Diatomic Array	101
2.1.3 The Three-Dimensional Crystal Case	105
2.1.4 Quantization of Ionic-Lattice Vibrations	109

2.2	The Specific-Heat Capacity of the Lattice	111
2.3	Allowance for Anharmonic Terms	120
2.3.1	Thermal Expansion of Crystals	120
2.3.2	Heat-Capacity Term Linear in Temperature	122
2.3.3	Thermal Conductivity of an Ionic Lattice	123
2.4	Localization of Phonons on Point Defects	124
2.5	Heat Capacity of Glasses at Low Temperatures	127
2.6	High-Frequency Permittivity of Ionic Crystals	131
2.7	Lattice Scattering and the Mössbauer Effect	134
2.7.1	Scattering Probability and the Correlation Function	134
2.7.2	Some Properties of the Phonon Operators and of the Averages Containing Them	138
2.7.3	Calculating the Dynamic Form Factor in the Harmonic Approximation	143
2.7.4	Elastic Scattering	147
2.7.5	Inelastic Scattering	149
2.7.6	The Mössbauer Effect	152
2.8	Conclusion	155
3.	Simple Metals: The Free Electron-Gas Model	157
3.1	Types of Metals	157
3.2	Physical Properties of the Metallic State. Conduction Electrons	158
3.3	Classical Conduction-Electron Theory (Drude-Lorentz Theory)	162
3.4	Itinerant Electron Theory According to Frenkel	168
3.5	Application of Fermi-Dirac Quantum Statistics to the Conduction-Electron Gas	170
3.5.1	The Case of $T = 0$ K	173
3.5.2	The Low-Temperature Case ($T > 0$ K, but $T \ll \Theta_{el}$)	176
3.5.3	Atomic Volume, Compressibility, and Strength of Metals	182
3.5.4	Paramagnetism of a Degenerate Electron Gas	185
3.5.5	Diamagnetism of a Degenerate Electron Gas According to Landau	191
3.5.6	Oscillatory Effects in the Fermi Gas	200
3.5.7	Thermionic Emission (the Richardson Effect)	203
3.6	Transport Phenomena	206
3.6.1	The Boltzmann Kinetic Equation	206
3.6.2	Electrical Conductivity	211
3.6.3	Thermal Conductivity and the Wiedemann-Franz Relation	213
3.6.4	Thermoelectric Phenomena	216
3.6.5	Galvanomagnetic Phenomena	221
3.7	High-Frequency Properties	228
3.7.1	Basic Equations	228
3.7.2	Skin Effect	231
3.7.3	Cyclotron Resonance	235
3.7.4	Electromagnetic Waves in Metals	238
3.8	Conclusions	243

4. Band Theory	245
4.1 Preliminary Observations and the One-Dimensional Model	245
4.1.1 Electron Waves in a Crystal	245
4.1.2 The Array of Rectangular Potential Barriers	248
4.1.3 Linear Atomic Array	253
4.1.4 Rigorous Theory of Electron Motion in a One-Dimensional Array	260
4.2 General Theory of the Electron Motion in a Three-Dimensional Crystal	274
4.2.1 Bloch's Theorem	274
4.2.2 Brillouin Zones	279
4.2.3 Electron Energy Spectrum	284
4.2.4 The Properties of Constant Energy Surfaces	289
4.2.5 Density of Electron States in Energy Bands. Topological Electronic Transitions	292
4.3 Nearly-Free-Electron Approximation	296
4.3.1 Statement of the Problem	296
4.3.2 Empty-Lattice Model	297
4.3.3 Allowance for a Weak Periodic Field	303
4.4 Effect of an Electric Field on Electronic States	310
4.4.1 Acceleration and Effective Electron Mass	310
4.4.2 Zener Breakdown	313
4.4.3 Quantum Theory of the Electric Inertia Effect	316
4.5 The Metal-Semiconductor Criterion	319
4.5.1 The Metal-Nonmetal Criterion in Band Theory	319
4.5.2 The Peierls Transition	325
4.5.3 The Mott Transition	327
4.5.4 Disordered Systems	328
4.6 Computing the Electron Energy Spectrum of Crystals	330
4.6.1 Self-Consistent Field Approximation	330
4.6.2 Solving the Schrödinger Equation. Formulation of the Problem and the Cellular Method	336
4.6.3 The LCAO Method and Tight-Binding Approximation	338
4.6.4 The Orthogonalized Plane Waves (OPW) Method. Pseudopotential	342
4.6.5 The Augmented Plane Waves (APW) Method	344
4.6.6 $\mathbf{k} \cdot \mathbf{p}$ Perturbation Theory	347
4.6.7 Fermi Surfaces in Real Metals	349
4.7 Band Electrons in a Magnetic Field	352
4.7.1 The Effective Hamiltonian	352
4.7.2 Classical Paths	359
4.7.3 Quasi Classical Energy Levels. Oscillatory Effects	364
4.8 Impurity States	368
4.8.1 A Simple Model	368
4.8.2 Green's Functions and the Density of States	371

4.8.3	Friedel Oscillations	376
4.9	The Electronic Structure of Disordered Systems	379
4.9.1	The Average Green's Function in the Diagonal Disorder Model	379
4.9.2	Approximate Methods of Computing the Average Green's Function in the Binary Alloy Model	383
4.9.3	Anderson Localization	388
4.10	Conclusion. The Role of Many-Particle Effects	393
5.	Many-Particle Effects	396
5.1	Plasma Phenomena. Screening	396
5.1.1	A Discussion of the Model	396
5.1.2	The Equation for a Self-Consistent Plasma Potential	397
5.1.3	Static Screening	402
5.1.4	Plasmons	406
5.1.5	Phonons in the Plasma Model	410
5.1.6	Fluctuation-Dissipation Theorem	411
5.2	The Fermi-Liquid Theory	415
5.2.1	Major Postulates of the Landau Theory	415
5.2.2	Thermodynamic Properties	419
5.2.3	Kinetic Equation for Quasiparticles	422
5.3	Electron-Phonon Interaction	427
5.3.1	Formulation of the Problem	427
5.3.2	Conditions for the Applicability of the Adiabatic Approximation	430
5.3.3	Temperature Dependence of the Electrical Conductivity in Metals	434
5.3.4	Polarons	438
5.3.5	The Cooper Phenomenon	448
5.4	Superconductivity	453
5.5	Excitons	460
5.6	Transition Metals and Their Compounds	463
5.6.1	Properties of d and f States	463
5.6.2	The Heisenberg Model	465
5.6.3	d Metals	476
5.6.4	Magnetism in the $4f$ Metals	480
5.7	Anderson's Orthogonality Catastrophe	482
5.8	Conclusion	487
	Addenda (Recent Developments)	488
	References	490
	Subject Index	499