

Contents

<i>Preface</i>	vii
1. Drude Theory of Metals	1
1-1 Electron speed distribution	2
1-2 Average and standard deviation of the collision time interval	2
1-3 Two successive collisions	3
1-4 Conductivity of a superconductor	4
1-5 Relative dielectric function of a metal	5
1-6 Propagation of electromagnetic radiation in a metal . . .	7
1-7 Thermal conduction of a one-dimensional metal	8
1-8 Metal in a uniform static electric field	9
2. Sommerfeld Theory of Metals	11
2-1 Fermi-Dirac distribution function at low temperatures . .	12
2-2 Effects of hydrostatic pressure	14
2-3 Approximate expression for the Fermi-Dirac distribution function	15
2-4 Uncertainty in the electron kinetic energy	16
2-5 Lindhard function	18
2-6 Boltzmann equation	21
2-7 Two-dimensional electron gas	24
2-8 Thermodynamics of an electron gas	25
3. Bravais Lattice	29
3-1 Primitive cells of five two-dimensional Bravais lattices . .	30
3-2 Wigner-Seitz cells of five two-dimensional Bravais lattices	31

3-3	Triangular and centered rectangular Bravais lattices	31
3-4	Packing fractions in two dimensions	32
3-5	Body-centered cubic crystal	33
3-6	Interstices in a face-centered cubic structure	34
3-7	Crystal structures and densities	36
3-8	Bond lengths and angles in BCC and FCC structures . .	36
3-9	Neighbors in cubic crystals	37
3-10	Volumes of primitive cells	38
3-11	Coulomb interaction energy in an SC structure	39
4.	Point Groups	43
4-1	Identification of groups	44
4-2	Group of Pauli matrices	44
4-3	Statements about groups	45
4-4	Identification of point groups	47
4-5	Expressions of rotations and reflections	48
4-6	Matrix representation of a point group	51
4-7	Invariant subgroup	52
4-8	Subgroups of point group C_{3v}	54
4-9	Abelian groups	56
4-10	Equivalence classes	56
4-11	Point group C_{4v}	57
5.	Classification of Bravais Lattices	63
5-1	Centerings in the hexagonal crystal system	64
5-2	Centerings in the cubic crystal system	68
5-3	Relations between symmetries of crystal systems	69
5-4	Lattice planes and directions in the cubic crystal system .	70
6.	Space Groups of Crystal Structures	71
6-1	Identification of crystals with symmorphic space groups .	73
6-2	Identification of crystals with nonsymmorphic space groups	73
6-3	Identification of crystals with symmorphic or nonsymmorphic space groups	73
6-4	Translation vectors in the diamond structure	74
6-5	Conventional and primitive unit cells of a monoclinic lattice	75
6-6	BCC and FCC structures of iron	76

6-7	Nearest and second-nearest neighbors in an HCP crystal	77
6-8	Diamond and body-centered tetragonal structures of gray tin	78
6-9	Wurtzite and zinblende structures of GaN	78
6-10	Crystal structure of diamond	79
6-11	Crystal structure of CaF_2	81
6-12	Monatomic BCC and FCC crystals	82
6-13	Hypothetical ceramic material of AX type	85
6-14	Crystal structure of CsCl	85
7.	Scattering of X-Rays by a Crystal	89
7-1	Evaluation of the differential scattering cross-section	89
7-2	Wave vector transfer in X-ray diffraction	90
7-3	Charged particle in a static magnetic field	90
7-4	Decay of a charged particle through radiation	92
7-5	Scattering by an atom	93
7-6	Incident and scattered X-ray beams	96
7-7	Motion of a bound electron in an atom under the influence of X-rays	98
7-8	Interaction of a bound electron with a plane electromagnetic wave	99
8.	Reciprocal Lattice	103
8-1	Reciprocal lattice of the reciprocal lattice	104
8-2	Symmetry of the reciprocal lattice	105
8-3	Reciprocal lattice of a two-dimensional Bravais lattice	105
8-4	Another two-dimensional Bravais lattice	107
8-5	First three Brillouin zones of a two-dimensional triangular lattice	108
8-6	Lengths of first eight reciprocal lattice vectors in SC, BCC, and FCC	109
8-7	Reciprocal lattice vectors and lattice planes	109
8-8	Structure factors of BCC and FCC crystals	110
8-9	First Brillouin zones and interplanar distances	111
8-10	Simple hexagonal lattice and its primitive cell and first Brillouin zone	113
8-11	Atom density in a lattice plane	115

8-12	Fourier series of a function with the periodicity of the Bravais lattice	116
8-13	Interplanar distances	117
8-14	Sizes of first Brillouin zones	119
8-15	First Brillouin zone of a simple orthorhombic Bravais lattice	120
8-16	Monatomic monovalent metal with an FCC structure . . .	121
9.	X-Ray Diffraction on Crystals	123
9-1	Powder diffraction on silicon	124
9-2	Powder diffraction on cubic CaF_2	125
9-3	Debye-Scherrer experiments on two cubic samples	126
9-4	Crystal structure of BaTiO_3	128
9-5	Temperature dependence of the Bragg angle for Al	129
9-6	Room-temperature superconductor	130
9-7	Powder diffraction on $\text{YBa}_2\text{Cu}_3\text{O}_{6.9}$	130
9-8	Three phases of iron	134
9-9	Powder diffraction on $\text{La}_{1.8}\text{Ba}_{0.2}\text{CuO}_{4-y}$	136
9-10	X-ray diffraction on Al	138
10.	Crystal Structure by Neutron Diffraction	141
10-1	Probe wavelengths proper for given structures	142
10-2	Reciprocal lattice vectors and families of lattice planes . .	143
10-3	Geometric structure factors	144
10-4	Structure factor of the HCP lattice	145
10-5	Neutron diffraction on the NaCl structure	147
10-6	Be as a neutron attenuator	148
10-7	Diffraction on Al of neutrons of energies below 15 meV . .	149
10-8	Neutron diffraction peak	150
11.	Bonding in Solids	153
11-1	Molecular orbitals for a hydrogen molecule	154
11-2	Energy of a hydrogen molecule in the bonding molecular orbital	155
11-3	Energy of a hydrogen molecule in the antibonding molecular orbital	158
11-4	Permanent dipole-permanent dipole interaction	159
11-5	Van der Waals bond in a diatomic molecule	160
11-6	Bond in a hypothetical diatomic molecule	161

12. Cohesion of Solids	163
12-1 Morse potential	164
12-2 One-dimensional crystal of a chain of alternating ions	165
12-3 Bonding in a three-dimensional ionic crystal	167
12-4 Born-Meyer theory of bonding in ionic crystals	167
12-5 Bonding in NaCl	169
12-6 Madelung constant of the CsCl crystal	170
12-7 Alkali metals	171
12-8 Exchange energy of the electron gas in an alkali metal	173
13. Normal Modes of Lattice Vibrations	177
13-1 Normal modes of a linear chain of ions	178
13-2 Simple one-dimensional crystal with a two-atom basis	181
13-3 One-dimensional crystal with next-nearest-neighbor interactions	183
13-4 Linear chain of atoms with damping	185
13-5 Polarizable molecules with internal degrees of freedom	186
13-6 Triatomic linear chain	188
13-7 Two-dimensional crystal with a square Bravais lattice	190
13-8 Simple cubic crystal	195
13-9 Three-dimensional monatomic crystal	199
13-10 Three-dimensional crystal with a two-atom basis	206
14. Quantum Theory of Lattice Vibrations	209
14-1 Quantum field operator of atomic momenta	211
14-2 Hamiltonian for a 3D crystal with a multi-atom basis	213
14-3 Thermodynamics of a gas of phonons	215
14-4 Lattice specific heat of a 1D crystal of inert gas atoms	217
14-5 Debye model for a 1D crystal of inert gas atoms	219
14-6 Electronic and lattice contributions to the specific heat of a metal	221
14-7 Specific heat of potassium at low temperatures	222
14-8 Phonon density of states for an optical branch	224
14-9 Phonon density of states for an acoustical branch	224
14-10 Number of phonons and its variance	225
14-11 Grüneisen parameter of a 1D crystal of inert gas atoms	229

15. Inelastic Neutron Scattering by Phonons	231
15-1 Debye-Waller factors in spaces of different dimensionality	232
15-2 Q - ω region accessible for inelastic neutron scattering . . .	236
15-3 Cumulant expansion	238
15-4 Property of the dynamical structure factor	240
16. Origin of Electronic Energy Bands	241
16-1 Quasi-momentum operator of Bloch electrons	242
16-2 Free-electron model	244
16-3 Infinite chain of atoms with a Peierls distortion	246
16-4 Densities of states in 1D and 2D tight-binding energy bands	247
16-5 Electron energies in a 2D metal with a square lattice . . .	249
16-6 Allowed wave vectors in a simple cubic crystal	250
16-7 Energy bands at the center of the first Brillouin zone for aluminum	251
16-8 Monovalent metal with an ideal HCP structure	251
16-9 Energy bands for an FCC lattice in the [111] direction . .	255
16-10 Band structure of a divalent FCC Sr metal	256
17. Electrons in a Weak Periodic Potential	259
17-1 Electrons in a 2D square lattice	259
17-2 Energy bands in a 1D crystal with a two-atom basis . . .	262
17-3 Energy gap at the M point in a 2D square lattice	264
17-4 Tight-binding band from localized orbitals	265
17-5 Energy band structure of aluminum	268
18. Methods for Band Structure Computations	273
18-1 Plane-wave method for a 1D crystal	274
18-2 Special $\mathbf{k}$ -points for a simple cubic Bravais lattice	279
18-3 Special $\mathbf{k}$ -points for a body-centered cubic crystal	282
18-4 Special $\mathbf{k}$ -points for a face-centered cubic crystal	285
18-5 Evanescent core potential	286
18-6 Green's function in the KKR method	287
18-7 $\mathbf{k} \cdot \mathbf{p}$ method for a semiconductor	290
18-8 Variational derivation of the tight-binding secular equation	292
18-9 Tight-binding approximation for a 1D crystal	293
18-10 Two-dimensional graphite sheet	294

19. Dynamics of Bloch Electrons in Electric Fields	299
19-1 Electrons in an ellipsoidal energy band	300
19-2 Electrons in the conduction band of a 1D metal	302
19-3 Electrons in a 1D tight-binding conductor	302
19-4 Electrons in a semiconductor superlattice	305
19-5 Effective mass approximation	307
19-6 Semi-classical equations of motion with damping	311
20. Fundamentals of Semiconductors	315
20-1 Conduction and valence bands of a hypothetical semiconductor	317
20-2 Effective mass, energy, momentum, and velocity of a hole	318
20-3 Effective mass of electrons at the conduction band edge .	319
20-4 Density of states for a single $\mathbf{k}$ -space ellipsoid in Si	319
20-5 Density of states in a nonparabolic conduction band . . .	320
20-6 Electron-hole pair excitations	321
20-7 Chemical potential of an intrinsic semiconductor	322
20-8 As-doped silicon crystal	322
20-9 Donors in indium antimonide	323
20-10 Band gap of InSb	324
20-11 Fermi levels in InP	326
20-12 Sb-doped silicon crystal	326
20-13 As-doped germanium	327
20-14 Concentrations of electrons and holes in a p -type semiconductor	328
20-15 Maximum concentration of donor atoms for intrinsic conduction	328
20-16 Conductivity and Fermi level of GaAs	330
21. Density Functional Theory	333
21-1 Electron densities in the Hartree and Fock-Hartree models	335
21-2 Pair densities and correlation functions in the Hartree-Fock model	338
21-3 Jellium model	339
21-4 Computation of one functional derivative	347
21-5 Computation of six functional derivatives	348
21-6 Action functional and Euler-Lagrange equation	351
21-7 One-electron system	352

21-8	Thomas-Fermi screening	354
21-9	N -representable density	357
21-10	Electron-ion interaction functional	359
21-11	Janak's Theorem	360
22.	Pseudopotentials	365
22-1	Smooth and oscillatory functions	366
22-2	Atom with a harmonic radial potential	369
22-3	Numerical solution of the radial Schrödinger equation	371
22-4	Kerker scheme for pseudopotentials	375
22-5	Spherical averages	379
22-6	Hedin-Lundqvist interpolation scheme for exchange and correlation	381
22-7	Simplified OPW pseudopotential	383
22-8	Equivalence of the norm-conservation condition	387
22-9	Perdew-Zunger parametrization of the correlation energy	388
23.	Projector-Augmented Plane-Wave Method	391
23-1	Kohn-Sham equations for auxiliary wave functions	392
23-2	General formula for local operators	395
24.	Determination of Electronic Band Structures	397
24-1	Quantization of electromagnetic fields	399
24-2	Quantum field operator of electrons	404
24-3	Poisson summation formula	406
24-4	Application of the Lifshits-Kosevich theory	408
24-5	Amplitude of dHvA oscillations in a free electron gas	409
25.	Crystal Defects	415
25-1	Deduction of the energy of vacancy formation from resistivity data	417
25-2	Energy of vacancy formation in gold	418
25-3	Number of vacant sites	419
25-4	Number of occupied lattice sites for every vacancy in Ni	419
25-5	Energy of vacancy formation in Al	420
25-6	Energy of vacancy formation in Mo	420
25-7	Schottky defects in copper	420
25-8	Schottky defects in an oxide ceramic	421

25-9	Burgers vectors of dislocations in FCC, BCC, and SC crystals	422
25-10	Two- and three-dimensional defects	424
25-11	Two perpendicular long edge dislocations	425
26.	Electron-Phonon Interaction	427
26-1	Perturbation computations for the electron-phonon system	430
26-2	Zeroth-order Green's functions from equations of motion	437
26-3	Field operators and single-electron Green's function	439
26-4	Feynman rules for the effective electron-electron interaction	442
26-5	Fourth-order corrections to the phonon Green's function	445
26-6	Spectral function, renormalization constant, and effective mass	449
26-7	Real and imaginary parts of the electron retarded self-energy	450
26-8	Periodic Anderson model	452
26-9	Fourth-order corrections to phonon Green's function at finite temperatures	457
26-10	Time-ordered product of three operators	462
26-11	Evaluation of Matsubara sums	464
26-12	Generalized spin susceptibility of a free electron gas	469
26-13	Pairing susceptibility	473
26-14	Localized electrons	475
26-15	Single impurity	481
26-16	Discontinuity of the momentum distribution	483
26-17	Multiparticle expectation value	483
26-18	Friedel oscillations	484
26-19	Plasma waves	488
26-20	Fermi gas in a spin-dependent external field	491
27.	Transport Properties of Solids	495
27-1	Equilibrium distribution function	497
27-2	Vector product of mechanical momentum with itself	498
27-3	DC conductivity of Bloch electrons in the presence of damping	498
27-4	Matthiessen's rule and its violation	501
27-5	Linear response theory and DC conductivity	502

27-6	Thermopower	506
27-7	Conductivity of a metal	508
27-8	Conductivity in terms of the effective mass	511
28.	Magnetic Properties of Solids	513
28-1	Localized magnetic moments in a weak magnetic field	515
28-2	Holstein-Primakoff transformation	518
28-3	Heisenberg-Weiss model for a ferromagnet	518
28-4	Two-site Hubbard model	520
28-5	Spin waves in a two-dimensional triangular ferromagnet	522
28-6	Double exchange model on two lattice sites	525
28-7	Specific heat of N noninteracting $1/2$ -spins in a magnetic field	528
28-8	Linear chain of three $1/2$ -spins	529
28-9	Landau's theory for the ferromagnetic phase transition	532
28-10	Spin operator in terms of electron annihilation and creation operators	535
28-11	Dot product of spin operators in terms of electron operators	536
28-12	One-dimensional spin- S Heisenberg quantum ferromagnet	536
28-13	Pauli susceptibility of a non-interacting Fermi gas	538
28-14	Instability of electron gas to ferromagnetism	540
28-15	Schwinger boson representation	542
28-16	Jordan-Wigner transformation	544
28-17	Matsubara susceptibility and Curie's law	546
28-18	One-dimensional anisotropic XY -model	548
28-19	Phonon-ferromagnon interaction	549
28-20	Weakly interacting dilute Bose gas	552
28-21	XY model for a one-dimensional quantum magnet	555
28-22	Schwinger-boson mean-field theory for a one-dimensional ferrimagnet	558
29.	Optical Properties of Solids	563
29-1	Properties of the electric susceptibility tensor	565
29-2	Reflectivity of a simple metal	568
29-3	Dielectric function of a free electron gas	570
29-4	Static dielectric function of a metal	572
29-5	Low-frequency response of electrons to an AC field	574

29-6	Dielectric function of an ideal metal	575
29-7	An isotropic solid modeled by Lorentz oscillators	577
29-8	Electric susceptibility in the Lorentz oscillator model	578
29-9	Optical properties of NaCl	579
29-10	Lyddane-Sachs-Teller relation for a crystal with a three-atom basis	583
29-11	Absorption coefficient of a nanowire	584
29-12	Model dielectric function for Ge	584
29-13	Analysis of reflectance data	586
30.	Superconductivity	589
30-1	Isotope effect in tin	592
30-2	Conductivity of a superconductor in the two-fluid model	594
30-3	Magnetic field inside an infinite superconducting plate	595
30-4	Critical field of a type-I superconductor in the Ginzburg- Landau theory	596
30-5	Ginzburg-Landau equation and superconducting current density	597
30-6	Proximity effect between two planar superconductors	598
30-7	Macroscopic quantum wave function of Cooper pairs	599
30-8	Phonon-mediated effective electron-electron attraction	602
30-9	Effect of the Fermi sea	607
30-10	Size of a Cooper pair	609
30-11	BCS superconducting ground state	612
30-12	Finite-momentum BCS state	615
30-13	Variational approach of the BCS theory	616
30-14	Average internal flux density in a triangular vortex lattice	620
30-15	Superconducting instability	620
	<i>References</i>	629
	<i>Index</i>	631