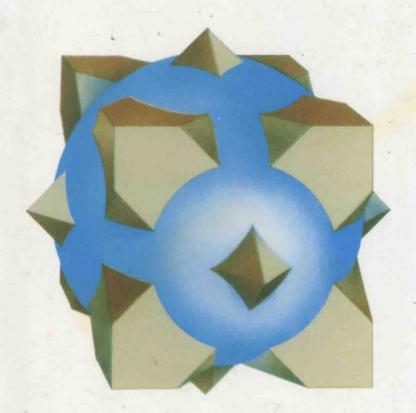
THOMSON

ASHCROFT/MERMIN

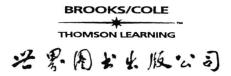


SOLID STATE PHYSICS 固态物理学

Solid State Physics

Neil W. Ashcroft N. David Mermin

Cornell University



Neil W.Ashcroft, N.David Mermin

Solid State Physics

EISBN: 0-03-083993-9

Copyright © 1976 Thomson Learning, Inc.

Original language published by Thomson Learning (a division of Thomson Learning Asia Pte Ltd). All Rights reserved. 本书原版由汤姆森学习出版集团出版。版权所有,盗印必究。

Beijing World Publishing Corporation is authorized by Thomson Learning to publish and distribute exclusively this English language reprint edition. This edition is authorized for sale in the People's Republic of China only (excluding Hong Kong, Macao SAR and Taiwan). Unauthorized export of this edition is a violation of the Copyright Act. No part of this publication may be reproduced or distributed by any means, or stored in a database or retrieval system, without the prior written permission of the publisher.

本书英文影印版由汤姆森学习出版集团授权世界图书出版公司北京公司独家出版发行。此版本仅限在中华人民共和国境内(不包括中国香港、澳门特别行政区及中国台湾)销售。未经授权的本书出口将被视为违反版权法的行为。未经出版者预先书面许可,不得以任何方式复制或发行本书的任何部分。

981-254-484-4

Preface

We began this project in 1968 to fill a gap we each felt acutely after several years of teaching introductory solid state physics to Cornell students of physics, chemistry, engineering, and materials science. In both undergraduate and graduate courses we had to resort to a patchwork array of reading assignments, assembled from some half dozen texts and treatises. This was only partly because of the great diversity of the subject; the main problem lay in its dual nature. On the one hand an introduction to solid state physics must describe in some detail the vast range of real solids, with an emphasis on representative data and illustrative examples. On the other hand there is now a well-established basic theory of solids, with which any seriously interested student must become familiar.

Rather to our surprise, it has taken us seven years to produce what we needed: a single introductory text presenting both aspects of the subject, descriptive and analytical. Our aim has been to explore the variety of phenomena associated with the major forms of crystalline matter, while laying the foundation for a working understanding of solids through clear, detailed, and elementary treatments of fundamental theoretical concepts.

Our book is designed for introductory courses at either the undergraduate or graduate level. Statistical mechanics and the quantum theory lie at the heart of solid state physics. Although these subjects are used as needed, we have tried, especially in the more elementary chapters, to recognize that many readers, particularly undergraduates, will not yet have acquired expertise. When it is natural to do so, we have clearly separated topics based entirely on classical methods from those demanding a quantum treatment. In the latter case, and in applications of statistical mechanics, we have proceeded carefully from explicitly stated first principles. The book is therefore suitable for an introductory course taken concurrently with first courses in quantum theory and statistical mechanics. Only in the more advanced chapters and appendices do we assume a more experienced readership.

The problems that follow each chapter are tied rather closely to the text, and are of three general kinds: (a) routine steps in analytical development are sometimes relegated to problems, partly to avoid burdening the text with formulas of no intrinsic interest, but, more importantly, because such steps are better understood if completed by the reader with the aid of hints and suggestions; (b) extensions of the chapter (which the spectre of a two volume work prevented us from including) are presented as problems when they lend themselves to this type of exposition; (c) further numerical and analytical applications are given as problems, either to communicate additional

¹ Suggestions for how to use the text in courses of varying length and level are given on pp. xviii-xxi.

information or to exercise newly acquired skills. Readers should therefore examine the problems, even if they do not intend to attempt their solution.

Although we have respected the adage that one picture is worth a thousand words, we are also aware that an uninformative illustration, though decorative, takes up the space that could usefully be filled by several hundred. The reader will thus encounter stretches of expository prose unrelieved by figures, when none are necessary, as well as sections that can profitably be perused entirely by looking at the figures and their captions.

We anticipate use of the book at different levels with different areas of major emphasis. A particular course is unlikely to follow the chapters (or even selected chapters) in the order in which they are presented here, and we have written them in a way that permits easy selection and rearrangement. Our particular choice of sequence follows certain major strands of the subject from their first elementary exposition to their more advanced aspects, with a minimum of digression.

We begin the book³ with the elementary classical [1] and quantum [2] aspects of the free electron theory of metals because this requires a minimum of background and immediately introduces, through a particular class of examples, almost all of the phenomena with which theories of insulators, semiconductors, and metals must come to grips. The reader is thereby spared the impression that nothing can be understood until a host of arcane definitions (relating to periodic structures) and elaborate quantum mechanical explorations (of periodic systems) have been mastered.

Periodic structures are introduced only after a survey [3] of those metallic properties that can and cannot be understood without investigating the consequences of periodicity. We have tried to alleviate the tedium induced by a first exposure to the language of periodic systems by (a) separating the very important consequences of purely translational symmetry [4, 5] from the remaining but rather less essential rotational aspects [7], (b) separating the description in ordinary space [4] from that in the less familiar reciprocal space [5], and (c) separating the abstract and descriptive treatment of periodicity from its elementary application to X-ray diffraction [6].

Armed with the terminology of periodic systems, readers can pursue to whatever point seems appropriate the resolution of the difficulties in the free electron model of metals or, alternatively, can embark directly upon the investigation of lattice vibrations. The book follows the first line. Bloch's theorem is described and its implications examined [8] in general terms, to emphasize that its consequences transcend the illustrative and very important practical cases of nearly free electrons [9] and tight binding [10]. Much of the content of these two chapters is suitable for a more advanced course, as is the following survey of methods used to compute real band structures [11]. The remarkable subject of semiclassical mechanics is introduced and given elementary applications [12] before being incorporated into the more elaborate semiclassical theory of transport [13]. The description of methods by which Fermi surfaces are measured [14] may be more suitable for advanced readers, but much of the survey

² The Table on pp. xix-xxi lists the prerequisites for each chapter, to aid those interested primarily in one aspect of the subject, or those preferring a different order of presentation.

³ References to chapter numbers are given in brackets.

of the band structures of actual metals [15] is readily incorporated into an elementary course.

Except for the discussion of screening, an elementary course might also bypass the essays on what is overlooked by the relaxation-time approximation [16] and by the neglect of electron-electron interactions [17].

Work functions and other surface properties [18] can be taken up at any time after the discussion of translational symmetry in real space. Our description of the conventional classification of solids [19] has been separated from the analysis of cohesive energies [20]. Both have been placed after the introduction to band structure, because it is in terms of electronic structure that the categories are most clearly distinguished.

To motivate the study of lattice vibrations (at whatever point after Chapter 5 readers choose to begin the subject) a summary [21] lists those solid properties that cannot be understood without their consideration. Lattice dynamics is given an elementary introduction, with the classical [22] and quantum [23] aspects of the harmonic crystal treated separately. The ways in which phonon spectra are measured [24], the consequences of anharmonicity [25], and the special problems associated with phonons in metals [26] and ionic crystals [27] are surveyed at an elementary level, though some parts of these last four chapters might well be reserved for a more advanced course. None of the chapters on lattice vibrations rely on the use of normal mode raising and lowering operators; these are described in several appendices for readers wanting a more advanced treatment.

Homogeneous [28] and inhomogeneous [29] semiconductors can be examined at any point after the introduction of Bloch's theorem and the elementary discussion of semiclassical mechanics. Crystalline defects [30] can be studied as soon as crystals themselves have been introduced, though parts of earlier chapters are occasionally referred to.

Following a review of atomic magnetism, we examine how it is modified in a solid environment [31], explore exchange and other magnetic interactions [32], and apply the resulting models to magnetic ordering [33]. This brief introduction to magnetism and the concluding essay on superconductivity [34] are largely self-contained. They are placed at the end of the book so the phenomena can be viewed, not in terms of abstract models but as striking properties of real solids.

To our dismay, we discovered that it is impossible at the end of a seven year project, labored upon not only at Cornell, but also during extended stays in Cambridge, London, Rome, Wellington, and Jülich, to recall all the occasions when students, postdoctoral fellows, visitors, and colleagues gave us invaluable criticism, advice, and instruction. Among others we are indebted to V. Ambegaokar, B. W. Batterman, D. Beaglehole, R. Bowers, A. B. Bringer, C. di Castro, R. G. Chambers, G. V. Chester, R. M. Cotts, R. A. Cowley, G. Eilenberger, D. B. Fitchen, C. Friedli, V. Heine, R. L. Henderson, D. F. Holcomb, R. O. Jones, B. D. Josephson, J. A. Krumhansl, C. A. Kukkonen, D. C. Langreth, W. L. McLean, H. Mahr, B. W. Maxfield, R. Monnier, L. G. Parratt, O. Penrose, R. O. Pohl, J. J. Quinn, J. J. Rehr, M. V. Romerio, A. L. Ruoff, G. Russakoff, H. S. Sack, W. L. Schaich, J. R. Schrieffer, J. W. Serene, A. J. Sievers, J. Silcox, R. H. Silsbee, J. P. Straley, D. M. Straus, D. Stroud, K. Sturm, and J. W. Wilkins.

x Preface

One person, however, has influenced almost every chapter. Michael E. Fisher, Horace White Professor of Chemistry, Physics, and Mathematics, friend and neighbor, gadfly and troubadour, began to read the manuscript six years ago and has followed ever since, hard upon our tracks, through chapter, and, on occasion, through revision and re-revision, pouncing on obscurities, condemning dishonesties, decrying omissions, labeling axes, correcting misspellings, redrawing figures, and often making our lives very much more difficult by his unrelenting insistence that we could be more literate, accurate, intelligible, and thorough. We hope he will be pleased at how many of his illegible red marginalia have found their way into our text, and expect to be hearing from him about those that have not.

One of us (NDM) is most grateful to the Alfred P. Sloan Foundation and the John Simon Guggenheim Foundation for their generous support at critical stages of this project, and to friends at Imperial College London and the Istituto di Fisica "G. Marconi," where parts of the book were written. He is also deeply indebted to R. E. Peierls, whose lectures converted him to the view that solid state physics is a discipline of beauty, clarity, and coherence. The other (NWA), having learnt the subject from J. M. Ziman and A. B. Pippard, has never been in need of conversion. He also wishes to acknowledge with gratitude the support and hospitality of the Kernforschungsanlage Jülich, the Victoria University of Wellington, and the Cavendish Laboratory and Clare Hall, Cambridge.

Ithaca June 1975 N. W. Ashcroft N. D. Mermin

Suggestions for Using the Book

It is in the nature of books that chapters must be linearly ordered. We have tried to select a sequence that least obscures several interwoven lines of development. The accompanying Table (pp. xix-xxi) is designed to help readers with special interests (in lattice vibrations, semiconductors, or metals, for example) or teachers of courses with particular constraints on time or level.

The prerequisites for each chapter are given in the Table according to the following conventions: (a) If "M" is listed after Chapter N, then the contents of Chapter M (as well, of course, as *its* essential prerequisites) are essential for understanding much or all of Chapter N; (b) If "(M)" appears after Chapter N, then Chapter M is not an *essential* prerequisite: either a small part of Chapter N is based on Chapter M, or a few parts of Chapter M may be of some help in reading Chapter N; (c) The absence of "M" or "(M)" after Chapter N does not mean that no reference back to Chapter M is made; however, such references as may occur are primarily because N illuminates the subject of M, rather than because M aids in the development of N.1

The rest of the Table indicates how the book might be used in a one semester (40 to 50 lectures) or two-semester (80 to 100 lectures) introductory undergraduate course. Chapters (or selections from a chapter) are listed for reading² if they are almost entirely descriptive, or, alternatively, if we felt that an introductory course should at least make students aware of a topic, even if time was not available for its careful exploration. The order of presentation is, of course, flexible. For example, although a two-semester course could follow the order of the book, one might well prefer to follow the pattern of the one-semester course for the first term, filling in the more advanced topics in the second.

An introductory course at the graduate level, or a graduate course following a onesemester undergraduate survey, would probably make use of sections omitted in the two-semester undergraduate course, as well as many of the sixteen appendices.

¹ Thus to proceed to Chapter 12 with a minimum of digression it is necessary to read Chapters 8, 5, 4, 2, and 1.

² Students would presumably be asked to read the chapters bearing on the lectures as well.

Chapter	Prerequisites	One-Semester Introduction	nester iction	I wo-Semester Introduction	nester ıction
		LECTURES	READING	LECTURES	READING
1. Drude	None	All		All	
2. Sommerfeld	1	All		All	
3. Failures of free-electron model	2		All		All
4. Crystal lattices	None	Summarize	All	All	
5. Reciprocal lattice	4	All		All	
6. X-ray diffraction	5	96-104		All	
7. Crystal symmetries	4				All
8. Bloch's theorem	5	132–143		All	
9. Nearly free electrons	8 (6)	152–166		All	
10. Tight binding	8		176	176–184	184–189
11. Computing band structure	8 (9)		192–193		All
12. Semiclassical dynamics	2, 8	214–233		214–233	
13. Semiclassical transport	12				244-246

Chu	Chapter	Prerequisites	One-Semester Introduction	nester ction	Two-Semester Introduction	nester ction
			LECTURES	READING	LECTURES	READING
14.	Measuring the Fermi surface	12	264-275		264-275	
15.	Band structure of metals	8 (2, 9, 10, 11, 12)		All	All	
16.	Beyond relaxation-time approximation	2 (13)				All
17.	Beyond independent electron approximation	2		337-342	330-344	345-351
18.	Surface effects	2, 4 (6, 8)		354-364	354-364	
19.	Classification of solids	2, 4 (9, 10)		All		All
20.	Cohesive energy	19 (17)	396-410		All	(1)
21.	Failures of static lattice model	(2, 4)		All		All
22.	Classical harmonic crystal	5	422–437		All	
23.	Quantum harmonic crystal	22	452-464		All	

24.	24. Measuring phonons	2, 23		470-481	All	
25.	25. Anharmonic effects	23		499-505	All	
26.	Phonons in metals	17, 23 (16)	523–526		512–519 523–526	
27.	Dielectric properties	19, 22		534-542	All	
28.	28. Homogeneous semiconductors	2, 8, (12)	562–580		All	
29.	29. Inhomogeneous semiconductors	28	290–600		All	
30.	30. Defects	4 (8, 12, 19, 22, 28, 29)		628–636		All
31.	Diamagnetism, Paramagnetism	(2, 4, 14)	661–665		All	
32.	Magnetic interactions	31 (2, 8, 10, 16, 17)	672–682		672–684	
33.	Magnetic ordering	4, 5, 32		694-700	All	
34.	34. Superconductivity	1, 2 (26)		726-736	All	

Contents

	Preface vii
	Important Tables xiv Suggestions for Using the Book xviii
1.	The Drude Theory of Metals 1
2.	The Sommerfeld Theory of Metals 29
3.	Failures of the Free Electron Model 57
4.	Crystal Lattices 63
5.	The Reciprocal Lattice 85
6.	Determination of Crystal Structures by X-Ray
	Diffraction 95
7.	Classification of Bravais Lattices and Crystal
	Structures 111
8.	Electron Levels in a Periodic Potential:
	General Properties 131
9.	Electrons in a Weak Periodic Potential 151
10.	The Tight-Binding Method 175
11.	Other Methods for Calculating Band
	Structure 191
12.	The Semiclassical Model of Electron
	Dynamics 213
13.	The Semiclassical Theory of Conduction in
	Metals 243
14.	Measuring the Fermi Surface 263
15.	Band Structure of Selected Metals 283
16.	
	Approximation 313
17.	Beyond the Independent Electron
	Approximation 329
18.	
	J JJ

19.	Classification of Solids 373
20.	Cohesive Energy 395
21.	Failures of the Static Lattice Model 415
22.	Classical Theory of the Harmonic
	Crystal 421
23.	Quantum Theory of the Harmonic
	Crystal 451
24.	Measuring Phonon Dispersion
	Relations 469
25.	Anharmonic Effects in Crystals 487
26.	Phonons in Metals 511
27.	Dielectric Properties of Insulators 533
28.	Homogeneous Semiconductors 561
29.	Inhomogeneous Semiconductors 589
30.	Defects in Crystals 615
31.	Diamagnetism and Paramagnetism 643
32.	Electron Interactions and Magnetic
	Structure 671
33.	Magnetic Ordering 693
34.	Superconductivity 725
	•
	ADDENDICES
	APPENDICES
A.	Summary of Important Numerical Relations is
	the Free Electron Theory of Metals 757
В.	The Chemical Potential 759
C.	The Sommerfeld Expansion 760
D.	Plane-Wave Expansions of Periodic Functions
	in More Than One Dimension 762
E.	The Velocity and Effective Mass of Bloch
	Electrons 765
F.	Some Identities Related to Fourier Analysis
	of Periodic Systems 767

G. The Variational Principle for Schrödinger's

769

Equation

797

H.	Hamiltonian Formulation of the
	Semiclassical Equations of Motion, and
	Liouville's Theorem 771
I.	Green's Theorem for Periodic
	Functions 772
J.	Conditions for the Absence of Interband
	Transitions in Uniform Electric or
	Magnetic Fields 773
K.	Optical Properties of Solids 776
L.	Quantum Theory of the Harmonic
	Crystal 780
M.	Conservation of Crystal Momentum 78
N.	Theory of the Scattering of Neutrons by a
	Crystal 790
O.	Anharmonic Terms and n-Phonon
	Puggessas 706

P. Evaluation of the Landé g-Factor

INDEX 799

Important Tables

The more important tables of data¹ or theoretical results are listed below. To aid the reader in hunting down a particular table we have grouped them into several broad categories. Theoretical results are listed only under that heading, and data on magnetic and superconducting metals are listed under magnetism and superconductivity, rather than under metals. Accurate values of the fundamental constants are given in the end paper and on page 757.

Theoretical Results

The noncubic crystallographic point groups 122

The cubic crystallographic point groups 121

Comparison of properties of Sommerfeld and Bloch electrons 214

Comparison of the general treatment of collisions with the relaxation-time approximation 318

Lattice sums of inverse *n*th powers for the cubic Brayais lattices 400

Madelung constants for some cubic crystal structures 405

Numbers of independent elastic constants for the seven crystal systems 445

Values of the Debye specific heat 461

Comparison of phonons and photons 466

Comparison of a gas of molecules and a gas of phonons 506

Characteristic lengths in a p-n junction 607

Ground states of ions with partially filled *d*- or *f*-shells 652

Comparison of exact and mean field critical temperatures for several Ising models 717

Major numerical formulas of free electron theory 757

¹ The data in the tables are presented with the aim of giving the reader an appreciation for orders of magnitude and relative sizes. We have therefore been content to quote numbers to one or two significant places and have not made special efforts to give the most precise values. Readers requiring data for fundamental research should consult the appropriate sources.

Crystal Structure

The face-centered cubic elements 70
The body-centered cubic elements 70

The trigonal (rhombohedral) elements 127

The tetragonal elements 127

The hexagonal close-packed elements 77

Elements with the diamond structure 76

Some compounds with the sodium chloride structure 80

Some compounds with the cesium chloride structure 81

Some compounds with the zincblende structure 81

Metals

Free electron densities and r_s/a_0 5

Electrical resistivities

Some typical relaxation times 10

Thermal conductivities 21

Fermi energies, temperatures, wave vectors, and

velocities 38

Bulk moduli 39

Low temperature specific heats 48

Work functions 364

Elastic constants 447

Debye temperatures 461

Linear expansion coefficients 496

Insulators and Semiconductors

Alkali halide ionic radii 384

Ionic radii of II-VI compounds 386

Lattice constants of some III-V compounds 389

xvi Important Tables

Radii of metallic ions compared with nearest-neighbor distances in the metal 391

Cohesive energies of the alkali halides 406

Bulk moduli of the alkali halides 408

Debye temperatures of some alkali halides 459

Grüneisen parameters and linear expansion coefficients for some alkali halides 494

Atomic polarizabilities of the noble gas atoms and the alkali halide ions 544

Static and optical dielectric constants and transverse optical phonon frequencies of the alkali halides 553

Lennard-Jones parameters for the noble gases 398

Lattice constants, cohesive energies, and bulk moduli of the solid noble gases 401

De Boer parameters for the noble gases 412

Elastic constants 447

Debye temperatures 459, 461

Static dielectric constants for covalent and covalent-ionic crystals 553

Ferroelectric crystals 557

Energy gaps of semiconductors 566

Impurity levels in silicon and germanium 580

Magnetism

Molar susceptibilities of the noble gas atoms and alkali halide ions 649

Effective Bohr magneton numbers for the rare earth ions 657

Effective Bohr magneton numbers for the iron group ions 658

Pauli susceptibilities of the alkali metals 664

Some dilute alloys with (and without) local moments 686

Critical temperatures and saturation magnetizations of ferromagnets 697