Solid State Theory

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Ulrich Rössler

Solid State Theory

An Introduction

With 110 Figures

Springer

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ISSN 0171-1873

ISBN 978-3-662-09942-1 ISBN 978-3-662-09940-7 (eBook)
DOI 10.1007/978-3-662-09940-7

Library of Congress Control Number: 2004106905

springeronline.com

Originally published by Springer-Verlag Berlin Heidelberg New York in 2004.
Softcover reprint of the hardcover 1st edition 2004

Typesetting by the author
Final Layout: Frank Herweg, Leutershausen
Cover production: *design & production* GmbH, Heidelberg

Printed on acid-free paper SPIN: 10859833 57/3141/ba - 5 4 3 2 1 0

To Erika

Preface

The history of my involvement in this book project starts more than 30 years ago. During the years 1969–1972, my thesis advisor, Otfried Madelung, wrote a series of three textbooks on Solid State Theory, entitled *Festkörpertheorie* I–III, which appeared in the Springer paperback series *Heidelberger Taschenbücher*. My fellow graduate students and friends Manfred Lietz, Rolf Sandrock, and Joachim Treusch and I, were the first to proof-read these books. Better still, we were given the unique opportunity to provide input based on insights gained during our studies. In 1978 when *Festkörpertheorie* I–III were partly rewritten and translated into English, Otfried Madelung again asked his former disciples, then already established in university positions, for comments and contributions based on their respective research and teaching experience in this field. The result, entitled *Introduction to Solid-State Theory*, became a widely used textbook, published in several further editions over the following years.

Like most textbooks on Solid-State Theory currently used in university physics courses all over the world, *Introduction to Solid-State Theory* has meanwhile become somewhat outdated. Solid State Physics has evolved significantly and many topics, which 30 years ago were still the subject of active research or even beyond its leading edge, have now become part of our standard knowledge. The idea of accounting for this development in a textbook has been lingering in the collective mind of the Solid State Physics community for quite a while, but it took an initiative by Springer to concretize the project. When Springer editors asked Otfried Madelung to rework *Introduction to Solid-State Theory* accordingly, he convinced them that it would make more sense to write a completely new book, proposing me as a potential author. This is how I got involved.

Due to the formative influence of Otfried Madelung and his approach to science, my research in Solid State Theory has from the very beginning been oriented towards experimental work, often directly stimulated by concrete experimental results. This tendency was solidified during a year as postdoctoral researcher with Manuel Cardona at Brown University in Providence, RI (USA). Quite commonly, my research projects were initiated by discussions with researchers renowned for their experimental work and have frequently been conducted in fruitful cooperations. It is to this continuous contact with the physics reality that I owe the down-to-earth approach which characterizes my research and teaching and which should also be noticeable in this book.

At the University of Regensburg, where I became professor in 1972, Solid State Physics has been a strong research field, both in experiment and theory. Over the years the topics evolved from magnetism, phase transitions, lattice dynamics, and electronic structure of bulk material to the upcoming fields of high-T_c superconductors, correlated electron systems, surface physics, quantum wells, nano-structures, and composite materials. Quite naturally, Solid State Theory has been a standard part of the physics curriculum in Regensburg. It started as a one-semester course with four weekly lectures in the fourth year of the German diploma curriculum (corresponding to the first year of the graduate education in the Anglo-American system). Soon it was supplemented by a second course on special topics, with the purpose of guiding the students into active research fields. For more than thirty years, I taught these courses on a regular basis, taking turns with my colleagues Joachim Keller, Uwe Krey, Ulrich Schröder, and Dieter Strauch. The exchange of teaching concepts and problems with these colleagues, and also our joint research projects considerably enriched my lectures. During the last decade I benefitted much from the expertise of my senior coworker Michael Suhrke. Further important input came from discussions with many colleagues from all over the world during conferences, visits, and sabbaticals in different places. My lecture notes for these courses, accumulated and continuously modified over the years, constitute the backbone of this book.

Clearly, the book follows a well-defined tradition. Target readers are those students in physics or material science who are interested in understanding the theoretical approach to Solid State Physics, while maintaining contact to the experimental facts. The contents are essentially comparable to those of other textbooks on the same subject, but emphasis is put on new aspects of the field that have resulted from more recent research. Extensive references to related literature in the form of textbooks, topical series, data collections, and selected original papers are provided to establish the connection with the sources of this subject and with active research fields. Each chapter contains a selection of problems and solutions, which are meant to help the reader gain practice with the concepts and the physics explained in the text. Since the number of pages is restricted, this book cannot claim completeness. Nevertheless, wherever possible, reference is given to those important topics that could be covered here only briefly or not at all. In short, this book is intended as an introduction to Solid State Theory, given from the perspective of more than 30 years of learning, teaching and research in this field.

It is a pleasure to thank all those who contributed in one way or the other to this project. I have already mentioned some friends and colleagues and would like to extend my acknowledgments to the students who attended my courses and enriched them by their constructive feedback. This applies especially to my diploma and Ph.D. students, who contributed ideas during many hours of discussion about their research projects. A highly visible contribution to this book came from Ingeburg Zirkl who prepared all the figures. A critical reading of parts of the manuscript by my friends and colleagues Joachim Keller and Dieter Strauch, and by my son Thomas has led to considerable improvements of the contents and the text. Finally, I express my gratitude to Springer, in particular to Dr. Claus Ascheron and Dr. Angela Lahee, for their expert help and advice but also for their patience in waiting for the final version of this book.

Regensburg,
April 2004

Ulrich Rössler

Contents

List of Symbols

a	lattice constant
$a_s^\dagger(\boldsymbol{q}),\ a_s(\boldsymbol{q})$	creation, annihilation operator of a phonon with quantum numbers $s, \boldsymbol{q}$
$a_i^\dagger, a_i$	creation, annihilation operator of spin excitations at site i
$\boldsymbol{a}_i,\ i = 1, 2, 3$	primitive lattice vectors
$\hat{A}$	observable
$\boldsymbol{A}$	vector potential
$\boldsymbol{b}_j,\ j = 1, 2, 3$	primitive reciprocal lattice vectors
$b_{\boldsymbol{k}}^\dagger, b_{\boldsymbol{k}}$	creation, annihilation operator of ferromagnetic magnons
$\boldsymbol{B}$	magnetic induction
$\hat{B}$	observable
B_0	bulk modulus
$\mathcal{B}_S(y)$	Brillouin function
c	velocity of light in vacuum
c_{V}	specific heat at constant volume
$c_{ijkl}(c_{IJ})$	components of the compliance tensor, elastic moduli (Voigt notation)
$c_{\boldsymbol{k}\sigma}^\dagger, c_{\boldsymbol{k}\sigma}$	creation, annihilation operator of Bloch electrons
$C_{nn}(\boldsymbol{r}, \boldsymbol{r}')$	density–density correlation function
$D, D_{1,2,3}$	deformation potentials
$D_{\boldsymbol{\tau} i, \boldsymbol{\tau}' j}(\boldsymbol{q})$	element of the dynamical matrix
$D(\omega),\ D(E)$	density of states
$\boldsymbol{D}, \boldsymbol{D}(\boldsymbol{q}, \omega)$	displacement field
e	elementary charge
e_{ijk}	piezoelectric tensor
$\boldsymbol{e}^s(\boldsymbol{q})$	normalized phonon eigenvector
E	energy Youngs modulus
$E_n(\boldsymbol{k}), \epsilon_{n\boldsymbol{k}\sigma}$	energy of Bloch electron
E_0	energy of ground state
E_{F}	Fermi energy

$E(T)$	thermal energy
$\mathcal{E}_{\mathrm{el}}$	energy eigenvalue of the many-body electron problem
$\boldsymbol{E}, \boldsymbol{E}(\boldsymbol{q}\omega)$	electric field
F	free energy
$g(g^*)$	Landé (effective) g factor
$g(\boldsymbol{r})$	pair–distribution function
G	rigidity modulus
$G_{\mathrm{AB}}, G(\alpha; t, t')$	retarded Green function
$\boldsymbol{G}_{\boldsymbol{m}}, \boldsymbol{G}$	reciprocal lattice vector
H	Hamiltonian of phonons or of electrons symmetry point of the *bcc* Brillouin zone, endpoint of the Δ axis
$\mathcal{H}, \mathcal{H}_0$	many-body Hamiltonian of the solid
$\mathcal{H}_{\mathrm{el}}$, $\mathcal{H}_{\mathrm{ion}}$, $\mathcal{H}_{\mathrm{el-ion}}$	parts of $\mathcal{H}$ describing electrons, ions, and the electron–ion interaction
$\mathcal{H}_{\mathrm{jell}}$	Hamiltonian of the jellium model
$\mathcal{H}_{\mathrm{so}}$	Hamiltonian of spin–orbit coupling
$\mathcal{H}_{\mathrm{spin}}$	Heisenberg's spin Hamiltonian
$\boldsymbol{H}$	magnetic field
$\boldsymbol{j}$	electric current density
$J, J_{\boldsymbol{RR}'}, J_{ij}$	exchange integrals
k_{B}	Boltzmann constant
k_{F}	radius of Fermi sphere
$\boldsymbol{k}$	wave vector (of electron)
L	symmetry point of the fcc Brillouin zone Lagragian of lattice vibrations
m	free electron mass
m^*	effective mass of an electron
$\boldsymbol{m}$	magnetic dipole moment
M_i, $M_{\boldsymbol{\tau}}$	mass of an ion
$\boldsymbol{M}^E$, $\boldsymbol{M}$	electric dipole moment
$\boldsymbol{M}$	magnetization or magnetic dipole density
$n(\boldsymbol{r})$	particle (electron) density
$\hat{n}$	density operator
$n_{\boldsymbol{q}}$	density or number fluctuation
$n_{\mathrm{s}}(\boldsymbol{q}, T)$	Bose–Einstein distribution function
N, N_0	number of electrons number of unit cells in the normalization volume
$N_{\pm}, N_{\uparrow\downarrow}$	number of electrons for different spin orientation
$\boldsymbol{p}$, $\boldsymbol{p}_l$	momentum of an electron
$\boldsymbol{P}$	dielectric polarization or electric dipole density
$\boldsymbol{P}_{\boldsymbol{n\tau}}$	momentum of an ion
$P_{\mathrm{s}}(\boldsymbol{q})$	conjugate momentum to $Q_s(\boldsymbol{q})$

$\boldsymbol{q}$	wave vector (of phonon)
Q_i, Q_{ext}	(point) charge
$Q_s(\boldsymbol{q})$	normal coordinate of lattice vibration
r_{s}	density parameter (radius of Wigner–Seitz sphere)
$\boldsymbol{r}$, $\boldsymbol{r}_l$	position vector of an electron
$\boldsymbol{R}_{\boldsymbol{n}}^0$	lattice vector, equilibrium position of an ion in a Bravais lattice
$\boldsymbol{R}_{\boldsymbol{n}}$	actual position of an ion in a Bravais lattice
$\boldsymbol{R}_{\boldsymbol{n\tau}}$	actual position of an ion in a lattice with basis
s_{ijkl}	components of the elastic or stiffness tensor
$S(\boldsymbol{q})$	static structure factor
$S(\boldsymbol{q}, \omega)$	dynamic structure factor
$\boldsymbol{S}_{\boldsymbol{R}}$	vector operator for spin at $\boldsymbol{R}$
$S^i, S^{\pm}$	components of vector spin operator
$t, t_{ij}, t_{\boldsymbol{RR}'}$	transfer integral
T	absolute temperature
T_{C}	critical (Curie) temperature
T_{N}	Néel temperature
$T_{\boldsymbol{R}_{\boldsymbol{n}}^0}$	translation operator
$\boldsymbol{u}_{\boldsymbol{n\tau}}(t)$	ion displacement from equilibrium position
U	exchange interaction, correlation energy (Hubbard)
$\mathcal{U}_\alpha(\{\boldsymbol{R}_{\boldsymbol{n}}\})$	adiabatic potential
$v_{\boldsymbol{q}}$	Fourier transform of (Coulomb) potential
v_{F}	Fermi velocity
v_{L}, v_{T}	longitudinal, transverse sound velocity
V, V_{c}	crystal or normalization volume
$V_{\text{eff}}(\boldsymbol{r})$	effective single particle potential
$V_{\text{xc}}(\boldsymbol{r})$	exchange–correlation potential
V_{ext}	external perturbation
$\mathcal{V}_s(\boldsymbol{q})$	matrix element of electron–phonon interaction
Z, Z_{G}	partition function of canonical and grand-canonical ensemble
α	thermal expansion coefficient
$\alpha_{\boldsymbol{k}}^\dagger, \alpha_{\boldsymbol{k}}; \beta_{\boldsymbol{k}}^\dagger, \beta_{\boldsymbol{k}}$	creation, annihilation operators of antiferromagnetic magnons
γ	Grüneisen parameter, Sommerfeld coefficient
Γ	center of the Brillouin zone, $\boldsymbol{k} = (0, 0, 0)$ damping parameter
Δ	symmetry line in the fcc(bcc) Brillouin zone connecting Γ and $X(H)$ gap parameter in superconductors
$\chi_{AB}(\omega)$	response function, susceptibility
$\boldsymbol{\chi}^E$, $\boldsymbol{\chi}^M$	dielectric, magnetic susceptibility
χ_{ij}^E, χ_{ij}^M	tensor components of $\boldsymbol{\chi}^E, \boldsymbol{\chi}^M$

$\chi^{\mathrm{M}}_{+-}(\boldsymbol{q},\omega)$	spin susceptibility
$\epsilon_{jl}(\varepsilon_J)$	components of the strain tensor (Voigt notation)
ϵ_0	average ground state energy per electron
ϵ_{c}	average correlation energy per electron
ε_0	vacuum dielectric constant
$\varepsilon(0)$	static or low-frequency dielectric constant
ε_∞	high-frequency dielectric constant
$\varepsilon(\boldsymbol{q},\omega)$	dielectric function
$\varepsilon_1,\ \varepsilon_2$	real, imaginary part of dielectric function
η	(transverse) effective charge
λ	localization length
$\mathit{\Lambda}$	symmetry line in the Brillouin zone connecting $\mathit{\Gamma}$ and L
μ	reduced mass chemical potential mobility
μ_{B}	Bohr's magneton
μ_0	magnetic field constant
ν	filling factor of Landau levels
ω_{c}	cyclotron frequency
ω_{D}	Debye frequency
$\omega_s(\boldsymbol{q})$	frequency of phonon with quantum numbers $s,\boldsymbol{q}$
$\omega_{\mathrm{L}},\ \omega_{\mathrm{T}}$	longitudinal, transverse phonon frequency at $\boldsymbol{q}=0$
$\omega_{\boldsymbol{k}}$	magnon frequency
ω_{p}	plasma frequency
$\mathit{\Omega}$	grand-canonical potential
$\psi(\boldsymbol{r})$	single-electron wave function
$\psi_{n\boldsymbol{k}}(\boldsymbol{r})$	Bloch function
$\mathit{\Psi},\tilde{\mathit{\Psi}}$	many-electron wave function (stationary, time-dependent)
$\phi_\nu(\boldsymbol{r}-\boldsymbol{R}^0_{\boldsymbol{n}})$	atomic orbital centered at $\boldsymbol{R}^0_{\boldsymbol{n}}$
$\mathit{\Phi}$	force constant magnetic flux
$\mathit{\Phi}_0$	elementary magnetic flux quantum
$\rho,\ \hat{\rho}$	statistical operator
ρ_0	statistical operator of thermal equilibrium
ρ_M	mass density
ρ_{AB}	spectral function
$\rho(\boldsymbol{r})$	charge density
$\boldsymbol{\rho}$	resistivity tensor
$\sigma_{ik}(\sigma_I)$	components of the stress tensor (Voigt notation)
$\boldsymbol{\sigma}$	conductivity tensor
$\mathit{\Sigma}$	symmetry line in the Brillouin zone connecting $\mathit{\Gamma}$ and K

$\Sigma(\alpha, E), \Sigma(\boldsymbol{k}, \sigma)$	electron self-energy
Θ_{D}	Debye temperature
$\tau_{\boldsymbol{k}}$	single-particle lifetime
τ_{tr}	transport relaxation time
$\boldsymbol{\tau}$	ion position relative to the lattice vector in a lattice with basis
ζ	degree of spin polarization
$\zeta_{\nu}(z)$	subband envelope function