BASIC ASPECTS OF THE QUANTUM THEORY OF SOLIDS

Order and Elementary Excitations

Aimed at graduate students and researchers, this book covers the key aspects of the modern quantum theory of solids, including up-to-date ideas such as quantum fluctuations and strong electron correlations. It presents the main concepts of the modern quantum theory of solids, as well as a general description of the essential theoretical methods required when working with these systems.

Diverse topics such as the general theory of phase transitions, harmonic and anharmonic lattices, Bose condensation and superfluidity, modern aspects of magnetism including resonating valence bonds, electrons in metals, and strong electron correlations, are treated using the unifying concepts of order and elementary excitations. The main theoretical tools used to treat these problems are introduced and explained in a simple way, and their applications are demonstrated through concrete examples.

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CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore,
São Paulo, Delhi, Dubai, Tokyo, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521835213

First published 2010

Printed in the United Kingdom at the University Press, Cambridge

A catalogue record for this publication is available from the British Library

Library of Congress Cataloguing in Publication data
Khomskii, Daniel, 1938–
Basic aspects of the quantum theory of solids : order and elementary excitations / Daniel Khomskii.
p. cm.
Includes bibliographical references and index.
ISBN 978-0-521-83521-3
1. Solid-state physics. 2. Quantum theory. I. Title.
QC176.K47 2010
530.4′1 – dc22 2010018879

ISBN 978-0-521-83521-3 Hardback

Cambridge University Press
978-0-521-83521-3 - Basic Aspects of the Quantum Theory of Solids: Order and Elementary Excitations
Daniel I. Khomskii
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Foreword and general introduction

Foreword

There are many good books describing the foundations and basics of solid state physics, such as *Introduction to Solid State Physics* by C. Kittel (2004) or, on a somewhat higher level, *Solid State Physics* by N. W. Ashcroft and N. D. Mermin (1976). However there is a definite lack of books of a more advanced level which would describe the modern problems of solid state physics (including some theoretical methods) on a level accessible for an average graduate student or a young research worker, including experimentalists.

Usually there exists a rather wide gap between such books written for theoreticians and those for a wider audience. As a result many notions which are widely used nowadays and which determine 'the face' of modern solid state physics remain 'hidden' and are not even mentioned in the available literature for non-specialists.

The aim of the present book is to try to fill this gap by describing the basic notions of present-day condensed matter physics in a way understandable for an average physicist who is going to specialize in both experimental and theoretical solid state physics, and more generally for everyone who is going to be introduced to the exciting world of modern condensed matter physics – a subject very much alive and constantly producing new surprises.

In writing this book I tried to follow a unifying concept throughout. This concept, which is explained in more detail below, may be formulated as the connection between an *order* in a system and *elementary excitations* in it. These are the notions which play a crucial role in condensed matter physics in general and in solid state physics in particular. I hope that this general line will help the reader to see different parts of condensed matter physics as different sides of a unified picture and not as a collection of separate unrelated topics.

The plan of the book is the following. After discussing the general theory of phase transitions (Chapter 2) which forms the basis for describing *order* in solids, I go step by step through different specific situations: systems of bosons (phonons in crystals – Chapter 4, and general Bose systems, including Bose condensation and superfluidity – Chapter 5). Then follows the important chapter on magnetism, Chapter 6 (strictly speaking dealing neither with bosons, nor with fermions), and after that we switch to the discussions of fermions – electrons in solids, Chapters 7–13. In each topic I have tried to follow the general line which I have already described above: to discuss first the type of order we have in one or the other situation, then introduce different types of elementary excitations in them, first independent excitations, but then paying most attention to the *interaction* between them and to their *quantum nature*. Thus altogether the material presented in the book is supposed to cover the main situations met in solids.

The theoretical methods used to describe these phenomena are introduced not so much separately, as such, but in the appropriate places where they are needed, and in a way which immediately shows how they work in specific problems. Thus, in studying Bose systems I introduce the widely used Bogolyubov canonical transformation, which later on is also used for treating magnons in antiferromagnets and for certain problems for electrons. Discussing spin waves, I introduce the method of equations of motion with corresponding decoupling, later on also used, e.g. for studying correlated electrons (the Hubbard model). When going to electron systems, I describe the Green function method and the Feynman diagram technique – without complete and rigorous derivations, but with the aim of demonstrating how these methods really *work* in different situations.

I hope the material covered in this book will give the reader a relatively complete picture of the main phenomena in modern solid state physics and of the main theoretical methods used to study them. But of course it is impossible to cover in one book of modest size this whole field. The most important and evident omissions are:

I do not practically touch on the broad and important field of *transport phenomena* (resistivity, thermal conductivity, thermopower, the Hall effect, etc.) This is a very big topic in itself, but it lies somewhat outside the main scope of this book. I also do not discuss specific features of such important, but well-known materials as semiconductors, ferroelectrics, etc. Also the wide field of superconductivity is touched upon only to the extent it is required to illustrate the general treatment.

Yet another relatively recent and very beautiful topic is missing – the phenomenon of the quantum Hall effect. Hopefully I can ‘repair’ this omission later.

On the theoretical side probably two important methods are not sufficiently discussed in the book. One is the renormalization group method used to treat complicated situations with strong interaction. I only briefly mention this method, but do not describe it in detail. Interested readers may find its description, e.g. in the books by Chaikin and Lubensky (2000) or Stanley (1987).

Another theoretical technique widely used nowadays is the use of different types of numerical calculations. This is a very broad and rapidly developing field which proved its efficiency for studying real materials and for theoretical investigations of many situations not accessible to analytical calculations. This is quite a special field, and it requires special treatment – although when appropriate I present some of the results obtained in this way.

With all these omissions, I still hope that the material which *is* included will be useful for a broad audience and will give the reader a relatively complete picture of the main phenomena and main problems in modern solid state physics.

A few words about the style of the presentation. This book has grown out of a lecture course which I gave for several years at Groningen University and at Cologne University. Therefore it still has some features of the lecture notes. I present in it all the main ideas, but often not the full derivations of corresponding results. This is also caused by the fact that the material touched upon in this book in fact covers a huge field, and it is impossible to present all the details in one book. There are many monographs and textbooks discussing in detail the separate subfields presented below. However I have tried to choose the topics and present them in such a way that the general ideas underlying modern solid state physics and the internal logic of this field become clear. For more detailed discussions of particular problems and/or corresponding methods of their theoretical treatment the readers should go to the specialized literature.

In accordance with this general concept of the book, I did not include in it a special 'problems' section. In some places, however, especially in the first part of the book, I formulate parts of the material, as Problems. Those who want to get a deeper understanding of the subject are recommended to stop reading the text at these places and try to find the answers themselves; the material presented before usually makes this task not too difficult. The answers, however, are usually given right after the problems, so that readers can also go on along the text if they do not have a desire, or time, to do these exercises themselves. Actually most of the problems, with their answers, form an integral part of the text.

In several places in the text I have also put some more special parts of the text in smaller type. These parts usually relate to more specialized (although useful) material.

In addition to the main material I have also included three very short chapters (Chapters 1, 3 and 7) with a short summary of some of the basic facts from statistical mechanics. I think it would be useful for readers to have this information at hand.

Some important notions are mentioned several times in different parts of the text. I did this intentionally, so that different chapters would become somewhat more independent – although of course there are a lot of cross-references in the text.

I hope that the book gives a coherent presentation of the main ideas and methods of the quantum theory of solids.

There are many good books which cover parts of the material contained in the present book (and actually much more!). I can recommend the following, already classical books:

1. J. M. Ziman (1979), *Principles of the Theory of Solids*. A very good and clear book covering the main topics in solid state physics. Highly recommended. However, it does not contain more modern methods.
2. N. W. Ashcroft and N. D. Mermin (1976), *Solid State Physics*. Also a very good and widely used book, covering the topics in more detail, on a somewhat more elementary level. Very transparent and useful.
3. M. P. Marder (2000), *Condensed Matter Physics*. A rather complete book describing the main phenomena in solid state physics, but not going into much theoretical detail.
4. C. Kittel (1987), *Quantum Theory of Solids*. Contains detailed discussion of many problems in quantum theory, using more modern methods such as diagram techniques. Somewhat more theoretical.
5. G. D. Mahan (2000), *Many-Particle Physics*. Gives a very complete treatment of the topics discussed; it is a kind of 'encyclopedia'. It uses the Green function method all the way through. Very useful for theoreticians, and contains all the necessary details and derivations, etc. However not all topics are discussed there.
6. L. D. Landau and I. M. Lifshits, *Course of Theoretical Physics*, especially *Statistical Physics* (old one-volume edition 1969, or new edition v. I 1980), and *Quantum Mechanics* (1977). These classical books contain virtually all the basic material necessary, and many particular topics important for our problems. If one can call the book by Mahan an encyclopedia, then the course of Landau and Lifshits is a 'bible' for all theoreticians, especially those working in condensed matter physics. But these books are very useful not just for theoreticians, but for everyone looking for clear and precise description of all the basic ideas of theoretical physics.
7. J. R. Schrieffer (1999), *Theory of Superconductivity*. A very clear book; contains in particular a very good and condensed treatment of the Green function method and diagram technique, in a form used now by most theoreticians.
8. A. A. Abrikosov, L. P. Gor'kov and E. Dzyaloshinsky (1975), *Methods of the Quantum Field Theory in Statistical Physics*. One of the first (and still the best) books on the modern methods applied to condensed matter physics. It gives a very detailed treatment of the theoretical methods and a good discussion of specific problems (Fermi and Bose liquids; plasma; electron–phonon interaction and the basics of the theoretical treatment of superconductivity).

9. P. M. Chaikin and T. C. Lubensky (2000), *Principles of Condensed Matter Physics*. A very good book containing in particular detailed discussion of different questions connected with phase transitions. The accent is on general statistical mechanics; specifically it contains a lot of material on soft condensed matter physics, but does not discuss such topics as electrons in metals, magnetism, etc.

Some other references will be given later, in the main body of the book. But, keeping in mind the character of the book (which is practically expanded lecture notes and which still retain that character), I deliberately refrained from including too many references – it would be simply impossible to cite all the relevant works. Therefore I mostly refer not to original publications but rather to monographs and review papers. Interested readers may find more detailed information on particular subjects in these references.

General introduction

The unifying concept in this book is the concept of *order* and *elementary excitations*; these are the key words.

One can argue as follows. In general in macroscopic systems with many degrees of freedom the internal state, or internal motion on the microscopic scale, is random. However as $T \to 0$ the entropy of the system should go to zero, $S \to 0$; this is the well-known Nernst theorem, or the third law of thermodynamics. Accordingly, at $T = 0$ there should exist *perfect order* of some kind.

Such ordering sets in at a certain characteristic temperature T^*, often with a phase transition, but not necessarily.

At $T \ll T^*$ we can describe the state of the system as predominantly ordered, or maybe in a weakly excited state. Such relatively weakly excited states will be thermally excited, but can appear also due to small external perturbations. Usually in such a state we can speak of a small number of *elementary excitations*, or *quasiparticles*. Examples are, e.g. *phonons* in crystals, *magnons* or *spin waves* in ferromagnets, *excitons* in semiconductors, etc.

Sometimes such elementary excitations are rather strange: instead of electrons they may be excitations with spin, but no charge (*spinons*), or vice versa (*holons*). There exist also *topological* excitations (solitons, vortices, etc.).

In a first approximation we can consider these excitations as *noninteracting*. Such are, e.g. phonons in a harmonic crystal, etc. However in the next step we have to include in general an *interaction* between quasiparticles.

There may exist interactions between the same quasiparticles. They lead, e.g. to anharmonic effects in crystals (phonon–phonon interactions); they are included in the Landau Fermi-liquid theory, and give rise to screening for electrons in metals; the magnon–magnon interaction can lead, e.g. to the formation of bound states of magnons, etc. There also exist interactions between different quasiparticles: electron–phonon interactions, pairing in conventional superconductors, and interactions between many other elementary excitations. Often due to these interactions the properties of quasiparticles are strongly changed, or renormalized: an example is the formation of polarons (electron + strong lattice distortion). Also new quasiparticles may be formed (plasmons due to the Coulomb interaction of electrons; excitons – bound states of electrons and holes in semiconductors). Even the ground state itself, the very type or ordering, may change because of such interactions. An example is the superconducting state instead of the normal state of a metal.

It is important that these quasiparticles, or elementary excitations, are *quantum* objects. Consequently, one should not visualize the order as completely classical: there are *quantum fluctuations* (zero-point motion, or zero-point oscillations) even at $T = 0$. Sometimes they lead only to minor numerical changes, but there are cases, especially in low-dimensional or frustrated systems, when they can completely modify the properties of a system, e.g. destroying the long-range order totally. They can also modify the properties of the phase transitions themselves, e.g. leading to *quantum phase transitions.* Thus the classical picture is always very useful, but one should be cautious and aware of its possible failures in some cases – but very often these cases are the most interesting!

In treating these problems a lot of different approaches were used, and different methods developed. These methods are often used not only in solid state physics or condensed matter physics in general; many of them are also widely used (and often have been developed!) in other parts of physics: in elementary particle physics, in field theory, and in nuclear physics. Methods such as the Green function method and Feynman diagrams were introduced in field theory, but are now widely used in condensed matter physics. On the other hand, some methods and concepts which first appeared in solid state physics (the mean field, or self-consistent field method, the concept of a phase transition) are now used in nuclear physics, in elementary particle physics (e.g. quark–gluon plasma), and even in cosmology.

In this book I will try to describe the main concepts and ideas used in modern many-particle physics, and the methods used to study these problems, such as the equation of motion method, canonical transformations, diagram techniques, and the Green function method. Once again, the key words will be *elementary excitations*, in connection with *order*. The illustrations will be predominantly given for the examples of solid state systems, although, as I said before, many concepts, notions and methods are also applicable in different fields, and even not only in physics! Thus, some of the ideas of many-particle physics are now widely used for treating problems in biology, and even economics and sociology. I hope that such a general view will help readers to form a unified concept of the main phenomena in condensed matter physics and related fields.