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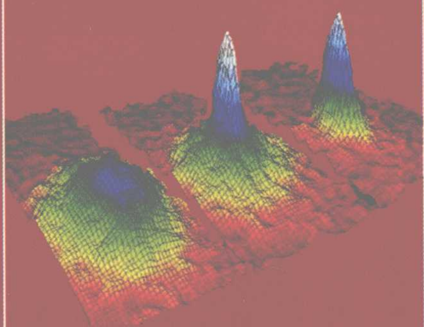
Band Theory and Electronic Properties of Solids

固体能带理论和电子性质

J. Singleton



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Preface

This book covers the important topic of band theory and electronic properties of materials. It is intended to be used by final-year undergraduates and first-year graduate students studying condensed matter physics as part of a physics or engineering degree. It may also be used as preparatory material for students starting a doctorate in condensed matter physics or semiconductor devices, or for recent graduates starting research in these fields in industry.

Why does this book exist?

Yet another book on the electronic properties of solids requires some explanation. In teaching final-year undergraduates and first-year graduate students, I have become frustrated with the scarcity of *general* texts which cover a wide range of material synoptically. Students at this point in their careers often have to embark on research projects, extended essays, literature searches, and so on, in very diverse topics; they tend to dive straight into a *specialised* text book covering one particular topic (one-dimensional solids, impurities in semiconductors etc.) and to forget that this topic is part of a wider whole. The outcome can be a blinkered attitude in which connections are missed, wheels are reinvented and so on.

Secondly, the 'old warhorses' by Kittel and Ashcroft and Mermin, although fine in many respects, have little connection with the huge explosion of research in condensed matter physics over the last 20 years. The leap from many such texts to current research topics is enormous; students, seeing illustrative data from the 1950s and 1960s are often convinced that condensed matter physics is no longer an active, glamorous research field.

Thirdly, there is a perceived gap between 'undergraduate' condensed matter physics texts, which often flounder at length in one dimension, concealing the wood with trees, and more advanced books such as Ashcroft and Mermin, which is often rather daunting for undergraduates.

I therefore planned a book which would treat band theory and its consequences at a simple level, but in three dimensions from the start, and which would provide pointers to recent developments. The book would give an overview of the field, suggesting literature which provided various routes into current research topics.

The task was made easier when the book became part of the wider *Oxford Master Series in Condensed Matter Physics*, a collection of six linked textbooks covering virtually all areas of the subject. Topics, such as superconductivity, which could lead to very lengthy diversions, could therefore be left to someone else, leaving what I hope is a much more focused book.

Background

Band theory is evident all around us, and yet is one of the most stringent tests of quantum mechanics. This book is therefore an attempt to reveal in a qualitative fashion how band theory leads to the everyday properties of materials around us.[1] It also provides many of the ideas and vocabulary necessary to understand the electronic, optical and structural properties of the materials met in science and technology.

[1] For example, silicon, calcite and copper all contain similar densities of electrons, and yet they have very different properties, all inexplicable without quantum mechanics.

An understanding of band theory has also led to an extraordinary burgeoning of solid state technology; the average resident of Europe, Japan or the USA interacts daily with hundreds of devices containing semiconductor logic, memory or optoelectronics. A huge amount of research world-wide is devoted to optimising and designing such devices. This book therefore aims to provide the vocabulary and quantum-mechanical training necessary to understand electronic, optoelectronic and other solid-state devices. Whilst not treating the operation of devices in detail, the book introduces holes, effective masses, doping, the use of reduced dimensionality, excitons etc. at the level required for advanced texts on the fundamental principles of device design.

The use of the book in a structured course

The book was designed to accompany a course of the same name in Oxford, and it may be useful to give a brief description of this process. The course comprises 12–16 lectures and three or four problems classes. Chapters 1–8 of the book, corresponding to perhaps the first 70 % of the lectures and first two classes, are intended to familiarise the student with the ideas and terminology of electronic bandstructure (e.g. bands, holes, Fermi surface, effective mass tensor, Landau quantisation, quasiparticles etc.). Thus equipped, the student can proceed to the rest of the book, corresponding to the final lectures and third (and fourth) classes, which deal with electron transport; i.e. the concepts derived in the first part are used in the second to study e.g. the transport of heat and electricity in metals and semiconductors, simple electronic devices and the quantum Hall effect.

In all of this, it should be emphasised that the exercises are very much an integral part of the book; they continue derivations and proofs started in the text, illustrate the new concepts encountered, and allow the student to become familiar with the typical sizes of important parameters. To gain maximum benefit from the book, the reader should attempt a substantial proportion of the exercises. Students vary greatly in ability, and I have included an appendix containing hints on how to tackle the more taxing problems, plus some numerical answers.

I have tended to assume that the reader will have already encountered some of the ideas of condensed matter physics, at the level of (say) *The Solid State* by Harry Rosenberg (OUP, Third Edition). However, this is not strictly necessary, and I hope that the appendices make the work reasonably self-contained, or at least provide a useful revision of related material.

In order to leave space for recent developments, the Drude model and the introduction of quantum statistics are treated synoptically, with an emphasis on the underlying assumptions and failings in Chapter 1. The need for a deeper understanding of bandstructure is thereby illustrated. Chapters 2–5 then introduce Bloch's theorem fairly rigorously in three dimensions, at a level slightly below that found in Ashcroft and Mermin; by this stage of their career, I believe that students are ready for such a rigorous treatment with 'no cheating'. The book then considers (in three dimensions) two tractable limits of Bloch's theorem, a very weak periodic potential and a very strong periodic potential (so strong that the electrons can hardly move from atom to atom). It is demonstrated that both extreme limits give rise to *bands*, with *band gaps* between them. In both extreme cases, the bands are qualitatively very similar; i.e. real potentials, which must lie somewhere between the two extremes, must also give rise to qualitatively similar bands and band gaps. The ideas of effective masses, band shapes and bandwidths are related to the *real space* arrangement of the atoms or molecules making up the substance in a qualitative way using the tight-binding model.

Having introduced the ideas of effective masses and holes, semiconductor bands are introduced in more detail, along with the idea of artificial structures such as superlattices and quantum wells, layered organic substances and oxides; again, all are qualitatively understandable using the ideas of the tight-binding model. In view of the presence of the book on soft condensed matter in the Master series, I did not consider it necessary to treat amorphous solids.

Most of the available condensed matter physics texts provide a very poor coverage of developments in the last twenty years. From Chapter 7 onwards I mention some of the current 'hot topics', and show that they can be understood using the techniques developed thus far in the book. In other words, by this stage the students have acquired enough background information to grasp the ideas behind recent research. Moreover, in illustrating examples of phenomena such as the de Haas–van Alphen effect, I have used recent experiments. For example, a crystalline organic metal is used as a 'case study' in Chapter 8. This is no accident; since 1998, more papers have been written on the physics of these materials than on the high-T_c cuprates.[2] However, in five years, the hot topics of condensed matter physics could be very different; if subsequent editions of this book are ever produced, I should expect to use different materials as my examples.[3]

I have tried wherever possible to use the standard symbols for quantities encountered in research papers and other fields, so that transferring from this book to other works is as painless as possible. Inevitably, this has led to one or two conflicting definitions,[4] but these are *always* made clear by the context. A list of the more commonly used symbols is given in one of the appendices.

In under three hundred pages, a book cannot be comprehensive.[5] Each chapter therefore ends with a section pointing out more detailed or differing treatments for the ambitious and simpler alternatives for the challenged. Relatively recent review articles and sources of supplementary data are also given; in this way, I hope that the book can function as a route to deeper, more specialised study.[6]

[2] I am grateful to Paul Chaikin of Princeton for this information.

[3] When reading these chapters, one of my older colleagues said 'but what about the seminal experiments on the magnetisation of metals in the 1930s?' My answer was that, whilst these examples are historically interesting, and worthy of considerable respect, they are not representative of this thriving field of research today. There are innumerable pictures of the oscillations in Bi and Cu in existing books, to which the student is referred if they are so inclined.

[4] For example, n is both the electron density and the quantum number of the Bohr atom; p is both the hole density and the momentum.

[5] As another John wrote 'And there are also many other things ..., the which, if they should be written every one, I suppose that even the world itself could not contain the books that should be written'.

[6] I believe that it is a mistake to make a book *too* comprehensive (e.g. some of the books which purport to contain the whole of 'University Physics'). This discourages the reader from seeking enlightenment elsewhere, and can eventually lead to the belief that one doesn't need any other text book or paper to 'know physics'. Gaining experience in sifting information, doing literature searches and seeking connections is invaluable and helps to develop the student's critical skills.

Acknowledgements

This book has been greatly improved by the suggestions of numerous friends and colleagues. In Oxford, Arzhang Ardavan, Steve Blundell, Geoff Brooker, Anne-Katrin Klehe and Mike Leask have read the various drafts of the book, making many useful comments, donating figures, doing the problems and correcting errors. Mike Glazer provided a critique of the appendices, ensuring (I hope) that I do not infuriate crystallographers and others. Elsewhere, Greg Boebinger (Los Alamos National Laboratory), Martyn Chamberlain (Engineering, Leeds University), Helen Fretwell (Physics, University of Wales), Marco Grioni (EPF, Lausanne), Neil Harrison (Los Alamos National Laboratory), Steve Hill (Montana State University, Bozeman), David Leadley (Physics, University of Warwick) and Jos Perenboom (Physics, Katholieke Universiteit Nijmegen) made excellent suggestions which I hope will make the book more widely applicable.

I have used various incarnations of the book in teaching undergraduate and graduate students in Oxford and elsewhere. I should like to thank the many victims of this process who have pointed out errors, typing mistakes and incomprehensibilities. Too much space would be consumed if I thanked *everyone* by name, but particularly enthusiastic or devastating in their suggestions were Lily Childress, Carol Gardiner, Paul Goddard, Eleanore Hodby, Lesley Judge, Brendon Lovett, Eleanore Lyons and Amalia Coldea, to whom I am very grateful. In spite of this enormous effort by others, some errors will inevitably remain, and these are entirely my responsibility.[7]

A substantial number of the figures in this book were drawn by Irmgard Smith, who made much of my rather wobbly initial sketches; I am very grateful to her for this enormous effort, which allowed me to spend more time on the text and the other figures. I should also like to thank Karen Dalton, Phil Gee, Phil Klipstein, Robin Nicholas and John Ward, who supplied data or images for use in the book. Mervyn Barnes of the Oxford Physics Practical Course deserves special mention for running his cryostats to provide some of the illustrative data in Chapters 8 and 9. Finally, I should like to thank Chuck Mielke (Los Alamos), who provided the cover picture and data.

Lastly, I am profoundly grateful to my wife Claire, and children, Louisa and Joe, for their support and love during the preparation of this book.

J. S.
Los Alamos

February 2001

[7] Please email corrections to j.singleton1@physics.ox.ac.uk.

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