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978-0-521-11711-1 — Quantum Theory of Materials
Efthimios Kaxiras , John D. Joannopoulos
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Quantum Theory of Materials

This accessible new text introduces the theoretical concepts and tools essential for graduate-level courses on the physics of materials in condensed matter physics, physical chemistry, materials science and engineering, and chemical engineering.

Topics covered range from fundamentals such as crystal periodicity and symmetry, and derivation of single-particle equations, to modern additions including graphene, two-dimensional solids, carbon nanotubes, topological states, and Hall physics. Advanced topics such as phonon interactions with phonons, photons, and electrons, and magnetism, are presented in an accessible way, and a set of appendices reviewing crucial fundamental physics and mathematical tools makes this text suitable for students from a range of backgrounds.

Students will benefit from the emphasis on translating theory into practice, with worked examples explaining experimental observations, applications illustrating how theoretical concepts can be applied to real research problems, and 242 informative full-color illustrations. End-of-chapter problems are included for homework and self-study, with solutions and lecture slides for instructors available online.

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Preface

Why do various materials behave the way they do? For instance, what makes a material behave like a good insulator, instead of being a good conductor or a semiconductor? What determines the strength of a material? How can we account for the color of different solids? Questions like these have attracted curious minds for centuries. Materials, after all, are of central importance to humanity: they define the stage of civilization, as in "Stone Age," "Bronze Age," "Iron Age," and the current "Silicon Age." The scientific study of the properties of materials in the last two centuries has produced a body of knowledge referred to as the "physics of materials" that goes a long way toward explaining and even *predicting* their properties from first-principles theoretical concepts. Our book aims to present these concepts in a concise and accessible manner.

The book emerged as the result of many years of teaching this subject at Harvard and MIT. The intended audience is graduate or advanced undergraduate students in physics, applied physics, materials science, chemistry, and related engineering and applied science fields. There are classic textbooks on the subject, the venerable work by N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, being a standard example; there are also numerous more recent works, for instance *Fundamentals of Condensed Matter Physics* by M. L. Cohen and S. G. Louie, a work of great depth and clarity, and the delightfully intuitive *Physics of Solids* by E. N. Economou. We mention most of these books as suggestions for further reading at the end of each chapter, as appropriate. Taken together, these sources quite nicely cover all important aspects of the subject. The present work aims to fill a gap in the literature, by providing a single book that covers all the essential topics, including recent advances, at a level that can be accessible to a wider audience than the typical graduate student in condensed matter physics. This is what prompted us to use the word "materials" (rather than "solids" or "condensed matter") in the title of the book. Consistent with this aim, we have included topics beyond the standard fare, like elasticity theory and group theory, that hopefully cover the needs, and address the interests, of this wider community of readers.

To facilitate accessibility, we have intentionally kept the mathematical formalism at the simplest possible level, for example, avoiding second quantization notation except when it proved absolutely necessary (the discussion of the BCS model for superconductivity, Chapter 8). Instead, we tried to emphasize physical concepts and supply all the information needed to motivate how they translate into specific expressions that relate physical quantities to experimental measurements.

The book concentrates on theoretical concepts and tools, developed during the last few decades to understand the properties of materials. As such, we did not undertake an extensive survey of experimental data. Rather, we compare the results of the theoretical models to key experimental findings throughout the book. We also give examples of how the theory can be applied to explain what experiment observes, as well as several compilations of experimental data to capture the range of behavior encountered in various types of materials.

The book can be used to teach a one-semester graduate-level course (approximately 40 hours of lecture time) on the physics of materials. For an audience with strong physics and math background and some previous exposure to solid-state physics, this can be accomplished by devoting an introductory lecture to Chapter 1, and covering the contents of Chapters 2–7 thoroughly. Topics from Chapters 8, 9, and 10 can then be covered as time permits and the instructor's interest dictates. An alternative approach, emphasizing more the applications of the theory and aimed at an audience with no prior exposure to solid-state physics, is to cover thoroughly Chapters 1 and 2, skip Chapter 3, cover Sections 4.1–4.7, Chapters 5 and 6, Sections 7.1–7.5, Sections 8.3 and 8.4, and selected topics from Chapters 9 and 10 as time permits.

Many examples and applications are carefully worked out in the text, illustrating how the theoretical concepts and tools can be applied to simple and more sophisticated models. Not all of these need to be presented in lectures; in fact, the reason for giving their detailed solutions was to make it possible for the student to follow them on their own, reserving lecture time for discussions of key ideas and derivations. We have also included several problems at the end of each chapter and we strongly encourage the interested student to work through them in detail, as this is the only meaningful way of mastering the subject.

Finally, we have included an extensive set of appendices, covering basic mathematical tools and elements from classical electrodynamics, quantum mechanics, and thermodynamics and statistical mechanics. The purpose of these appendices is to serve as a reference for material that students may have seen in a different context or at a different level, so that they can easily refresh their memory of it, or become familiar with the level required for understanding the discussion in the main text, without having to search a different source.

Acknowledgments

When trying to explain something, it is often difficult to keep track of how your own understanding of the ideas was formed. Acknowledging all the sources of inspiration and insight can therefore be an impossible task, but some of these sources definitely stand out.

We wish to thank our teacher and mentor Marvin Cohen as an especially important influence on our thinking and understanding of physics. EK wishes to express a deep debt of gratitude to his teachers at various stages of his career, John Joannopoulos, Kosal Pandey, and Lefteris Economou, all of whom served as role models and shaped his thinking. Many colleagues have played an equally important role, including Bert Halperin, David Nelson, Nihat Berker, and Stratos Manousakis.

The students who patiently followed several iterations of the manuscript, helping to improve it in ways big and small, are the ultimate reason for putting a vast collection of hand-written notes into a coherent text – we thank them sincerely, and hope they benefitted from the experience. Some of them put an extraordinary amount of energy and care into writing solutions to the problems at the end of the chapters, for which we are thankful. The most recent and careful compilation was made by Cedric Flamant, who also corrected some problem statements and several inaccuracies in the text – he deserves special thanks. Daniel Larson read Chapter 9 very carefully, and provided much useful feedback and suggestions for improving the presentation. We also thank Eugene Mele for many useful comments on the physics of topological states.

Last but not least, we wish to acknowledge the essential, or more appropriately, existential role that our partners Eleni and Kyriaki played in this endeavor; they have put up with innumerable hours of distraction while we were working out some idea to include in the book. Without their support and patience, the book would simply not exist; we gratefully dedicate it to them.