

Preface

This is a book detailing the theory of a band-structure method. The three most common empirical band-structure methods for semiconductors are the tight-binding, the pseudopotential, and the $k \cdot p$ method. They differ in the choice of basis functions used to represent Schrödinger's equation: atomic-like, plane-wave, and Bloch states, respectively. Each have advantages of their own. Our goal here is not to compare the various methods but to present a detailed exposition of the $k \cdot p$ method.

One always wonder how a book got started. In this particular case, one might say when the two authors were postdoctoral fellows in the Cardona *Abteilung* at the Max Planck Institut für Festkörperforschung in Stuttgart, Germany in 1994–1995. We started a collaboration that got us to use a variety of band-structure methods such as the $k \cdot p$, tight-binding and ab initio methods and has, to date, led to over 50 joint publications. The first idea for a book came about when one of us was visiting the other as a Balslev research scholar and, fittingly, the final stages of the writing were carried out when the roles were reversed, with Morten spending a sabbatical at Wright State University.

This book consists of two main parts. The first part concerns the application of the theory to bulk crystals. We will spend considerable space on deriving and explaining the bulk $k \cdot p$ Hamiltonians for such crystal structures. The second part concerns the application of the theory to “perturbed” and nonperiodic crystals. As we will see, this really consists of two types: whereby the perturbation is gradual such as with impurities and whereby it can be discontinuous such as for heterostructures.

The choice of topics to be presented and the order to do so was not easy. We thus decided that the primary focus will be on showing the applicability of the theory to describing the electronic structure of intrinsic semiconductors. In particular, we also wanted to compare and contrast the main Hamiltonians and $k \cdot p$ parameters to be found in the literature. This is done using the two main methods, perturbation theory and the theory of invariants. In the process, we have preserved some historical chronology by presenting first, for example, the work of Dresselhaus, Kip and Kittel prior to the more elegant and complete work of Luttinger and Kane. Partly biased by our own research and partly by the literature, a significant part of the explicit derivations and illustrations have been given for the diamond and zincblende semiconductors, and to a lesser extent for the wurtzite semiconductors. The impact of external strain and static electric and magnetic fields on the electronic

structure are then considered since they lead to new $k \cdot p$ parameters such as the deformation potentials and g -factors. Finally, the problem of inhomogeneity is considered, starting with the slowly-varying impurity and exciton potential followed by the more difficult problem of sharp discontinuities in nanostructures. These topics are included because they lead to a direct modification of the electron spectrum. The discussion of impurities and magnetic field also allows us to introduce the third theoretical technique in $k \cdot p$ theory, the method of canonical transformation. Finally, the book concludes with a couple of appendices that have background formalism and one appendix that summarizes some of the main results presented in the main text for easy reference. In part because of lack of space and because there exists other excellent presentations, we have decided to leave out applications of the theory, e.g., to optical and transport properties.

The text is sprinkled with graphs and data tables in order to illustrate the formal theory and is, in no way, intended to be complete. It was also decided that, for a book of this nature, it is unwise to try to include the most “accurate” material parameters. Therefore, most of the above were chosen from seminal papers. We have attempted to include many of the key literature and some of the more recent work in order to demonstrate the breadth and vitality of the theory. As much as is possible, we have tried to present a uniform notation and consistent mathematical definitions. In a few cases, though, we have decided to stick to the original notations and definitions in the cited literature.

The intended audience is very broad. We do expect the book to be more appropriate for graduate students and researchers with at least an introductory solid state physics course and a year of quantum mechanics. Thus, it is assumed that the reader is already familiar with the concept of electronic band structures and of time-independent perturbation theory. Overall, a knowledge of group representation theory will no doubt help, though one can probably get the essence of most arguments and derivations without such knowledge, except for the method of invariants which relies heavily on group theory.

In closing, this work has benefitted from interactions with many people. First and foremost are all of our research collaborators, particularly Prof. Dr. Manuel Cardona who has always been an inspiration. Indeed, he was kind enough to read a draft version of the manuscript and provide extensive insight and historical perspectives as well as corrections! As usual, any remaining errors are ours. We cannot thank our family enough for putting up with all these long hours not just working on this book but also throughout our professional careers. Last but not least, this book came out of our research endeavors funded over the years by the Air Force Office of Scientific Research (LCLYV), Balslev Fond (LCLYV), National Science Foundation (LCLYV), the Danish Natural Science Research Council (MW), and the BHH Foundation (MW).

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