Preface

This book is aimed at second-year graduate students in physics, electrical engineering (EE), or materials science (MS). Its main goal is to present a rigorous introduction to electronic transport in solids, especially at the nanometer scale, within a self-contained text (and course) and with a not-so-hidden emphasis on computational aspects.

Understanding electronic transport in solids requires some basic knowledge of Hamiltonian classical mechanics, quantum mechanics, condensed matter theory, and statistical mechanics. Thus, usually, four "heavy" courses are required to acquire this background knowledge. Unfortunately, in practice, EE and MS students may only attend a quick course on quantum mechanics at best; they are unlikely to have ever seen the Hamiltonian formulation of classical mechanics or to have been exposed to statistical mechanics or condensed matter beyond some quick preview, especially as far as electronic (band) structure is concerned. MS students may be required to enroll in a class on the electrical and optical properties of solids but this is often only a superficial introduction. Finally, not all physics students will have seen these subjects at the depth needed. Our aim is to provide a deep discussion of those specific subtopics of these four disciplines which are required to deal with electronic transport, so that a single, self-contained class may suffice. This will be useful for students who intend to work in academia or the nano-/microelectronics industry.

We assume some basic knowledge of classical mechanics (of course) and of quantum mechanics. Therefore, only the Lagrangian and Hamiltonian formulations of classical mechanics are reviewed. Similarly, the principles of quantum mechanics are revisited only formally, with emphasis on canonical quantization, since this leads to its generalization to systems with infinitely many degrees of freedom (fields) and so to second quantization, elementary excitations in solids, and scattering processes. A bird's-eye view of the structure of atoms, bonds, and molecules serves the purpose of introducing some useful mathematical tools and concepts used in the text.

Topics covered in this book are: the theory of energy bands in crystals, second quantization and elementary excitations in solids, dielectric properties of semiconductors, with an emphasis on dielectric screening, electron scattering with phonons, plasmons, electrons, and photons, the derivation of transport equations in semiconductors and semiconductor nanostructures, both at the quantum and semiclassical level. The text presents examples relevant to current research, not only about Si, but also III–V compound semiconductors, nanowires, graphene, and graphene nanoribbons. In particular, the text gives major emphasis to plane-wave methods regarding the electronic structure of solids, both Density Functional Theory (DFT) and empirical pseudopotentials, always paying attention to their effect on (and numerical implementation in a description of) electron transport. The core of the text deals with electronic transport, as we said above, with ample discussions of the transport equations derived both in the quantum picture (the Liouville–von Neumann equation) and semiclassically (the Boltzmann transport equation, BTE). Several methods for solving the semiclassical BTE are also

reviewed, including the method of moments, expansions into orthogonal functions, iterative methods, Monte Carlo, cellular automata, and direct matrix inversion.

Four appendices conclude the text. The first one presents time-independent and time-dependent perturbation theory, as well as the Born approximation. The second appendix provides full information, and references, about the empirical pseudopotentials that are commonly used for fcc semiconductors. The third appendix, a quick-and-dirty introduction to the principles of special relativity, is required to understand the "minimal" electromagnetic coupling between electrons and photons. It also introduces the relativistic wave equation for spin-1/2 particles which, in its massless version, describes approximately the electron dispersion in graphene. The fourth appendix pays tribute to our emphasis on computational aspects and lists the source code of a simple computer program to compute the band structure of Si using empirical pseudopotentials. We hope that students will enjoy running and modifying this program.

The breath and length of the subjects presented in this text makes it impossible to cover the totality of material presented here in a single one-semester course (typically 28 lectures of 75 min each) and even less so in a one-quarter course. In our experience, only the basic subjects can be covered in such a class. Subjects that may be covered "optionally," if time allows or in a sequel of this course, have been highlighted by an asterisk. Some are simple historical remarks or curiosities, but those that deal with advanced topics are intentionally treated at a slightly deeper, more research-oriented level. In these chapters and/or sections, more frequent reference is made to journal papers than to textbooks. In the second year of a graduate program, we find it appropriate to start exposing graduate students to the more terse and concise style used in research papers, while the students are preparing to perform research on their own.

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