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Fausto Rossi

Theory of Semiconductor Quantum Devices

Microscopic Modeling and Simulation Strategies

With 125 Figures

Springer
dedicato a Elena, la luce della mia vita

(devoted to Elena, the light of my life)
Primary goal of the present volume is to provide a cohesive description of the vast area of semiconductor quantum devices, with special emphasis on basic quantum-mechanical phenomena governing the electro-optical response of new-generation nanomaterials. The book covers within a common theoretical framework different types of optoelectronic nanodevices, including quantum-cascade laser sources and detectors, few-electron/exciton quantum devices, and semiconductor-based quantum logic gates. Distinguished feature of the present volume is a unified microscopic treatment of quantum-transport and coherent-optics phenomena on ultrasmall space- and time-scales, as well as of their semiclassical counterparts.

The book, mainly devoted to graduate students as well as researchers working in the field, presents a unified theoretical treatment of semiconductor nanodevices; indeed, the primary goal of this volume is to cover within a common language two different classes of quantum devices, i.e., systems where the quantum nature manifests itself in terms of discrete energy spectra but their dynamics may still be treated within a semiclassical scenario (e.g., infrared laser sources and detectors) and semiconductor devices whose behavior is entirely governed by electronic quantum coherence (e.g., semiconductor-based quantum logic gates).

The field of semiconductor quantum devices is so active and extensive that an exhaustive treatment of the many diverse research areas is nearly impossible; we shall therefore limit ourselves to a discussion of selected theoretical and experimental issues, including recent developments, which have led to fundamental new insights as well as to relevant advances in semiconductor quantum physics and technology. In particular, we shall focus on nonequilibrium carrier dynamics in open quantum devices. Furthermore, we shall not address the vast area of quantum-optics phenomena; the only exception will be the case of carrier-cavity mode coupling in semiconductor microcavities.

The book is organized into 11 chapters plus 4 appendices. In Chap. 1 we shall recall the basic concepts and fundamental properties of semiconductor bulk materials as well as of low-dimensional semiconductor structures like,
e.g., superlattices, quantum wells, wires, and dots; in addition, we shall discuss in very general and qualitative terms the link between nanomaterials and corresponding optoelectronic quantum devices. Chapter 2 will focus on the basic assumptions of the conventional semiclassical picture, showing that the latter are not always justified in new-generation semiconductor nanomaterials and nanodevices and therefore fully quantum-mechanical treatments of the problem are imperative. In Chap. 3 we shall recall the fundamentals of the well-known density-matrix formalism applied to the investigation of the electro-optical properties of semiconductor nanomaterials and nanodevices, while in Chap. 4 the same formalism will be extended to quantum systems with open spatial boundaries, corresponding to the case of a generic quantum device inserted into an electric circuit. Chapter 5 will introduce the basic concepts as well as key instruments related to the numerical modeling of semiconductor nanomaterials and nanodevices. In Chap. 6 we shall discuss in very general terms the most effective approaches for the study of unipolar transport in nanodevices; to this end, we shall address separately the low- and the high-field regimes, and for both regimes we shall provide a semiclassical treatment of the problem as well as its quantum-mechanical generalization. Chapter 7 will address the basic physical processes as well as open technological problems related to the design and optimization of new-generation quantum-well infrared photodetectors, focusing on the development of efficient quantum devices for the terahertz spectral region. In Chap. 8 we shall discuss the basic features of quantum-cascade coherent-light sources; to this aim, we shall review a few simulated experiments focusing on the microscopic explanation of the gain regime, both in the mid-infrared and in the far-infrared spectral regions. Chapter 9 will discuss the basic properties and unique features of few-electron/exciton quantum systems, namely single and coupled semiconductor macroatoms, pointing out their potential role in designing a completely new class of optoelectronic quantum devices, like electron-state detectors and quantum logic gates. In Chap. 10 we shall review a few potential implementation strategies for the concrete realization of quantum information processing using specifically designed semiconductor nanostructures, namely quantum dots and wires. In Chap. 11 we shall briefly address two extremely active and stimulating research topics, namely molecular and spin-transport electronics, whose development may lead to completely new paradigms in semiconductor-based electronic and optoelectronic physics and technology.

This volume is the result of about 20 years of research activity on fundamental issues related to quantum-transport as well as coherent-optics phenomena in semiconductor bulk and nanostructures; the latter have been performed at the University of Modena (Italy), at the Philipps University of Marburg (Germany), and mostly at the Polytechnic University of Torino (Italy), involving a number of worldwide collaborations with several leading research groups in the field.

Let me take this unique opportunity to thank a number of people that in many ways and at different stages have contributed significantly to this
research effort. First of all, I am grateful to Carlo Jacoboni, the person that opened my young mind to the magic world of quantum mechanics; his enthusiasm, scientific curiosity, and intellectual rigor have strongly influenced my personal as well as professional life. Let me thank Paolo Lugli and Elisa Molinari; their innovative viewpoint on scientific research as well as their continuous help and support played a crucial role during the first stages of my scientific career. I am grateful to Tilmann Kuhn and Paolo Zanardi; they gave key contributions in developing many of the ideas on the theoretical description of quantum devices presented in this book. Let me thank Rita Claudia Iotti for her essential role in setting up and developing our current research group at the Physics Department of the Polytechnic University of Torino, together with a number of Ph.D. students and researchers, including Eliana Biolatti, Remo Proietti Zaccaria, Emanuele Ciancio, Irene D’Amico, Ehoud Pazy, Radu Ionicioiu, Stefano Portolan, Fabrizio Castellano, and David Taj; she has contributed significantly to a large fraction of the research activity reviewed in this book. Let me finally thank Traiano Rossi (my father) for his invaluable help in setting out the manuscript layout. Last but not least, I am profoundly grateful to my family for their never-ending support and patience.

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1

Fundamentals of Semiconductor Materials and Devices

In this chapter we shall recall basic concepts and fundamental properties of semiconductor bulk materials as well as of low-dimensional semiconductor structures like superlattices, quantum wells, wires, and dots. In addition, we shall discuss in very general and qualitative terms the link between nanomaterials and corresponding optoelectronic quantum devices.

1.1 An Introductory Overview on Semiconductor Physics and Technology

The following introductory overview by Martin Stutzmann [1] has been written in 2008 for the celebration of the 20th anniversary of the Walter Schottky Institute (WSI) of the Technische Universität München.

On the 14th of November, 1876, the high school teacher Ferdinand Braun gave a presentation entitled “Experiments concerning deviations from Ohm’s law in metallic conductors” in front of the illustrious Naturforschende Gesellschaft zu Leipzig. Neither Mr. Braun nor his critical audience were aware of the fact that they were just witnessing the birth of Semiconductor Physics. Indeed, what Ferdinand Braun had discovered by a long series of meticulous experiments, at first sight did not appear too exciting: if one equipped a solid crystal with two metallic contacts and applied an electric voltage, two basic kinds of behavior could be observed. Either no measurable electric current passed through the crystal. Then this crystal obviously was an electric insulator and, therefore, was no longer of interest for further investigation of its electric properties. Or, for the second type of crystals, a sizeable current could be measured. Then this crystal was a metallic conductor and obeyed Ohm’s law. If one doubled the applied voltage, also the observed current was doubled. And if one inverted the electric voltage applied to the two contacts, also the current was inverted. At least, that was the way it used to be until 1876...