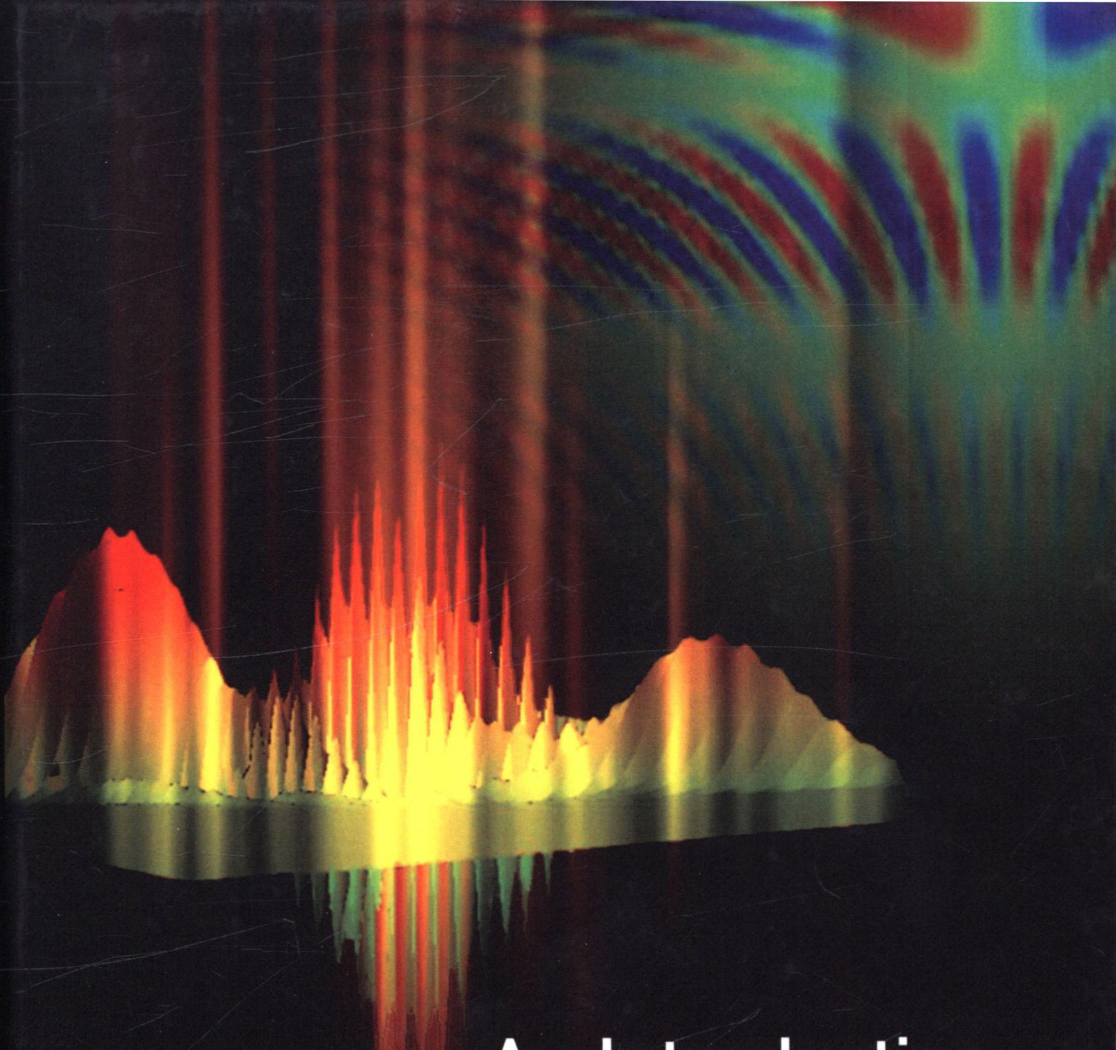

An Introduction to Quantum Transport in Semiconductors

David K. Ferry

"Prof. Ferry is a highly respected expert in quantum transport of nanoscale devices. He has used a vast number of different theoretical tools to model the fascinating transport physics of these systems. He has now collected results of his scholarship in this volume, where the reader will learn about the pragmatic use of various sophisticated techniques, including Green's functions (both in equilibrium and in nonequilibrium incarnations), density matrices, and Wigner functions. This is probably the first time all this material is available in a single volume using a unified notation, giving the interested reader a unique and self-contained view of the entire field. The reader will also benefit from the many personal and insightful discussions that interlace the technical material. A researcher with a solid command of the theoretical techniques in condensed matter and who wants to work in the borderline of physics and nanoelectronics will find this volume highly useful."

Prof. Antti-Pekka Jauho
Technical University of Denmark, Denmark

"Prof. Ferry has transferred into this book his extensive knowledge about problems, and possible solutions, arising in electronic transport in semiconductors when the dimensions of the physical system at hand are such that a quantum treatment is required. The reading of this text will be of benefit to both physicists interested in basic problems and to engineers interested in understanding the functioning principles of modern nanoelectronic devices and designing new ones."

Prof. Carlo Jacoboni
University of Modena and Reggio Emilia, Italy

"This book is an invaluable addition to the literature for many device physicists and engineers. The device simulations based on Green's functions are now widely employed for analyzing actual device characteristics, yet the physics behind the formalism has been hardly accessible to many device engineers. The book thoroughly discusses the physics and methodology of quantum transport in a lucid style."

Prof. Nobuyuki Sano
University of Tsukuba, Japan

This book moves beyond the basics to highlight the full quantum-mechanical nature of the transport of carriers through nanoelectronic structures. It is unique in that it addresses quantum transport only in the materials that are of interest to microelectronics—semiconductors, with their variable densities and effective masses. It describes all approaches to quantum transport in semiconductors, thus becoming an essential textbook for advanced graduate students in electrical engineering or physics.

David K. Ferry is regents' professor in the School of Electrical, Computer and Energy Engineering, Arizona State University (ASU), USA. He is also a faculty member in the Department of Physics and for the graduate program in Materials Science and Engineering at ASU and a visiting professor at Chiba University, Japan. He joined ASU in 1983 following shorter stints at Texas Tech University, the Office of Naval Research, and Colorado State University, USA. He enjoys teaching, which he refers to as "warping young minds," and his research focuses on semiconductors, particularly as they apply to nanotechnology and integrated circuits as well as quantum effects in devices.

V565
ISBN 978-981-4745-86-4

PAN STANFORD PUBLISHING
www.panstanford.com

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Pan Stanford Publishing

Published by

Pan Stanford Publishing Pte. Ltd.
Penthouse Level, Suntec Tower 3
8 Temasek Boulevard
Singapore 038988

Email: editorial@panstanford.com
Web: www.panstanford.com

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

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ISBN 978-981-4745-86-4 (Hardcover)
ISBN 978-1-315-20622-6 (eBook)

Printed in the USA

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Preface

The density of transistors in integrated circuits has grown exponentially since the first circuit was created. This growth has been dubbed Moore's Law. Now, why should this be of interest to the engineer or scientist who wants to study the role of quantum mechanics and quantum transport in today's world? Well, if you think about the dimensions that are intrinsic to an individual transistor in modern integrated circuits, about 5–20 nm, then it is clear that these are really quantum mechanical devices. In fact, we live in a world in which basically all of our modern microelectronics have become quantum objects, ranging from these transistors to the world of lasers and light-emitting diodes. It is also not an accident that this world is created from semiconductor materials, because these materials provide a canvas upon which we can paint our quantum devices as we wish. Of course, silicon is the dominant material since it is the base for the integrated circuits. But, optical devices are created from a wide range of semiconducting materials in order to cover the wide spectrum of light that is desired; from the ultraviolet to the far infrared.

I have had the good fortune to be an observer, and occasional contributor, to this ever-increasing world of microelectronics. I have followed the progress from the very first transistor radio to today's massive computing machines which live on a chip of about 1 cm^2. Over these years, I have become involved in the study of quantum devices and the attempts to try to write down the relevant theoretical expressions and find their solutions. As an educator, this led to many attempts to devise a course in which to teach these complicated (both then and now) quantum approaches to device physics. As with most people, the effort began with Kadanoff and Baym's excellent but small book on Green's functions. It became easier when Steve Goodnick and I undertook to write the book *Transport in Nanostructures*, which appeared in 1997. But, neither this book, nor its later second edition, was a proper textbook, and it contained far too much material to contemplate a one semester course on the topic. Nevertheless, we pressed forward with its use as a text several times in the intervening years. As age has crept not so slowly upon me, it became evident that it was time to try to put down my vision of a textbook on the topic. I guess it became evident that it was going to be now or never, and so I undertook to create this textbook (and I have to thank Stanford Chong for pushing me to do this). There are, of course, many other textbooks on Green's functions, but not so many that each one of them can treat all of the approaches to quantum transport. According to me, a more thorough coverage is essential. Despite the glorious claims of its practioners, nonequilibrium Green's functions are not the entire answer to the problem, and this is becoming evident as we experimentally probe more and more into questions of quantum coherence in real systems.

As evidenced by this book, I have finished the task with this version. I am sure that no author has ever finished a science text without immediately (or at least within a few minutes of seeing the published book) being worried that they have missed important points or should have said it differently. I know from my other books that, in looking back at them (which is often with the textbooks), I wonder what I was thinking when I wrote certain passages, especially as there are better ways to express something, which also crop up in retrospect. Nevertheless, I hope that this book will serve as a good reference for others as well as myself. It is designed to be more than a one semester course, so that the teacher can pick and choose among the topics and still have enough to fill a semester. It is not a first-year graduate course, as the student should have a good background in quantum mechanics itself. Typically, the prior attempts to put the course together have suggested that the student be "a serious-minded doctoral student," a phrase my own professor used to describe a one semester course out of the old 1100+ page Morse and Feshbach. The field has a lot of mathematical detail, but sometimes the simpler aspects have been blurred by confusing presentations. I don't know if I can claim that I have overcome this, but I have tried. Hopefully, the readers will find this book easier to use than some others.

I have benefitted from the interaction with a great many very bright people over the years, who have pushed me forward in learning about quantum transport. To begin with, there were John Barker, Gerry Iafrate, Hal Grubin, Carlo Jacoboni, Antti-Pekka Jauho, and Richard Akis, who remain friends to this day, in spite of my inherent grumpy nature. In addition, I have learned with and from Wolf Porod,

Walter Pötz, Jean-Jacques Niez, Jacques Zimmermann, Al Kriman, Bob Grondin, Steve Goodnick, Chris Ringhofer, Yukihiko Takagaki, Kazuo Yano, Paolo Bordone, Mixi Nedjalkov, Anna Grincwajg, Roland Brunner, and Max Fischetti, as they passed through my group or were collaborators at Arizona State University. Then, there were my bright doctoral students who worked on quantum theory and simulations: Tampachen Kunjunny, Bob Reich, Paolo Lugli, Umberto Ravaioli, Norman "Mo" Kluksdahl, Rita Bertoncini, Jing-Rong Zhou, Selim Günçer, Toshishige Yamada, Dragica Vasileska, Nick Holmberg, Lucian Shifren, Irena Knezevic, Matthew Gilbert, Gil Speyer, Aron Cummings, and Bobo Liu.

In addition, I have had the good fortune to collaborate with a number of excellent experimentalists, particularly John Bird, but also over the years with Yuichi Ochiai, Koji Ishibashi, and Nobuyuki Aoki in Japan. Then, there are my doctoral students who labored on the quantum device experiments: Jun Ma, David Pivin, Kevin Connolly, Neil Deutscher, Carlo da Cunha, and Adam Burke. These are long lists, both here and in the previous paragraph, but the present work is really the result of their work. Of course, I have to thank my long persevering wife, who puts up with my shenanigans, and without whom I probably wouldn't have amounted to much.

David K. Ferry

Fall 2017

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Chapter 1

Introduction

The transport of carriers, electrons and holes, in semiconductors has been of interest for quite some time. It certainly became a subject of central interest when the inventors of the transistor were trying to understand the properties of the carriers in this new device [1]. But almost immediately, there was interest in the behavior of the carriers at high electric fields, in efforts to understand the breakdown of the oxides in use at that time [2]. Of course, there was increased interest in the materials important to the new semiconductor devices, such as silicon [3]. By understanding the transport properties of the carriers, one could certainly understand more about the physics governing the interactions between the carriers and their environment—the surfaces, the phonons, and so on. Over the decades since, we have found that the careful modeling of transport and the semiconductor devices has contributed to the ability to push the technology to ever smaller physical sizes. Today, the critical length in a modern tri-gate transistor is approaching the distance between the individual atoms of the underlying semiconductor. Indeed, we have seen the fabrication of a device in which the active region consists of a single phosphorus atom [4]! If the atoms of the semiconductor are held together by quantum mechanical forces, then it is quite likely that we will need to describe the transport in such small transistors via

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a fully quantum mechanical approach (and, indeed, this was done to gain understanding of the physics within the single-atom transistor).

Thus, it is clear that more detailed modeling of the quantum contributions in modern semiconductor devices is required. These contributions appear in many forms: (1) changes in the statistical thermodynamics within the devices themselves as well as in its connection and interaction with the external world, (2) new critical length scales, (3) an enlarged role for ballistic transport and quantum interference, and (4) new sources of fluctuations, which will affect device performance. Indeed, many of these effects have already been studied at low temperatures where the quantum effects appear more readily in such devices [5].

A fair question to ask at this point is why are not quantum effects seen in today's very small devices? In fact, quantum effects are an integral part of the design of today's devices, but they are not seen in the observed output characteristics for one good reason. Most of the important quantum effects are in a direction normal to that in which the current flows. But this does not diminish their importance. For example, strain is a common part of every device in a modern microprocessor. This strain is used to distort the band structure and improve the mobility of the electrons and holes. So controlled introduction of quantum modifications has been a part of the fabrication of devices for more than a decade. And there has been an ongoing effort to design and create simulation tools for the semiconductor world, which incorporate the quantum effects in the very base of the physics included within the tool. On the other hand, many people have studied quantum transport (and written books on the subject) in metals for quite a long time. But semiconductors are not metals. The differences are large and significant. So while one would like to extrapolate from what is known in metals, this can be taken only so far. What we would like to do here is to examine what approaches work for semiconductors and to try to learn from the many places where studies have been done for these materials and the resulting devices. In the following sections, we will try to describe what the key features are that differentiate quantum transport from the classical transport world that has been used so successfully in semiconductors and semiconductor devices.