ELECTRICAL TRANSPORT IN NANOSCALE SYSTEMS

In recent years there has been a huge increase in the research and development of nanoscale science and technology, with electrical transport playing a central role. This graduate textbook provides an in-depth description of the transport phenomena relevant to systems of nanoscale dimensions.

In this textbook the different theoretical approaches are critically discussed, with emphasis on their basic assumptions and approximations. The book also covers information content in the measurement of currents, the role of initial conditions in establishing a steady state, and the modern use of density-functional theory. opics are introduced by simple physical arguments, with particular attention to the non-equilibrium statistical nature of electrical conduction, and followed by a detailed formal derivation. This textbook is ideal for graduate students in physics, chemistry, and electrical engineering.

Massimiliano Di Ventra is Professor of Physics at the University of California, San Diego. He has published over 70 papers in refereed journals, co-edited the textbook *Introduction to Nanoscale Science and Technology* (Springer, 2004), and has delivered more than 100 invited talks worldwide on the subject of this book.

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Massimiliano Di Ventra
Frontmatter
More information

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Contents

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Preface

"The important thing is not to stop questioning.
Curiosity has its own reason for existing."
Albert Einstein

About ten years ago I was resting between session breaks of a busy American Physical Society March meeting. A colleague, whom I had not seen in ears, was with me and inquired about my work. I told him I was working on understanding transport in nanoscale systems. He replied, "Aren't the most important facts already understood?"

As unsettling as that question was, I realized he was simply echoing a sentiment in the community: the field of mesoscopic systems – larger "cousins" of nanoscale systems – had provided us with a wealth of experimental results, and a theoretical construct – known as the single-particle scattering approach to conduction – that had almost assumed the characteristics of a "dogma". Many transport properties of mesoscopic systems could be understood in terms of this approach. Books on the subject had appeared which enumerated the successes of this theory. Nanoscale systems were nothing else than smaller versions of mesoscopic systems. All we needed to do was transfer the established experimental knowledge – and proven theoretical and computational techniques – to this new length scale. Or so it seemed.

The past decade has shown that the field of transport in nanoscale systems is *not* a simple extension of mesoscopic physics. Thanks to improved experimental capabilities and new theoretical approaches and viewpoints, it has ecome clear that novel transport properties emerge at the nanometer scale. In addition, many physical assumptions and approximations we reasonably make to describe mesoscopic systems may not hold for nanoscale structures. Most importantly, it is now starting to sink in that we need to treat the many-body transport problem for what it truly is: a *non-equilibrium statis-*

tical problem. Conducting electrons – and the background ionic structure – are in a state of non-equilibrium, whose properties are known, at best, statistically, even at steady state. By neglecting the true non-equilibrium statistical nature of this problem, we may neglect important dynamical phenomena of particular relevance in nanostructures.

This book attempts to reframe the transport problem with this perspective in mind. Therefore, attention is given to questions that are often overlooked in the literature, e.g., how electrical current is generated, what do we measure when we measure currents, what is the role of initial conditions in establishing a steady state, etc. The language of information theory is used throughout the book to quantify the amount of information one can gather from either the measurement of the current, or the various descriptions of electrical conduction. In addition, I have tried to critically point out the underlying physical assumptions and approximations of the different approaches to transport. It is my opinion that some of the concepts we generally take for granted need to be applied with more care in the case of nanoscale systems, and novel physics may emerge if some of these approximations/assumptions are lifted.

Transport theories belong to the field of non-equilibrium statistical mechanics and are, first and foremost, based on *viewpoints*, not sets of equations. Each of these viewpoints contributes bits of information to our understanding of electrical conduction. The book is thus roughly divided into the description of these viewpoints, the similarities and differences among them, and the physical phenomena one can predict from them. In addition, due to the growing importance of density-functional theory (DFT) – in both its ground-state and dynamical formulations – in transport, the book contains a description of DFT so that it is as self-contained as possible. In particular, the fundamental limitations of ground-state DFT in approaches to electrical conduction are highlighted, and several theorems on the total current are formulated and demonstrated within dynamical density-functional theories. The inclusion of these theorems is not a tribute to mathematics. Rather, it shows the conceptual and formal strengths of these theories in describing electrical transport.

A colleague of mine, who has written textbooks, once told me: "A book is useful to at least one person: its own author." While this statement is definitely true in my case – in the sense that by writing it I have deepened my knowledge and understanding of the subject beyond what everyday research would have probably allowed me – I truly hope this textbook will be of use to its readership, especially those students and researchers who approach the subject for the first time. I have tried to write it at a level accessible to graduate students with a good background in quantum mechanics and statistical mechanics. Some knowledge of solid state physics may help but is not necessary. The derivations of almost all the main results are written explicitly. When this would have resulted in an unnecessary increase in length, I left them as exercises for the reader, or in few cases referred to other textbooks. In this respect, the most difficult topic is probably the non-equilibrium Green's function formalism of Chapter 4. As a compromise etween synthesis and clarity, I have written enough about this many-body technique for the reader to follow its basic tenets and results, and referred to other textbooks whenever the level of details seemed to overshadow the main physics. Finally, some of the exercises add to the topics discussed in the main text, or provide useful reference to some mathematical statements use but have no space to prove.

I have left out topics like superconductivity, the Kondo problem, Luttinger liquid, weak localization, and universal conductance fluctuations. This is not ecause I believe they are not important but because a comprehensive description of these phenomena would have resulted in a very lengthy extension of the manuscript, with the addition of advanced mathematical formalisms. There are other excellent textbooks that cover these topics. I also apologize in advance to all the authors who feel their work has not been properly credited, and remind them that this is intended as a textbook not a review.

Despite all my efforts and the amount of energy spent to write this book with as much care as I could possibly muster, it would be foolish of me to think that with more than 1200 equations – and a comparable num-er of concepts – this manuscript would be free of errors. I will therefore ost any correction I uncover after its publication on a link to my website **http://physics.ucsd.edu/∼diventra/**, and take comfort in the old saying: "Those who never make mistakes make the biggest mistake of all: they never try anything new."

There are too many people who directly or indirectly have contributed to my personal understanding of the subject, and have helped me in this endeavor. I particularly wish to thank Norton Lang, who introduced me to the topic of transport in nanoscale systems. My gratitude also goes to Hardy Gross, Doug Natelson, Nongjian Tao, Tchavdar Todorov, Jan an Ruitenbeek, and Giovanni Vignale, for enlightening discussions, and to Congjun Wu for taking time off his busy schedule to read most of the manuscript. His suggestions and criticisms have helped me improve it. I am also indebted to Dan Arovas who has shared with me his lecture notes on mesoscopic physics. Some topics of Chapter 3 have been inspired by these notes.

I feel fortunate to have worked over the years with talented students and post-doctoral associates. They have shared with me the difficulties and excitement of some of the research that has made it through the pages of this book. Those directly involved in the topics presented here are Neil Bushong, Yu-Chang Chen, Roberto D'Agosta, Yonatan Dubi, John Gamble, Matt Krems, Johan Lagerqvist, Yuriy Pershin, Na Sai, Eric Wright, Zhongqin Yang, and Mike Zwolak. Many of them have also read parts of the manuscript, found several misprints, and made valuable suggestions. Needless to say, any remaining error is due solely to the author.

I also wish to thank the National Science Foundation, the Department of Energy, the National Institutes of Health, and the Petroleum Research Fund for generously funding my research over the years. These funding agencies are, however, not responsible for the ideas expressed in this manuscript.

Finally, the writing of a book takes an enormous amount of energy and time at the expense of the relationships that are most dear to one's life. It is the loving support, understanding, and patience of my wife, Elena, and of my two children, Francesca and Matteo, that have made this project possible. Their presence and encouragement have sustained me during the most difficult times, when it would have been so easy to simply give up. A thank you does not make full justice of my feelings of gratitude and love towards them.

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