

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. Topics 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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To
Elena, Matteo and Francesca

Contents

1	A primer on electron transport	<i>page</i> 1
1.1	Nanoscale systems	1
1.2	Generating currents	3
1.2.1	Finite versus infinite systems	8
1.2.2	Electron sources	9
1.2.3	Intrinsic nature of the transport problem	10
1.3	Measuring currents	11
1.3.1	Microscopic states	12
1.3.2	The current operator	13
1.3.3	The measurement process	16
1.3.4	Complete measurement and pure states	17
1.4	The statistical operator and macro-states	19
1.4.1	Pure and mixed states	21
1.4.2	Quantum correlations	22
1.4.3	Time evolution of the statistical operator	23
1.4.4	Random or partially specified Hamiltonians	24
1.4.5	Open quantum systems	25
1.4.6	Equilibrium statistical operators	29
1.5	Current measurement and statistical operator truncation	32
1.6	One current, different viewpoints	34
	Summary and open questions	36
	Exercises	36
2	Drude model, Kubo formalism and Boltzmann equation	39
2.1	Drude model	39
2.2	Resistance, coherent and incoherent transport	42
2.2.1	Relaxation vs. dephasing	44

viii	<i>Contents</i>	
	2.2.2 Mean-free path	48
	2.2.3 The meaning of momentum relaxation time	49
2.3	Kubo formalism	50
	2.3.1 The current-current response function	55
	2.3.2 The use of Density-Functional Theory in the Kubo approach	57
	2.3.3 The fluctuation-dissipation theorem	60
	2.3.4 Ohmic vs. ballistic regimes	66
2.4	Chemical, electrochemical and electrostatic potentials	68
2.5	Drift-diffusion equations	72
	2.5.1 Diffusion coefficient of an ideal electron gas in the non-degenerate limit	73
	2.5.2 Generalization to spin-dependent transport	75
2.6	Distribution functions	77
2.7	Boltzmann equation	79
	2.7.1 Approach to local equilibrium	82
2.8	Entropy, loss of information, and macroscopic irreversibility	83
	2.8.1 The classical statistical entropy	85
	2.8.2 Quantum statistical entropy	86
	2.8.3 Information content of the N - and one-particle statistical operators	89
	2.8.4 Entropy of open quantum systems	90
	2.8.5 Loss of information in the Kubo formalism	91
	2.8.6 Loss of information with stochastic Hamiltonians	92
	2.8.7 Entropy associated with the measurement of currents	93
	Summary and open questions	94
	Exercises	95
3	Landauer approach	101
	3.1 Formulation of the problem	102
	3.2 Local resistivity dipoles and the “field response”	113
	3.3 Conduction from transmission	115
	3.3.1 Scattering boundary conditions	115
	3.3.2 Transmission and reflection probabilities	119
	3.3.3 Total current	123
	3.3.4 Two-probe conductance	128
	3.4 The Lippmann–Schwinger equation	132
	3.4.1 Time-dependent Lippmann–Schwinger equation	132
	3.4.2 Time-independent Lippmann–Schwinger equation	140
	3.5 Green’s functions and self-energy	145

	<i>Contents</i>	ix
	3.5.1 Relation to scattering theory	154
3.6	The $\mathcal{S}$ matrix	159
	3.6.1 Relation between the total Green's function and the $\mathcal{S}$ matrix	162
3.7	The transfer matrix	167
	3.7.1 Coherent scattering of two resistors in series	169
	3.7.2 Incoherent scattering of two resistors in series	171
	3.7.3 Relation between the conductance and the transfer matrix	173
	3.7.4 Localization, ohmic and ballistic regimes	174
3.8	Four-probe conductance in the non-invasive limit	178
	3.8.1 Single-channel case	179
	3.8.2 Geometrical "dilution"	181
	3.8.3 Multi-channel case	182
3.9	Multi-probe conductance in the invasive limit	185
	3.9.1 Floating probes and dephasing	187
3.10	Generalization to spin-dependent transport	190
	3.10.1 Spin-dependent transmission functions	194
	3.10.2 Multi-probe conductance in the presence of a magnetic field	195
	3.10.3 Local resistivity spin dipoles and dynamical effects	196
3.11	The use of Density-Functional Theory in the Landauer approach	198
	Summary and open questions	202
	Exercises	203
4	Non-equilibrium Green's function formalism	209
	4.1 Formulation of the problem	211
	4.1.1 Contour ordering	215
	4.2 Equilibrium Green's functions	217
	4.2.1 Time-ordered Green's functions	218
	4.2.2 Dyson's equation for interacting particles	221
	4.2.3 More Green's functions	223
	4.2.4 The spectral function	225
	4.3 Contour-ordered Green's functions	231
	4.3.1 Equations of motion for non-equilibrium Green's functions	233
	4.4 Application to steady-state transport	236
	4.5 Coulomb blockade	244
	4.6 Quantum kinetic equations	250

	Summary and open questions	255
	Exercises	257
5	Noise	258
5.1	The moments of the current	261
5.2	Shot noise	263
5.2.1	The classical (Poisson) limit	264
5.2.2	Quantum theory of shot noise	266
5.3	Counting statistics	274
5.4	Thermal noise	275
	Summary and open questions	277
	Exercises	277
6	Electron-ion interaction	280
6.1	The many-body electron-ion Hamiltonian	281
6.1.1	The adiabatic approximation for a current-carrying system	282
6.1.2	The phonon subsystem	284
6.1.3	Electron-phonon coupling in the presence of current	288
6.2	Inelastic current	290
6.2.1	Inelastic current from standard perturbation theory	291
6.2.2	Inelastic current from the NEGF	296
6.3	Local ionic heating	312
6.3.1	Lattice heat conduction	319
6.4	Thermopower	323
6.5	Current-induced forces	328
6.5.1	Elastic vs. inelastic contribution to electro-migration	328
6.5.2	One force, different definitions	330
6.5.3	Local resistivity dipoles and the force sign	333
6.5.4	Forces at equilibrium	333
6.5.5	Forces out of equilibrium	335
6.5.6	Are current-induced forces conservative?	340
6.6	Local ionic heating vs. current-induced forces	343
	Summary and open questions	344
	Exercises	344
7	The micro-canonical picture of transport	346
7.1	Formulation of the problem	347
7.1.1	Transport from a finite-system point of view	347
7.1.2	Initial conditions and dynamics	349
7.2	Electrical current theorems within dynamical DFTs	351
7.2.1	Closed and finite quantum systems in a pure state	351

<i>Contents</i>		xi
7.2.2	Closed quantum systems in a pure state with arbitrary boundary conditions	353
7.2.3	Current in open quantum systems	354
7.2.4	Closure of the BBGKY hierarchy	356
7.2.5	Functional approximations and loss of information	357
7.3	Transient dynamics	358
7.4	Properties of quasi-steady states	360
7.4.1	Variational definition of quasi-steady states	360
7.4.2	Dependence of quasi-steady states on initial conditions	364
7.5	A non-equilibrium entropy principle	365
7.6	Approach to steady state in nanoscale systems	369
7.7	Definition of conductance in the micro-canonical picture	374
	Summary and open questions	375
8	Hydrodynamics of the electron liquid	376
8.1	The Madelung equations for a single particle	378
8.2	Hydrodynamic form of the Schrödinger equation	380
8.2.1	Quantum Navier–Stokes equations	382
8.3	Conductance quantization from hydrodynamics	388
8.4	Viscosity from Time-Dependent Current Density-Functional Theory	391
8.4.1	Functional approximation, loss of information, and dissipative dynamics	394
8.4.2	Effect of viscosity on resistance	395
8.5	Turbulent transport	397
8.6	Local electron heating	403
8.6.1	Electron heat conduction	405
8.6.2	Hydrodynamics of heat transfer	406
8.6.3	Effect of local electron heating on ionic heating	410
	Summary and open questions	412
	Exercises	413
Appendices		
<i>Appendix A</i>	A primer on second quantization	415
<i>Appendix B</i>	The quantum BBGKY hierarchy	420
<i>Appendix C</i>	The Lindblad equation	423
C.1	The Lindblad theorem	424
C.2	Derivation of the Lindblad equation	426
C.3	Steady-state solutions	430

xii	<i>Contents</i>	
Appendix D	Ground-state Density-Functional Theory	431
D.1	The Hohenberg–Kohn theorem	431
D.2	The Kohn–Sham equations	432
D.3	Generalization to grand-canonical equilibrium	434
D.4	The local density approximation and beyond	434
Appendix E	Time-Dependent DFT	436
E.1	The Runge–Gross theorem	436
E.2	The time-dependent Kohn–Sham equations	437
E.3	The adiabatic local density approximation	437
Appendix F	Time-Dependent Current DFT	439
F.1	The current density as the main variable	439
F.2	The exchange-correlation electric field	440
F.3	Approximate formulas for the viscosity	442
Appendix G	Stochastic Time-Dependent Current DFT	444
G.1	The stochastic Schrödinger equation	444
G.2	Derivation of the quantum master equation	446
G.3	The theorem of Stochastic TD-CDFT	449
Appendix H	Inelastic corrections to current and shot noise	451
Appendix I	Hydrodynamic form of the Schrödinger equation	454
Appendix J	Equation of motion for the stress tensor	458
Appendix K	Cut-off of the viscosity divergence	461
Appendix L	Bernoulli’s equation	463
	<i>References</i>	464
	<i>Index</i>	470

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 years, 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 become 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 between 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 because 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 number of concepts – this manuscript would be free of errors. I will therefore post 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 van 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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