Quantum Transport: Atom to Transistor

This book presents the conceptual framework underlying the atomistic theory of matter, emphasizing those aspects that relate to current flow. This includes some of the most advanced concepts of non-equilibrium quantum statistical mechanics. No prior acquaintance with quantum mechanics is assumed. Chapter 1 provides a description of quantum transport in elementary terms accessible to a beginner. The book then works its way from hydrogen to nanostructures, with extensive coverage of current flow. The final chapter summarizes the equations for quantum transport with illustrative examples showing how conductors evolve from the atomic to the ohmic regime as they get larger. Many numerical examples are used to provide concrete illustrations and the corresponding MATLAB codes can be downloaded from the web. Videostreamed lectures, keyed to specific sections of the book, are also available through the web. This book is primarily aimed at senior and graduate students.

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* Asterisked sections indicate those that I use for undergraduate teaching.

Preface

The purpose of this book is to convey the conceptual framework that underlies the microscopic or atomistic theory of matter, emphasizing those aspects that relate to electronic properties, especially current flow. Even a hundred years ago the atomistic viewpoint was somewhat controversial and many renowned scientists of the day questioned the utility of postulating entities called atoms that no one could see.[1] What no one anticipated was that by the end of the twentieth century, scientists would actually be "seeing" and taking pictures of atoms and even building "nanostructures" engineered on a nanometer length scale.[2] The properties of such nanostructures cannot be modeled in terms of macroscopic concepts like mobility or diffusion. What we need is an atomic or microscopic viewpoint and that is what this book is about.

The microscopic theory of matter was largely developed in the course of the twentieth century following the advent of quantum mechanics and is gradually becoming an integral part of engineering disciplines, as we acquire the ability to engineer materials and devices on an atomic scale. It is finding use in such diverse areas as predicting the structure of new materials, their electrical and mechanical properties, and the rates of chemical reactions, to name just a few applications. In this book, however, I will focus on the flow of current through a nanostructure when a voltage is applied across it. This is a problem of great practical significance as electronic devices like transistors get downscaled to atomic dimensions. It is a rapidly evolving field of research and the specific examples I will use in this book may or may not be important twenty years from now. But the problem of current flow touches on some of the deepest issues of physics and the concepts we will discuss represent key fundamental concepts of quantum mechanics and non-equilibrium statistical mechanics that should be relevant to the analysis and design of nanoscale devices for many years into the future. This book is written very much in the spirit of a text-book that uses idealized examples to clarify general principles, rather than a research monograph that does justice to specific real-world issues.

[1] For an interesting description see Lindley (2001).
[2] The distance between two atoms is ~0.25 nm.

Describing the flow of current involves a lot more than just quantum mechanics – it requires an appreciation of some of the most advanced concepts of non-equilibrium statistical mechanics. Traditionally these topics are spread out over many physics/chemistry courses that take many semesters to cover. My aim is to condense the essential concepts into a book that can be covered in a one-semester graduate course. I have also used a subset of this material to teach a senior-level undergraduate course. The only background I will assume is a knowledge of partial differential equations and matrix algebra including familiarity with MATLAB (or an equivalent mathematical software package).

The first chapter and the appendix are somewhat distinct from the rest of the book, but they have been included because I believe they should help the reader connect with the "big picture." The first chapter motivates the concepts covered in this book by laying out the factors that enter into a description of quantum transport in terms that are accessible to a beginner with no background in quantum mechanics. The appendix on the other hand is intended for the advanced reader and describes the same concepts using advanced formalism ("second quantization"). Both these chapters have been adapted from a longer article (Datta, 2004).

When I finished my last book, *Electronic Transport in Mesoscopic Systems* (*ETMS*) (Datta, 1995), I did not think I would want to write another. But *ETMS* was written in the early 1990s when quantum transport was a topic of interest mainly to physicists. Since then, electronic devices have been shrinking steadily to nanometer dimensions and quantum transport is fast becoming a topic of interest to electrical engineers as well. I owe it largely to my long-time friend and colleague Mark Lundstrom, that I was convinced to write this book with an engineering audience in mind. And this change in the intended audience (though I hope physicists too will find it useful) is reflected in my use of "q" rather than "e" to denote the electronic charge. However, I have not replaced "i" with "−j", since a Schrodinger equation with "$-j\partial\psi/\partial t$" just does not look right!

Anyway, this book has more substantial differences with *ETMS*. *ETMS* starts from the effective mass equation, assuming that readers had already seen it in a solid-state physics course. In this book, I spend Chapters 2 through 7 building up from the hydrogen atom to $E(k)$ diagrams and effective mass equations. Most importantly, *ETMS* was largely about low-bias conductance ("linear response") and its physical interpretation for small conductors, emphasizing the transmission formalism. In this book (Chapters 1, 8–11) I have stressed the full current–voltage characteristics and the importance of performing self-consistent calculations. I have tried to inject appropriate insights from the transmission formalism, like the Landauer formula and Buttiker probes, but the emphasis is on the non-equilibrium Green's function (NEGF) formalism which I believe provides a rigorous framework for the development of quantum device models that can be used to benchmark other simplified approaches. It bridges the gap between the fully coherent quantum transport models of mesoscopic physicists and the fully incoherent Boltzmann transport models of device physicists.

The NEGF formalism is usually described in the literature using advanced many-body formalism, but I have tried to make it accessible to a more general audience. In its simplest form, it reduces to a rate equation for a one-level system that I can teach undergraduates. And so in this book, I start with the "undergraduate" version in Chapter 1, develop it into the full matrix version, illustrate it with examples in Chapter 11, and provide a more formal justification using second quantization in the appendix. This book thus has a very different flavor from *ETMS*, which was primarily based on the transmission formalism with a brief mention of NEGF in the last chapter.

Another important distinction with *ETMS* is that in this book I have made significant use of MATLAB. I use many numerical examples to provide concrete illustrations and, for the readers' convenience, I have listed my MATLAB codes at the end of the book, which can also be downloaded from my website.[3] I strongly recommend that readers set up their own computer program on a personal computer to reproduce the results. This hands-on experience is needed to grasp such deep and diverse concepts in so short a time.

Additional problems designed to elaborate on the text material are posted on my website and I will be glad to share my solutions with interested readers. I plan to add more problems to this list and welcome readers to share problems of their own with the rest of the community. I will be happy to facilitate the process by adding links to relevant websites.

This book has grown out of a graduate course (and recently its undergraduate version) that I have been teaching for a number of years. The reader may find it useful to view the videostreamed course lectures, keyed to specific sections of this book, that are publicly available through the web, thanks to the Purdue University E-enterprise Center, the NSF Network for Computational Nanotechnology, and the NASA Institute for Nanoelectronics and Computing.

[3] http://dynamo.ecn.purdue.edu/~datta

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Symbols

Fundamental constants

q	electronic charge	1.602×10^{-19} C
h	Planck constant	6.626×10^{-34} J s
$\hbar$	$h/2\pi$	1.055×10^{-34} J s
m	free electron mass	9.11×10^{-31} kg
ε_0	permittivity of free space	8.854×10^{-12} F/m
a_0	Bohr radius, $4\pi\varepsilon_0\hbar^2/mq^2$	0.0529 nm
$G_0 = q^2/h$	conductance quantum	38.7×10^{-6} S (S $= 1/\Omega$ $=$ A/V) $= 1/(25.8 \times 10^3\ \Omega)$

We will use rationalized MKS units throughout the book, with energy in electron-volts: 1 eV $= 1.602 \times 10^{-19}$ J.

E_0	$q^2/8\pi\varepsilon_0 a_0$	13.6 eV

Some of the other symbols used

		Units
I	current (external)	amperes (A)
J	current (internal)	amperes (A)
V	voltage	volts (V)
R	resistance	ohms ($\Omega = $ V/A)
G	conductance	siemens (S $=$ A/V)
a	lattice constant	meters (m)
t_0	$\hbar^2/2m^*a^2$	electron-volts (eV)
t	time	seconds (s)
m^*	effective mass	kilograms (kg)
m_c	conduction band effective mass	kilograms (kg)
$\gamma_{1,2,3}$	Luttinger parameters	dimensionless
ε_r	relative permittivity	dimensionless
$\vec{F}$	electric field	V/m
L	channel length	m
S	cross-sectional area	m^2

$\vec{k}$	wavevector		/m
$\vec{v}$	velocity		m/s
n_S	electron density per unit area		/m^2
n_L	electron density per unit length		/m
N	number of electrons or number of photons		dimensionless
ρ	density matrix		dimensionless
ε	energy level		eV
H	Hamiltonian		eV
U	self-consistent potential		eV
E	energy		eV
μ	electrochemical potential		eV
$f(E)$	Fermi function		dimensionless
$n(E)$	electron density per unit energy		/eV
$D(E)$	density of states (DOS)		/eV
$A(E)$	spectral function		/eV
$G^n(E)$	(same as $-iG^<$) correlation function		/eV
$G^p(E)$	(same as $+iG^>$) hole correlation function		/eV
$G(E)$	Green's function (retarded)		/eV
$\overline{T}(E)$	transmission function		dimensionless
$T(E)$	transmission probability (<1)		dimensionless
γ, $\Gamma(E)$	broadening		eV
$\Sigma(E)$	self-energy (retarded)		eV
$\Sigma^{in}(E)$	(same as $-i\Sigma^<$) inscattering		eV
$\vartheta(E)$	unit step function	$\begin{cases} = 1, E > 0 \\ = 0, E < 0 \end{cases}$	dimensionless
$\delta(E)$	Dirac delta function		/eV
δ_{nm}	Kronecker delta	$\begin{cases} = 1, n = m \\ = 0, n \neq m \end{cases}$	dimensionless
t	Superscript to denote conjugate transpose		
T	Superscript to denote transpose		