

Lessons from Nanoscience:
A Lecture Note Series

Vol. **1**

Lessons from **Nanoelectronics**

A New Perspective on Transport

Supriyo Datta

Lessons from Nanoscience:
A Lecture Note Series

Vol. **1**

Lessons from **Nanoelectronics**

A New Perspective on Transport

常州大学图书馆
藏书章

Supriyo Datta

Purdue University, USA

 **World Scientific**

NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI

Published by

World Scientific Publishing Co. Pte. Ltd.

5 Toh Tuck Link, Singapore 596224

USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601

UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

Lessons from Nanoscience: A Lecture Note Series — Vol. 1

LESSONS FROM NANOELECTRONICS

A New Perspective on Transport

Copyright © 2012 by World Scientific Publishing Co. Pte. Ltd.

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the Publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN-13 978-981-4335-28-7

ISBN-10 981-4335-28-2

ISBN-13 978-981-4335-29-4 (pbk)

ISBN-10 981-4335-29-0 (pbk)

Printed in Singapore by B & Jo Enterprise Pte Ltd

Lessons from **Nanoelectronics**

A New Perspective on Transport

Lessons from Nanoscience: A Lecture Note Series

ISSN: 2301-3354

Series Editors: Mark Lundstrom and Supriyo Datta

(Purdue University, USA)

This series is intended to address a very different need, namely the need to develop conceptual frameworks that can help unify the diverse phenomena being discovered. Such frameworks may not yet be in final form but this series will provide a forum for them to evolve and develop into the textbooks of tomorrow that train our students and guide young researchers as they turn nanoscience into nanotechnology. The focus of the series is on electronics, but volumes in areas of nanoscience and technology broadly related to electronics will be also be considered, as long as they are driven by a quest for unifying principles that embed a diversity of phenomena or techniques.

Published:

Vol. 1 **Lessons from Nanoelectronics: A New Perspective on Transport**
by Supriyo Datta

To
Malika, Manoshi
and
Anuradha

Preface

Everyone is familiar with the amazing performance of a modern smart phone, powered by a billion-plus nanotransistors, each having an active region that is barely a few hundred atoms long.

These lectures, however, are about a less-appreciated by-product of the microelectronics revolution, namely the deeper understanding of current flow, energy exchange and device operation that it has enabled, which forms the basis for what we call the bottom-up approach.

I believe these lessons from nanoelectronics should be of broad relevance to the general problems of non-equilibrium statistical mechanics which pervade many different fields. To make these lectures accessible to anyone in any branch of science or engineering, we assume very little background beyond linear algebra and differential equations. We hope to reach all those who have an interest in basic physics, even if they are not specializing in devices or transport theory.

For dedicated graduate students and the experts, I have written extensively in the past. But they too may enjoy these notes taking a fresh look at a familiar subject, emphasizing the insights from mesoscopic physics and nanoelectronics that are of general interest and relevance.

Finally I should stress that these are *lecture notes* in unfinished form, with typos included to enhance the readers' attention, as my colleague Gerhard likes to put it. With your feedback and suggestions, I hope to have a better version in the future, one that requires less attention!

April 21, 2012

Supriyo Datta
Purdue University

Acknowledgements

Thanks to World Scientific Publishing Corporation and, in particular, our series editor, Zvi Ruder for joining us in this partnership.

The precursor to this lecture note series, namely the *Electronics from the Bottom Up* initiative on www.nanohub.org was funded by the U.S. National Science Foundation (NSF), the Intel Foundation, and Purdue University.

The nanoHUB-U recently offered its first online course based on these notes and I am thankful for the feedback I received from many online students whom I have never met. We gratefully acknowledge Purdue and NSF support for this program, along with the superb team of professionals who made nanoHUB-U a reality (<https://nanohub.org/groups/u>).

A special note of thanks to Mark Lundstrom for his leadership that made it all happen and for his encouragement and advice.

I am indebted to Ashraf Alam, Kerem Camsari, Deepanjan Datta, Vinh Diep, Samiran Ganguly, Seokmin Hong, Changwook Jeong, Bhaskaran Muralidharan, Angik Sarkar, Srikant Srinivasan for their valuable feedback and suggestions.

Finally I would like to express my deep gratitude to all who have helped me learn, a list that includes not only those named above, but also many teachers, colleagues and students over the years, starting with the late Richard Feynman whose classic lectures on physics, I am sure, have inspired many like me.

Some Symbols Used

Constants

| | | |
|--------------------|--------------------|---------------------------------------|
| Electronic charge | $-q$ | - 1.6e-19 coul. |
| Unit of Energy | 1 eV | + 1.6e-19 Joules |
| Planck's constant | h | 6.626e -34 Joule-sec |
| | $\hbar = h / 2\pi$ | 1.055e -34 Joule-sec |
| Boltzmann constant | k | 1.38e-23 Joule / K ~ 25 meV / 300K |
| Free electron mass | m_0 | 9.11e-31 Kg |
| Effective mass | m | |

Other Symbols

| | | |
|-------------|---|----------------------|
| I | Electron Current (See Fig.3.2) | amperes (A) |
| V | Electron Voltage | volts (V) |
| U | Electrostatic Potential | eV |
| μ | Electrochemical Potential (also called Fermi level or quasi-Fermi level) | eV |
| μ_0 | Equilibrium Electrochemical Potential | eV |
| R | Resistance | Ohms (V/A) |
| G | Conductance | Siemens (A/V) |
| $G(E)$ | Conductance at 0K with $\mu_0=E$ | Siemens (A/V) |
| \bar{D} | Diffusivity | m^2 /sec |
| $\bar{\mu}$ | Mobility | m^2 /V-sec |
| ρ | Resistivity | Ohm-m (3D), Ohm (2D) |
| σ | Conductivity | S/m (3D), S (2D) |

| | | |
|---|--|---|
| A | Area | m^2 |
| W | Width | m |
| L | Length | m |
| E | Energy | eV |
| $f(E)$ | Fermi Function | Dimensionless |
| $\left(-\frac{\partial f}{\partial E}\right)$ | Thermal Broadening Function (TBF) | $/\text{eV}$ |
| $kT\left(-\frac{\partial f}{\partial E}\right)$ | Normalized TBF | Dimensionless |
| $D(E)$ | Density of States | $/\text{eV}$ |
| $N(E)$ | Number of States with Energy $< E$ Equals Number of Electrons at 0K with $\mu_0=E$ | Dimensionless |
| N | Electron Density (3D or 2D or 1D) | $/\text{m}^3$ or $/\text{m}^2$ or $/\text{m}$ |
| $M(E)$ | Number of Channels (also called transverse modes) | Dimensionless |
| T | Temperature | degrees Kelvin (K) |
| t | Transfer Time | seconds |
| ν | Transfer Rate | $/\text{second}$ |
| $\gamma \equiv \hbar \nu$ | Energy Broadening | eV |
| $[X]^+$ | Complex conjugate of transpose of matrix | $[X]$ |
| H | (Matrix) Hamiltonian | eV |
| $G^R(E)$ | (Matrix) Retarded Green's function | $/\text{eV}$ |
| $G^A(E)=[G^R(E)]^+$ | (Matrix) Advanced Green's function | $/\text{eV}$ |
| $G^n(E)/2\pi$ | (Matrix) Electron Density | $/\text{eV}$, per gridpoint |
| $A(E)/2\pi$ | (Matrix) Density of States | $/\text{eV}$, per gridpoint |
| $\Gamma(E)$ | (Matrix) Energy Broadening | eV |

Contents

| | |
|---|-----|
| <i>Preface</i> | vii |
| <i>Some Symbols used</i> | ix |
| I. <i>The New Ohm's Law</i> | 1 |
| 1. The Bottom-Up Approach | 3 |
| 2. Why Electrons Flow | 15 |
| 3. The Elastic Resistor | 27 |
| 4. Ballistic and Diffusive Transport | 39 |
| 5. Conductivity | 47 |
| 6. Diffusion Equation for Ballistic Transport | 65 |
| 7. What about Drift? | 79 |
| 8. Electrostatics is Important | 93 |
| 9. Smart Contacts | 111 |
| II. <i>Old Topics in New Light</i> | 123 |
| 10. Thermoelectricity | 125 |
| 11. Phonon Transport | 145 |
| 12. Measuring Electrochemical Potentials | 155 |
| 13. Hall Effect | 173 |
| 14. Spin Valve | 191 |
| 15. Kubo Formula | 221 |
| 16. Second Law | 229 |
| 17. Fuel Value of Information | 251 |
| III. <i>Contact-ing Schrödinger</i> | 265 |
| 18. The Model | 267 |
| 19. Non-Equilibrium Green's Functions (NEGF) | 293 |

| | | |
|---|---|-----|
| 20. | Can Two Offer Less Resistance than One? | 321 |
| 21. | Quantum of Conductance | 337 |
| 22. | Rotating an Electron | 355 |
| 23. | Does NEGF Include “Everything”? | 389 |
| 24. | The Quantum and the Classical | 409 |
| <i>References /Further Reading</i> | | 423 |
| <i>Appendices</i> | | 433 |

Detailed Contents

| | |
|--|-----|
| <i>Preface</i> | vii |
| <i>Some Symbols used</i> | ix |
| I. The New Ohm's Law | 1 |
| 1. The Bottom-Up Approach | 3 |
| 2. Why Electrons Flow | 15 |
| 2.1. Two Key Concepts | 18 |
| 2.2. Fermi Function | 18 |
| 2.3. Non-equilibrium: Two Fermi Functions | 21 |
| 2.4. Linear Response | 22 |
| 2.5. Difference in "Agenda" Drives the Flow | 24 |
| 3. The Elastic Resistor | 27 |
| 3.1. How an Elastic Resistor Dissipates Heat | 30 |
| 3.2. Conductance of an Elastic Resistor | 32 |
| 3.3. Why an Elastic Resistor is Relevant | 35 |
| 4. Ballistic and Diffusive Transport | 39 |
| 4.1. Ballistic and Diffusive Transfer Times | 42 |
| 4.2. Channels for Conduction | 45 |
| 5. Conductivity | 47 |
| 5.1. $E(p)$ or $E(k)$ Relations | 52 |
| 5.2. Counting States | 53 |
| 5.3. Drude Formula | 55 |
| 5.4. Is Conductivity proportional to Electron Density? | 59 |
| 5.5. Quantized Conductance | 61 |
| 6. Diffusion Equation for Ballistic Transport | 65 |
| 6.1. Electrochemical Potentials Out of Equilibrium | 72 |
| 6.2. Currents in Terms of Non-Equilibrium Potentials | 76 |

| | | |
|------------|---|------------|
| 7. | What about Drift? | 79 |
| 7.1. | <i>Boltzmann Transport Equation, BTE</i> | 82 |
| 7.2. | <i>Diffusion Equation from BTE</i> | 85 |
| 7.3. | <i>Equilibrium Fields Do Matter</i> | 88 |
| 7.4. | <i>The Two Potentials</i> | 89 |
| 8. | Electrostatics is Important | 93 |
| 8.1. | <i>The Nanotransistor</i> | 94 |
| 8.2. | <i>Why the Current Saturates</i> | 96 |
| 8.3. | <i>Role of Charging</i> | 98 |
| 8.4. | <i>Rectifier Based on Electrostatics</i> | 102 |
| 8.5. | <i>Extended Channel Model</i> | 104 |
| 9. | Smart Contacts | 111 |
| 9.1. | <i>Why p-n Junctions are Different</i> | 112 |
| 9.2. | <i>Contacts are Fundamental</i> | 119 |
| II. | <i>Old Topics in New Light</i> | 123 |
| 10. | Thermoelectricity | 125 |
| 10.1. | <i>Seebeck Coefficient</i> | 129 |
| 10.2. | <i>Thermoelectric Figures of Merit</i> | 131 |
| 10.3. | <i>Heat Current</i> | 133 |
| 10.4. | <i>“Delta Function” Thermoelectric</i> | 138 |
| 11. | Phonon Transport | 145 |
| 11.1. | <i>Phonon Heat Current</i> | 147 |
| 11.2. | <i>Thermal Conductivity</i> | 151 |
| 12. | Measuring Electrochemical Potentials | 155 |
| 12.1. | <i>The Landauer Formulas</i> | 161 |
| 12.2. | <i>Büttiker Formula</i> | 165 |
| 13. | Hall Effect | 173 |
| 13.1. | <i>Why n- and p- Conductors Are Different</i> | 178 |
| 13.2. | <i>Spatial Profile of Electrochemical Potential</i> | 179 |
| 13.3. | <i>Measuring the Potential</i> | 184 |
| 13.4. | <i>Non –Reciprocal Circuits</i> | 188 |

| | | |
|-------------|---|------------|
| 14. | Spin Valve | 191 |
| 14.1. | <i>Mode Mismatch and Interface Resistance</i> | 194 |
| 14.2. | <i>Spin Potentials</i> | 201 |
| 14.3. | <i>Spin-Torque</i> | 209 |
| 14.4. | <i>Polarizers and Analyzers</i> | 217 |
| 15. | Kubo Formula | 221 |
| 15.1. | <i>Kubo Formula for an Elastic Resistor</i> | 224 |
| 15.2. | <i>Onsager Relations</i> | 227 |
| 16. | Second Law | 229 |
| 16.1. | <i>Asymmetry of Absorption and Emission</i> | 233 |
| 16.2. | <i>Entropy</i> | 235 |
| 16.3. | <i>Law of Equilibrium</i> | 240 |
| 16.4. | <i>Fock Space States</i> | 242 |
| 16.5. | <i>Alternative Expression for Entropy</i> | 246 |
| 17. | Fuel Value of Information | 251 |
| 17.1. | <i>Information-Driven Battery</i> | 255 |
| 17.2. | <i>Fuel Value Comes From Knowledge</i> | 258 |
| 17.3. | <i>Landauer's Principle</i> | 260 |
| 17.4. | <i>Maxwell's Demon</i> | 261 |
| III. | <i>Contact-ing Schrödinger</i> | 265 |
| 18. | The Model | 267 |
| 18.1. | <i>Schrödinger Equation</i> | 270 |
| 18.2. | <i>Electron-Electron Interactions</i> | 275 |
| 18.3. | <i>Differential to Matrix Equation</i> | 278 |
| 18.4. | <i>Choosing Matrix Parameters</i> | 281 |
| 19. | Non-Equilibrium Green's Functions (NEGF) | 293 |
| 19.1. | <i>One-level Resistor</i> | 299 |
| 19.2. | <i>Multi-level Resistors</i> | 308 |
| 19.3. | <i>Conductance Functions for Coherent Transport</i> | 314 |
| 19.4. | <i>Elastic Dephasing</i> | 315 |
| 20. | Can Two Offer Less Resistance than One? | 321 |
| 20.1. | <i>Modeling 1D Conductors</i> | 322 |

| | | |
|-------------------------------------|--|-----|
| 20.2. | <i>Quantum Resistors in Series</i> | 326 |
| 20.3. | <i>Potential Drop Across Scatterer(s)</i> | 331 |
| 21. | <i>Quantum of Conductance</i> | 337 |
| 21.1. | <i>2D Conductor as 1D Conductors in Parallel</i> | 337 |
| 21.2. | <i>Contact self-energy for 2D Conductors</i> | 343 |
| 21.3. | <i>Quantum Hall Effect</i> | 349 |
| 22. | <i>Rotating an Electron</i> | 355 |
| 22.1. | <i>One-level Spin Valve</i> | 359 |
| 22.2. | <i>Rotating Magnetic Contacts</i> | 363 |
| 22.3. | <i>Spin Hamiltonians</i> | 366 |
| 22.4. | <i>Vectors and Spinors</i> | 369 |
| 22.5. | <i>Spin Precession</i> | 374 |
| 22.6. | <i>From NEGF to Diffusion</i> | 380 |
| 23. | <i>Does NEGF Include “Everything”?</i> | 389 |
| 23.1. | <i>Coulomb Blockade</i> | 392 |
| 23.2. | <i>Fock Space Description</i> | 397 |
| 23.3. | <i>Entangled States</i> | 402 |
| 24. | <i>The Quantum and the Classical</i> | 409 |
| 24.1. | <i>Spin coherence</i> | 410 |
| 24.2. | <i>Pseudo-spins</i> | 412 |
| 24.3. | <i>Quantum Entropy</i> | 415 |
| 24.4. | <i>Does Interaction Increase the Entropy?</i> | 417 |
| 24.5. | <i>Spins and magnets</i> | 419 |
| References / Further Reading | | 423 |
| Appendices | | 433 |
| A. | <i>Fermi and Bose Function Derivatives</i> | 433 |
| B. | <i>Angular Averaging</i> | 435 |
| C. | <i>Hamiltonian with E- and B-Fields</i> | 437 |
| D. | <i>Transmission Line Parameters from BTE Equations</i> | 439 |
| E. | <i>NEGF Equations</i> | 443 |
| F. | <i>MATLAB Codes for Text Figures</i> | 449 |

I. The New Ohm's Law

| | |
|---|-----|
| 1. The Bottom-Up Approach | 3 |
| 2. Why Electrons Flow | 15 |
| 3. The Elastic Resistor | 27 |
| 4. Ballistic and Diffusive Transport | 39 |
| 5. Conductivity | 47 |
| 6. Diffusion Equation for Ballistic Transport | 65 |
| 7. What about Drift? | 79 |
| 8. Electrostatics is Important | 93 |
| 9. Smart Contacts | 111 |