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W. C. J. Magnus
W. J. Schoenmaker

Quantum Transport in Sub-Micron Devices

A Theoretical Introduction

Springer

Wim Magnus Wim Schoenmaker

Quantum Transport in Submicron Devices

A Theoretical Introduction

With 40 Figures

Springer

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ISSN 0171-1873

ISBN 3-540-43396-1 Springer-Verlag Berlin Heidelberg New York

Library of Congress Cataloging-in-Publication Data.
Magnus, Wim, 1954- . Quantum transport in submicron devices: a theoretical introduction/
Wim Magnus, Wim Schoenmaker. p. cm. – (Springer series in solid-state sciences, ISSN 0171-1873; 137)
Includes bibliographical references and index. ISBN 3-540-43396-1 (alk. paper)
1. Electron transport. 2. Holes (Electron deficiencies) I. Schoenmaker, Wim. II. Title. III. Series.
QC176.8.E4 M34 2002 530.4'16–dc21 2002021663

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Springer-Verlag Berlin Heidelberg New York
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Printed in Germany

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Typesetting made by the author
Cover concept: eStudio Calamar Steinen
Cover production: *design & production* GmbH, Heidelberg

Printed on acid-free paper SPIN: 10859825 57/3141/tr - 5 4 3 2 1 0

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To our beloved wives Marie-Paule and Vee
for lending their husbands to science

Preface

In this book the problem of transport of electrons and holes is approached from the point of view that a coherent and consistent physical theory can be constructed for transport phenomena. Along the road we will visit various exciting citadels in theoretical physics. The authors will guide the reader in this tour along the strong and weak aspects of the various theoretical constructions. Moreover, our goal is to make clear the mutual coherence and to put each theoretical model in an appropriate perspective. Merely the fact that so many partial solutions have been proposed to describe transport, be it in condensed matter, fluids, or gases, illustrates that we are entering a world of physics with a rich variety of phenomena. Moreover, the subject is not closed and the final theory of transport has still to be written down. Unavoidably, some aspects are commented by us with remarks that contain our personal views and there is room for discussion. Theoretical physics always aims at a unifying picture, but so far this ultimate goal has not been reached. However, this situation should not withhold us from working towards this goal. By presenting this tour among the many very inventive attempts to build this unifying picture, we hope that the reader is inspired and encouraged to help find the unifying principle behind the many faces of transport.

The present work grew out of a series of lectures that we have presented at IMEC, a research center for microelectronics and populated by a mixture of engineers, physicists, chemists and computer scientists, as far as the scientific staff is concerned. The underlying text reflects this audience. The first part of the book describes a series of physical concepts that can be found in numerous text books in physics libraries. One does not possess an operational knowledge of the Schrödinger equation, if one has no knowledge about the Hamiltonian operator. The latter one can only be properly understood within a realm of analytical mechanics.

Each chapter of Part I describes the essential knowledge that is needed to catch up with the present-day language in device engineering. For example, for engineers, these chapters should trigger interest in further reading physics books. Gradually, the text moves towards engineering problems and the second part of this work should convince physicists that there are numerous fundamental problems to be addressed that originate from microelectronic and mesoscopic physics. Therefore, it is our hope that physicists will find their way to engineering libraries.

Whereas Part I describes well-established result in physics, the second part of this work (Chaps. 11 to 17) contain our research results that can be found in the recent physics literature.

A multidisciplinary text book always runs the risk that a specialist in one field is disappointed by that piece of the text that covers his field of expertise, whereas the areas that are outside his field of interest remain hidden in a layer of fog, because the treatment is too condensed. Being aware of this risk, we have put serious effort into presenting the text in such a way that the reader can follow the line of thoughts. As a consequence, the text is occasionally 'narrative'. The intention of some sections is to introduce the reader to a terminology. The goal of these sections is to encourage further study and to provide access to the modern literature in the field.

Acknowledgment

The writing of this book was triggered by the request of a number of researchers at IMEC with a strong desire to gain a better understanding of what is going on in submicron devices. We have benefited substantially from numerous discussions which have also sharpened our views. In particular we would like to express our gratitude to Serge Biesemans, Stefan Kubicek, Carlos Augusto, Bart Sorée, Brahim Elattari, Marc Van Rossum, Kristin De Meyer, Karl-Heinz Bock, An de Keersgieter and many others scientists who contributed in one way or another to our knowledge of transport theory in the way as it became formulated in this book. We would like to thank our directors Herman Maes and Gilbert Declerck for creating the stimulating environment and support. We also benefited from numerous discussions with co-workers outside IMEC. In particular, we mention Jozef Devreese, Volodya Fomin, Sergei Balaban, Volodya Gladilin, Eugene Pokatilov of the University of Antwerp and the University of Moldova. Their impact can hardly be overrated. We are grateful to many research colleagues for sharing their views. To mention a few: Bob Dutton, Zhiping Yu (Stanford University), Wolfgang Fichtner, Andreas Schenk (ETH Zurich), Andreas Wettstein (ISE-AG), Siegfried Selberherr (TU Vienna), Gilles Le Carval (LETI Grenoble) and Marcel Profirescu (Technical University Bucharest). Some of the results that are presented in this book were obtained in research projects funded by Flemish Institute for Science and Technology (IWT) and the European Commission (IST). Last but not least we would like to express our thanks to Claus Ascheron, Angela Lahee and Elke Sauer (Springer-Verlag) for the smooth collaboration that helped to get this monograph off/on the shelf.

Leuven
April 2002

Wim Magnus
Wim Schoenmaker

List of Symbols

$\boldsymbol{A}$	vector potential
$a_q, a_{\boldsymbol{Q}}$	phonon annihilation operator
$a_q^\dagger, a_{\boldsymbol{Q}}^\dagger$	phonon creation operator
$\boldsymbol{B}$	magnetic induction
C	set of complex numbers
$c_{\boldsymbol{k}\sigma}, c_{\alpha l \boldsymbol{k}\sigma}, c_{n\sigma}$	electron annihilation operator
$c_{\boldsymbol{k}\sigma}^\dagger, c_{\alpha l \boldsymbol{k}\sigma}^\dagger, c_{n\sigma}^\dagger$	electron creation operator
$\mathrm{d}\boldsymbol{r}$	line element
$\mathrm{d}\boldsymbol{S}$	surface element
$\mathrm{d}\tau$	volume element
D_{AC}	acoustic deformation potential
D_{it}	density of interface states
$\boldsymbol{E}$	electric field
$\boldsymbol{E}_{\mathrm{C}}$	conservative electric field
$\boldsymbol{E}_{\mathrm{NC}}$	non-conservative electric field
$E, \mathcal{E}$	energy
E_{F}	Fermi energy
E_{L}	longitudinal electric field
$E_{\alpha \boldsymbol{k}}$	one-electron energy
$H, H_0, H_1, H', H_{\mathrm{int}}$	Hamiltonian
h	Planck's constant
$\hbar$	reduced Planck constant ($h/2\pi$)
I	electric current
$I_{\alpha l}$	leakage current carried by a virtual bound state
$\boldsymbol{J}$	electric current density
$J_{\alpha l}^z$	leakage current density carried by a virtual bound state
$k, k_1, k_2, \ldots$	single-particle quantum numbers
$k_{\mathrm{g},\alpha}, k_{1,\mathrm{ox},\alpha}, k_{2,ox,\alpha}, \ldots,$ $k_{1,\mathrm{w},\alpha}, k_{2,w,\alpha}, \ldots, k_{\mathrm{s},\alpha}$	electron wave number

$\boldsymbol{k}$	electron wave vector
k_{B}	Boltzmann's constant
L	Lagrangian
$\boldsymbol{L}$	total angular momentum
l	subband index
$\boldsymbol{l}$	one-particle angular momentum
m_0	free electron mass
$m_{\mathrm{g}\alpha x}, m_{\mathrm{g}\alpha y}, m_{\mathrm{g}\alpha z}, m_\alpha^{\parallel}, m_\alpha^{\perp}$, $m^{\parallel}, m^{\perp}, m_{1,\mathrm{ox},\alpha}, m_{2,ox,\alpha}, \ldots$, $m, m_{\mathrm{n}}, m_{\alpha x}, m_{\alpha y}, m_{\alpha z}$	electron effective masses
m_{p}	hole effective masses
$M(\boldsymbol{Q})$, v_q	electron–phonon coupling strength
N	number of particles, coordinates or modes
N_A	acceptor doping density
n	electron concentration
N_{ox}	number of gate stack layers
N_{w}	number of sublayers in the inversion layer
Φ	wave function, magnetic flux
$\|\Phi\rangle$	state vector
$\phi_{\alpha l}(z)$	subband wave function
$p_1, p_2, \ldots$	generalized momenta
$\boldsymbol{p}$	one-particle momentum
$\boldsymbol{P}$	total momentum
p	hole concentration
q_{D}	Debye wave number
$q_1, q_2, \ldots$	generalized coordinates
$\boldsymbol{q}, \boldsymbol{Q}$	phonon or photon wave vector
$\mathbf{R}$	set of real numbers
$\boldsymbol{r}, \boldsymbol{r}_1, \boldsymbol{r}_2, \ldots$	position vector
$\boldsymbol{S}$	spin vector operator
S	entropy
s	spin index
T	lattice temperature
T_{e}	electron temperature
$T_{\mathrm{g},\alpha} T_{1,\mathrm{ox},\alpha}, T_{1,\mathrm{ox},\alpha}, \ldots$, $T_{1,\mathrm{w},\alpha}, T_{2,\mathrm{w},\alpha}, \ldots$	transfer matrices
$t_{\mathrm{g}}, t_{\mathrm{ox}}, t_{1,\mathrm{w}}, t_{2,\mathrm{w}}, \ldots$	layer thicknesses
U	potential energy
V	scalar electric potential
$\boldsymbol{v}$	velocity, one-particle velocity operator
v_{D}	electron drift velocity
v_{S}	velocity of sound
V_ε	electromotive force
w	electron energy density

$W_{\alpha l}$	subband energy
α	valley index
$\partial\Omega$	boundary surface of Ω
ε_{S}	silicon permittivity
ε_k	one-electron energy
ε_0	vacuum permittivity
$\Gamma_{\alpha l}$	resonance width of virtual bound state
μ	chemical potential
μ_0	vacuum permeability
$\phi_k, \psi_{\alpha \boldsymbol{k}}$	electron wave function
ψ	field operator
Ω	connected subset of $\mathbf{R}^3$
ω_{D}	Debye frequency
ω_q	phonon, photon frequency
ϱ	density matrix, statistical operator, charge density
ϱ_{Si}	silicon mass density
σ	spin index
$\tau_{\alpha l}$	lifetime of a virtual bound state

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