

H. Haug  
A.-P. Jauho

**Quantum  
Kinetics  
in Transport  
and Optics  
of Semi-  
conductors**

**半导体输运  
和光学中的量子动力学**

Springer-Verlag

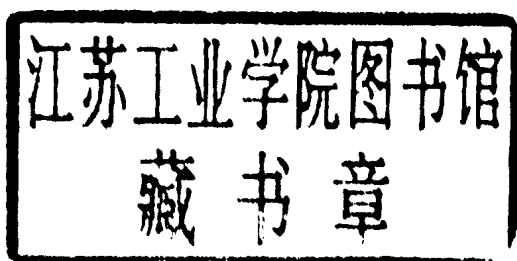
世界图书出版公司

Hartmut Haug Antti-Pekka Jauho

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# Quantum Kinetics in Transport and Optics of Semiconductors

With 94 Figures



Springer

Professor Dr. Hartmut Haug  
Institut für Theoretische Physik, J. W. Goethe Universität  
Robert-Mayer-Strasse 8, D-60325 Frankfurt am Main, Germany

Dr. Antti-Pekka Jauho  
Mikroelektronik Centret (MIC), Technical University of Denmark  
Bygning 345Ø, DK-2800 Lyngby, Denmark

*Series Editors:*

Professor Dr., Dres. h. c. Manuel Cardona  
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Professor Dr., Dres. h. c. Klaus von Klitzing  
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Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany  
\* Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38  
D-01187 Dresden, Germany

*Managing Editor:*

Dr.-Ing. Helmut K.V. Lotsch  
Springer-Verlag, Tiergartenstrasse 17, D-69121 Heidelberg, Germany

Corrected Printing 1998

ISSN 0171-1873

ISBN 3-540-61602-0 Springer-Verlag Berlin Heidelberg New York

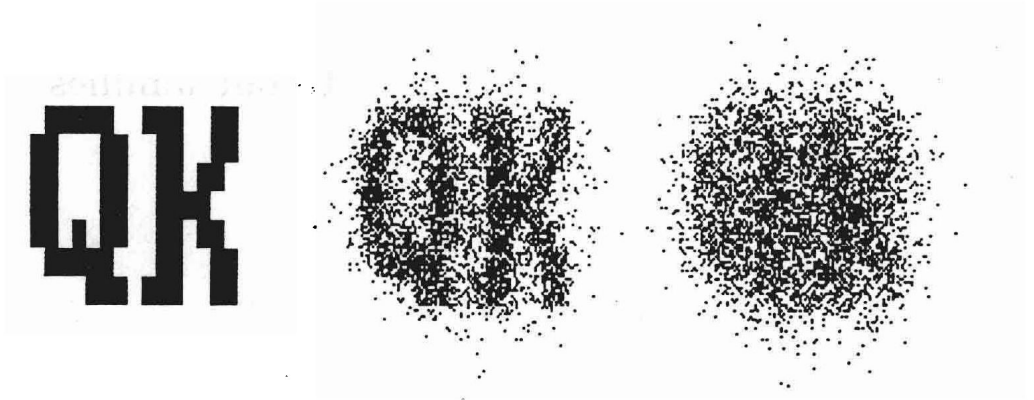
Library of Congress Cataloging-in-Publication Data. Haug, Hartmut: Quantum kinetics in transport and optics of semiconductors / Hartmut Haug ; Antti-Pekka Jauho. – 1st ed. p. cm. – (Springer series in solid-state sciences ISSN 0171-1873: 123) Includes bibliographical references and index. ISBN 3-540-61602-0 (hc : alk. paper) 1. Semiconductors—Optical properties. 2. Green's functions. 3. Quantum theory. I. Jauho, Antti-Pekka. 1952– II. Title. III. Series. QC611.6.O6H38 1996 537.6'22—dc20 96-34054

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**To our families**



The figure shows a Monte Carlo simulation of the Coulomb relaxation kinetics of a 2D electron gas, calculated by K. El Sayed. Each dot in the 2D momentum space corresponds to an electron. The initial distribution of the 3600 electrons forms the initial letters of Quantum Kinetics (QK). This distribution relaxes under Coulomb scattering into a thermal distribution. The three snapshots are taken at  $t = 0, 55,$  and 145 femtoseconds. In the last picture, 3000 scattering events, i.e., roughly one scattering event per particle, produce a nearly thermal distribution.

## Preface

New textbooks on various aspects of theoretical physics seem to overflow the market. A prospective author must be able to provide convincing answers to at least the following questions (posed by the publisher, colleagues, and last but not least, by him/herself and the associated family members). (i) Why bother writing the book? (ii) Is there a sufficient audience for the text? (iii) Isn't the topic already covered by a number of books, and isn't the author's best hope just to add a new wrinkle to the existing lore (and perhaps enhance his/her own publication record)? (iv) Is there any practical need for the book? (v) Are there any important open problems that the book will contribute to finding solutions to (or, at least, be able to identify points where the present understanding is insufficient).

We have thought carefully about the above questions, and have become convinced (at least between ourselves), that indeed there is a purpose in writing the book that you are holding in your hands.

In what follows we will try to outline reasons why we feel that this book might be useful, and define its scope and ultimate goals. First of all, this is a book on a *technique*. More precisely, this is a book on nonequilibrium Green functions (NGF). Narrowing the definition down even more precisely, this is a book about how NGF are applied in *semiconductor science*. To identify the final qualifier, we are mostly interested in systems where *extremely short* length scales ( $\simeq 1$  nm) and *extremely fast* time scales ( $\simeq 1$  fs) play a crucial role. In these short length and time scales the electrons exhibit their quantum mechanical wave nature: the quantum coherence of the electronic excitations becomes important. To properly describe phenomena of this kind, one needs a quantum theory of nonequilibrium phenomena, and the NGF provide such a technique. One of the purposes of this book is to show how deeply the quantum coherence modifies the physics in short time and length scales: the relaxation and dephasing dynamics differ radically from their semiclassical counterparts, and the collision terms of the quantum kinetic equations have a non-Markovian memory structure.

Equilibrium Green functions (EGF) have been one of the central items in the toolbox of a theoretical physicist for many years, and the interested student can find many excellent treatises on the topic (a brief bibliography is given in Chap. 3). Many of these books are written by the very people

who invented the formalism, and obviously our ambitions must be set on a lower level. Nonequilibrium Green functions, on the other hand, are much less frequently mentioned in the canonical textbooks. An exception is, of course, the classic work by Kadanoff and Baym, where the whole topic was introduced, but this work is now more than thirty years old, and obviously should be followed by a more modern treatise.

One may wonder why the beautiful techniques developed by Kadanoff and Baym (and, independently, by Keldysh), have so far not acquired the same popularity as equilibrium Green functions. For some reason there seems to be a rather widespread prejudice to the effect that the nonequilibrium techniques are accessible to only a very small select group of experts. We strongly disagree with this standpoint; in fact one of the main goals of our work is to emphasize that NGF are conceptually no more difficult (or easy) than normal Green functions are. In our opinion there are several factors that have contributed to this misconception. The first is that the physics of *degenerate Fermi systems* has defined the central topic of interest for the majority of many-body theorists. For this particular class of problems an extremely powerful formalism exists: *quasi-classical Green functions*, which take advantage of the fact that the electronic momenta are confined to the neighborhood of the Fermi surface, and thus allow the development of an essentially linear (in terms of the external driving field) theory. Consequently, the full potential power of the Kadanoff-Baym-Keldysh theory has not been called for. The second reason is that once the Fermi energy does not provide the overall largest energy scale, the all-important (in sense of the Landau school of theoretical physics) "small parameter" is not so easy to define. Thus applying rigorous many-body techniques to semiconductors under nonequilibrium conditions is, by definition, a topic that purists would be hesitant to touch. To quote a remark attributed to W. Pauli: "One should not work on semiconductors, that is a filthy mess; who knows whether they really exist", and this remark was made long before highly nonequilibrium semiconductors were even considered. We are fully aware that some of the theories described in this book suffer from this lack of rigor; nevertheless we have taken the risks of writing down expressions that later developments may require to be modified. Our philosophy has consistently been that we try to expose our topic as it stands today, and not have any false pretense in that what we are saying would be the final truth. (Paranetically, if everything was well-known and understood, would there be a real challenge in writing the book?!)

Perhaps another reason for the not-so-widespread use of nonequilibrium Green functions is that there are relatively few texts available that offer a systematic treatment. In book form we, of course, have the classic work of Kadanoff and Baym (1962), but in addition to that, it has been necessary to look for journals. A few review articles exist; we have particularly benefitted from those by Langreth (1976), Chou et al. (1985), and Rammer and Smith (1986), but these works are written for an experienced scientist and not for

a (graduate) student. It is interesting to note that during the last few years several books addressing many-body physics in general have added sections on NGF, [Datta (1995); Enz (1992); Ferry (1991); Mahan (1990)], but always as a kind of side remark. Many authors still feel that it is necessary to add an appendix or two in their research papers explaining the basic notions of NGF whenever they are needed in their research. If our book contributes towards a weakening of this feeling, one of our main goals has been achieved.

Semiconductor microscience has developed dramatically throughout the 1980s and 1990s. Many laboratories have access to samples and instruments that probe new and exciting effects in parameter ranges where standard theories, such as the Boltzmann equation or the Kubo formula, are not applicable. Hence there is a strong experimental motivation to search for theories that can be applied in these new situations. We feel that nonequilibrium Green functions are a good candidate for such a theoretical framework. It was already mentioned that this is a book on a *technique*, and not on a *topic*. A highly respected approach among the theoretical community is to attack a *problem* and then use whatever technique is necessary to sort out the problem. This is at the same time the distinction between a monograph and a textbook (in our definition): we do not attempt to cover a single topic in all its variations; what we do attempt to do is to take a given technique (NGF in our case) and use it in a number of carefully chosen topics. The textbook approach has dictated rather stringently the choice of topics: throughout the book we have chosen a level of presentation where a diligent student can follow all steps with a finite amount of pencils and paper. This may have occasionally led to rather trivial algebraic steps, at least for some of our sophisticated colleagues, but we have deliberately chosen this route. Our justification is based on the experience that students learn more from a text, and feel more secure about its essential contents, if they know that all the material is carefully chosen so that no essential steps are hidden behind elusive statements like "it can be shown", etc. Thus we are essentially providing an engineering approach: take our book, make sure that you can reproduce every single equation in it, and we will guarantee that you have acquired the weaponry to attack many as of yet unresolved issues in contemporary physics! Or, more modestly, after studying our book you should not be intimidated by a reference to NGF, and will be prepared to continue the conversation on whatever *physics* that was discussed..

The pedagogical approach chosen in this book has necessarily had its price. We do not show many experimental curves and their best theoretical fits. Rather, we focus on different theoretical approaches, and compare their interrelations. In particular this means that our "semiconductor" seldom has a real band structure with several (anisotropic) conduction and/or valence bands, or that we do not dwell in detail on various aspects of the self-consistent calculations (where the dynamical quantities determine the effective parameters that define the structures under investigation), nor do



we dwell in detail on the many possible different scattering mechanisms that take place in a real semiconductor (thus we consider only “impurities”, not worrying about their charge or internal degrees of freedom, and most of our “phonons” are of the dispersionless optical variety). We hope that this somewhat weakened connection to real materials is compensated for by the ability to carry out the calculations analytically, as far as it is possible, and that whenever the practical need arises, the general *structure* of the theory, as it is outlined here, can be applied to the real materials one is interested in.

We also need to comment about the prerequisites for the students approaching our text. A solid command of statistical physics and quantum mechanics is necessary. Some familiarity with second quantization would certainly be helpful, even though we give a brief summary on the topic. The hardest issue concerns the required background knowledge on equilibrium Green functions. This topic is viewed as a rather advanced issue in standard curricula, and we have no way of approaching the topics that lie at the core of our book without assuming some prior knowledge of EGF. However, we do provide a summary of EGF in Chap. 3, and since one of our most important messages is that NGF are conceptually *no more difficult* than EGF, our hope is that even a reader with a slightly rusty command of EGF will not shy away from our book; rather our hope is that this reader will learn more about EGF as a by-product of studying our book!

There is yet another philosophical point that has contributed to the birth of this book. We are strong believers that different disciplines in science can learn and benefit from a forced contact with each other. In this day and age of ever increasing specialization, different physics communities find it ever more difficult to communicate with each other, even though the mathematical principles underlying their respective research topics can be (once stripped of the everyday jargon) actually quite similar. To make a point in case, one of the standard books in Green function theory, Fetter and Walecka (1971), nicely talks about common themes in solid-state physics and nuclear physics. We have tried to follow the same route, but with a much more restrictive definition: we emphasize throughout our book that the *optical* and *transport* communities in semiconductor physics are actually tackling very similar problems. Thus we conceive as one of our main tasks the abolishment of any artificial barriers between these two groups of scientists.

The structure of this book is very clear cut: the text is divided into four parts, the first of which serves as a summary of some the concepts needed later, and also gives some Boltzmann-level results relevant to our topic; Part II develops the the general theoretical framework; Part III applies it to transport in semiconductor microstructures, and, finally, Part IV discusses optical applications. Parts III and IV are independent of each other, but our belief is that a serious student will greatly benefit by comparing the similar theoretical structures arising from superficially different physical starting points.

Last, but not least, it is our great pleasure to thank the many colleagues we have worked together with, and without whose expertise and (at times) friendly criticism we would not have been able to complete the book. (Naturally, the responsibility for all errors and inaccuracies lies with us.) Our special thanks go to Laci Bányai, Rita Bertoncini, John Davies, Claudia Ell, Karim El Sayed, David Ferry, Karsten Flensburg, Klaus Henneberger, Ben Hu, Kristian Johnsen, Leonid Keldysh, Stephan Koch, Tillman Kuhn, David Langreth, Pavel Lipavský, Gerry Mahan, Yigal Meir, Jørgen Rammer, Lino Reggiani, Ernst Reitsamer, Christian Remling, Wilfried Schäfer, Stefan Schuster, Henrik Smith, Pablo Tamborenea, Bao Tran Thoi, Bedřich Velický, Andreas Wacker, Martin Wegener, John Wilkins, Ned Wingreen, and Roland Zimmermann.

Frankfurt and Copenhagen  
August 1996

*Hartmut Haug*  
*Antti-Pekka Jauho*

# Contents

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## Part I Introduction to Kinetics and Many-Body Theory

---

<b>1. Boltzmann Equation</b>	<b>3</b>
1.1 Heuristic Derivation of the Semiclassical Boltzmann Equation	3
1.2 Approach to Equilibrium, H-Theorem	5
1.3 Linearization, Eigenfunction Expansion	8
<b>2. Numerical Solutions of the Boltzmann Equation</b>	<b>11</b>
2.1 Linearized Coulomb Boltzmann Kinetics of a 2D Electron Gas	12
2.2 Ensemble Monte Carlo Simulation	20
2.2.1 General Theory	20
2.2.2 Simulation of the Relaxation Kinetics of a 2D Electron Gas	23
2.3 $N^+N^-N^+$ -Structure: Boltzmann Equation Analysis	30
<b>3. Equilibrium Green Function Theory</b>	<b>35</b>
3.1 Second Quantization	35
3.2 Green Functions	38
3.2.1 Examples of Measurable Quantities	39
3.3 Fluctuation-Dissipation Theorem	41
3.4 Perturbation Expansion of the Green Function	44
3.5 Examples of Simple Solvable Models	46
3.5.1 Free-Particle Green Function	46
3.5.2 Resonant-Level Model	47
3.6 Self-Energy	49
3.6.1 Electron-Phonon Interaction	49
3.6.2 Elastic Impurity System; Impurity Averaging	51
3.7 Finite Temperatures	55

---

**Part II Nonequilibrium Many-Body Theory**


---

<b>4. Contour Ordered Green Functions</b>	59
4.1 General Remarks	59
4.2 Two Transformations	60
4.3 Analytic Continuation	65
<b>5. Basic Quantum Kinetic Equations</b>	71
5.1 The Kadanoff-Baym Formulation	71
5.2 The Keldysh Formulation	73
<b>6. Boltzmann Limit</b>	75
6.1 Gradient Expansion	75
6.2 Quasiparticle Approximation	77
6.3 Recovery of the Boltzmann Equation	78
<b>7. Gauge Invariance</b>	79
7.1 Choice of Variables	79
7.2 Gauge Invariant Quantum Kinetic Equation	81
7.2.1 Driving Term	81
7.2.2 Collision Term	83
7.3 Retarded Green Function	85
<b>8. Quantum Distribution Functions</b>	87
8.1 Relation to Observables, and the Wigner Function	87
8.2 Generalized Kadanoff-Baym Ansatz	88
8.3 Summary of the Main Formal Results	91

---

**Part III Quantum Transport in Semiconductors**


---

<b>9. Linear Transport</b>	95
9.1 Quantum Boltzmann Equation	95
9.2 Linear Conductivity of Electron-Elastic Impurity Systems	98
9.2.1 Kubo Formula	98
9.2.2 Quantum Kinetic Formulation	102
9.3 Weak Localization Corrections to Electric Conductivity	104
<b>10. A Model for Dynamical Disorder:</b>	
<b>The Gaussian White Noise Model</b>	109
10.1 Introduction	109
10.2 Determination of the Retarded Green Function	109

10.3 Kinetic Equation for the GWN .....	111
10.4 Other Transport Properties .....	115
<b>11. Quantum High-Field Transport in Semiconductors .....</b>	<b>119</b>
11.1 Introduction .....	119
11.2 Free Green Functions and Spectral Functions in an Electric Field .....	120
11.3 Resonant-Level Model in High Electric Fields .....	130
11.3.1 Introduction .....	130
11.3.2 Retarded Green Function: Single Impurity Problem ..	131
11.3.3 Retarded Green Function: Dilute Concentration of Impurities .....	133
11.3.4 Analytic Continuation .....	140
11.3.5 Quantum Kinetic Equation .....	141
11.4 Quantum Kinetic Equation for Electron-Phonon Systems ..	144
11.5 An Application: Collision Broadening for a Model Semiconductor .....	148
11.5.1 Analytical Considerations .....	148
11.5.2 A Simple Model: Optical Phonon Emission at $T = 0$ .....	150
11.6 Spatially Inhomogeneous Systems .....	152
<b>12. Transport in Mesoscopic Semiconductor Structures .....</b>	<b>157</b>
12.1 Introduction .....	157
12.2 Nonequilibrium Techniques in Mesoscopic Tunneling Structures .....	160
12.3 Model Hamiltonian .....	160
12.4 General Expression for the Current .....	162
12.5 Non-Interacting Resonant-Level Model .....	165
12.6 Resonant Tunneling with Electron-Phonon Interactions ...	168
12.7 Transport Through a Coulomb Island .....	170
<b>13. Time-Dependent Phenomena .....</b>	<b>179</b>
13.1 Introduction .....	179
13.2 Applicability to Experiments .....	180
13.3 Mathematical Formulation .....	181
13.4 Average Current .....	183
13.5 Time-Dependent Resonant-Level Model .....	184
13.5.1 Response to Harmonic Modulation .....	187
13.5.2 Response to Step-Like Modulation .....	190
13.6 Linear-Response .....	193
13.7 Fluctuating Energy Levels .....	195

---

**Part IV Theory of Ultrafast Kinetics  
in Laser-Excited Semiconductors**


---

<b>14. Optical Free-Carrier Interband Kinetics in Semiconductors</b>	199
14.1 Interband Transitions in Direct-Gap Semiconductors	199
14.2 Free-Carrier Kinetics Under Laser-Pulse Excitation	202
14.3 The Optical Free-Carrier Bloch Equations	205
<b>15. Interband Quantum Kinetics with LO-Phonon Scattering</b>	209
15.1 Derivation of the Interband Quantum Kinetic Equations	209
15.2 Approximations for the Green Functions $G_{\mu\nu}^r$ and $G_{\mu\nu}^a$	213
15.3 Intraband Quantum Kinetics	216
15.4 Linear Polarization Kinetics, Phonon Sidebands	218
15.5 Coupled Interband Kinetic Equations in Diagonal Approximation	219
15.6 Numerical Studies	221
<b>16. Exciton Quantum Kinetics in Polar Semiconductors</b>	227
16.1 Interband Quantum Kinetic Equations with Excitonic Effects	227
16.2 Quantum Beats and Urbach Tail	229
16.2.1 LO-Phonon Quantum Beats	229
16.2.2 Urbach Tail Absorption	236
16.3 Excitonic Optical Stark Effect	238
16.4 Coupled Quantum Kinetics of Electrons and Phonons	241
16.5 Quantum Coherence of the Green Functions	244
<b>17. Two-Pulse Excitation</b>	253
17.1 Calculation of the Photon Echo	253
17.2 Calculation of the Four-Wave Mixing Signal	255
17.3 Comparison with Four-Wave Mixing Experiments	258
<b>18. Coulomb Quantum Kinetics in a Dense Electron Gas</b>	261
18.1 Introduction	261
18.2 Derivation of a Closed Quantum Kinetic Description	263
18.3 Simplifying Approximations	268
18.3.1 Initial Time Regime Without Screening and Energy Conservation	268
18.3.2 Time-Dependent Plasmon Pole Approximation	269
18.3.3 Instantaneous Static Potential Approximation	272

<b>19. Interband Coulomb Quantum Kinetics,</b>	
<b>Optical Dephasing</b> .....	277
19.1 Interband Quantum Kinetic Equations	
with Coulomb Interaction .....	277
19.2 Early Stage of the Coulomb Quantum Kinetics .....	280
19.3 Quasi-Classical Theory of the Polarization Decay .....	288
<b>20. The Build-Up of Screening</b>	
<b>After Ultra-Short Pulse Excitation</b> .....	293
20.1 The Model .....	293
20.2 Numerical Results .....	295
<b>References</b> .....	301
<b>Subject Index</b> .....	309

Part I

**Introduction to Kinetics  
and Many-Body Theory**



