SOLID-STATE SCIENCES

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Quantum Kinetics in Transport and Optics of Semiconductors

半导体输运和光学中的量子动力学

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With 94 Figures

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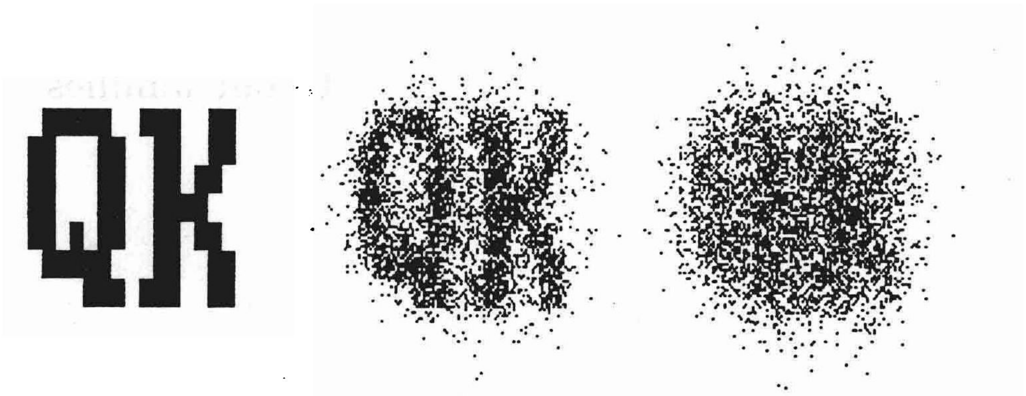
To our families



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 intitial distribution of the 3600 electrons forms the intitial 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. (Paranthetically, 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 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 aquired 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 Flensberg, 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 Thoai, Bedřich Velický, Andreas Wacker, Martin Wegener, John Wilkins, Ned Wingreen, and Roland Zimmermann.

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Part I

Introduction to Kinetics and Many-Body Theory