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Hartmut Haug   Antti-Pekka Jauho

Quantum Kinetics in Transport and Optics of Semiconductors

Second, Substantially Revised Edition

With 98 Figures

Springer

Professor Dr. Hartmut Haug
Institut für Theoretische Physik, J. W. Goethe Universität
Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Professor Dr. Antti-Pekka Jauho
Department of Micro and Nanotechnology (MIC), Technical University of Denmark
Building 345 E, 2800 Kongens Lyngby, Denmark

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* Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38
01187 Dresden, Germany

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Department of Physics, 5000 East University, University of Michigan
Ann Arbor, MI 48109-1120, USA

Professor Dr. Horst Störmer
Dept. Phys. and Dept. Appl. Physics, Columbia University, New York, NY 10027 and
Bell Labs., Lucent Technologies, Murray Hill, NJ 07974, USA

ISSN 0171-1873

ISBN 978-3-540-73561-8 2nd Edition Springer Berlin Heidelberg New York
ISBN 3-540-61602-0 1st Edition Springer Berlin Heidelberg New York

Library of Congress Control Number: 2007931202

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Typesetting: Data prepared by SPI Kolam using a Springer LaTeX macro package
Cover: eStudio Calamar Steinen

Printed on acid-free paper SPIN: 12081660 57/3180/SPI - 5 4 3 2 1 0

To our families

Preface

During the 11 years since the first edition was published the field of quantum kinetics has experienced a great expansion, and the methods described in the first edition are now widely used in a large number of different subfields. Literally thousands of papers have been published in this area and an attempt to give an exhaustive review is clearly beyond the present scope. In this revised edition we have attempted to include some examples of modern topics, essentially from the research areas we have been active in. We are fully aware of the fact that this approach will leave many important topics untouched, and our hope is that the leading researchers in those areas write their own books! [1] More specifically, in our revision we have left the first nine chapters essentially unchanged, only supplying a few updated references, and correcting misprints. On the other hand, the last nine chapters have been substantially revised, reorganized, and expanded. In the sections describing transport phenomena we have included a number of new topics, such as transport in a superlattice, molecular electronics (and inelastic interactions), and noise calculations. We have added a new chapter, describing the dynamical Franz–Keldysh effect, which follows directly from the field-dependent Green functions, originally introduced to describe high-field transport in semiconductors. In the sections dealing with optical properties we emphasize that the concepts of quantum kinetics have proved to be extremely fruitful for the analysis of new experiments in ultrafast semiconductor spectroscopy. Some highlights included in the new edition are: The femtosecond build-up of screening and of polaron correlations, four-wave mixing studies of the plasma-density dependent dephasing, the femtosecond formation of phonon–plasmon mixed modes, detection of light-induced band gaps, and non-Markovian relaxation in the short femtosecond regime. None of these fascinating new observations can be understood in the framework of a semiclassical Markovian Boltzmann kinetics, but require for their description the theory of quantum kinetics as demonstrated

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[1] Recent progress in research using nonequilibrium Green functions is reviewed in a very useful series of edited volumes due to M. Bonitz and co-workers [55–57].

in the new edition. Even with these new topics we have attempted to keep the total page number essentially unchanged, which naturally has led to omission of some material which we no longer felt was necessary. Our hope is that the readers, new and old, will find the revised book useful in their research work.

We have worked with many colleagues on the new topics included here. We would particularly like to mention Mads Brandbyge, Thomas Frederiksen, Paul Gartner, Alfred Leitenstorfer, Bernhard Mieck, Tomáš Novotný, Gloria Platero, Arne Schmenkel, Oli Schmidt, Fabricio Souza, Alexandra Stein, and Tuyen Vu. Also, the many students who have found mistakes and misprints, and suggested improvements, deserve our sincere thanks.

Frankfurt and Copenhagen, *Hartmut Haug*
July 2007 *Antti-Pekka Jauho*

Preface to the First Edition

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). (1) Why bother writing the book? (2) Is there a sufficient audience for the text? (3) Is not the topic already covered by a number of books, and is not the author's best hope just to add a new wrinkle to the existing lore (and perhaps enhance his/her own publication record)? (4) Is there any practical need for the book? (5) 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 (NEGF). Narrowing the definition down even more precisely, this is a book about how NEGF are applied in *semiconductor science*. To identify the final qualifier, we are mostly interested in systems where *extremely short* length scales ($\simeq 1\,\mathrm{nm}$) and *extremely fast* time scales ($\simeq 1\,\mathrm{fs}$) play a crucial role. In these short length and timescales 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 NEGF 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 [191], where the whole topic was introduced, but this work is now more than 30 years old, and obviously should be followed by a more modern treatise.

One may wonder why the beautiful techniques developed by Kadanoff and Baym [191] (and, independently, by Keldysh [198]), 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 NEGF 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. (Parenthetically, if everything was well-known and understood, would there be 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 [191], 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 [231], Chou et al. [80], and Rammer and Smith [287], 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 NEGF, (see, e.g., books by Datta [93], Enz [105], Ferry [109], or Mahan [254]), 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 NEGF 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 (NEGF 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 materials are 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 NEGF, 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 NEGF are conceptually *no more difficult* than EGF, our hope is that even a reader with a slightly rusty command of EGF will not shun away from our book; rather our hope is that this reader will learn more about EGF's 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 [110], 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 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 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 Bertoncinı, John Davies, Claudia Ell, Karim El Sayed, David Ferry, Karsten Flensberg, Klaus Henneberger, Ben Hu, Kristinn 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, Bao Tran Thoai, Bedřich Velický, Andreas Wacker, Martin Wegener, John Wilkins, Ned Wingreen, and Roland Zimmermann.

Frankfurt and Copenhagen, *Hartmut Haug*
August 1996 *Antti-Pekka Jauho*

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Part I

Introduction to Kinetics and Many-Body Theory

1

Boltzmann Equation

Summary. We review some of the general properties of the semiclassical Boltzmann equation - not necessarily restricting ourselves to the dilute electron gas - paying special attention to its irreversible properties.

1.1 Heuristic Derivation of the Semiclassical Boltzmann Equation

The kinetic theory of Boltzmann which connects the regime of dynamics with that of thermodynamics has been a milestone in the development of theoretical physics. In order to describe the kinetics of, e.g., an atomic gas, Boltzmann [51] introduced, with great intuition, more than half a century before the rise of quantum mechanics, a probabilistic description for the evolution of a single-particle distribution which anticipated atomistic scattering concepts. Boltzmann introduced a single-particle probability distribution in the phase space of the canonical variables $\boldsymbol{r}$ and $\boldsymbol{p}$. This Boltzmann distribution function is usually denoted as $f(\boldsymbol{r}, \boldsymbol{p}, t)$. Obviously, this object is classical, because in quantum mechanics $\boldsymbol{r}$ and $\boldsymbol{p}$ are noncommuting operators so that they cannot be simultaneously measured with arbitrary precision. We will analyze in the following chapter how this conceptual difficulty affects the limits of validity of the Boltzmann equation. Here we will first present a heuristic derivation of the semiclassical Boltzmann equation. Later in this book we will pay special attention to the more detailed quantum mechanical justifications of the Boltzmann kinetics, present discussions of the limits of this semiclassical theory, and, most importantly, derive and study the quantum kinetics which has to be used instead of the Boltzmann kinetics on small length and/or short timescales. In the framework of the classical Hamilton theory the total change in time of this distribution function is

$$\begin{aligned}\frac{\mathrm{d}f(\boldsymbol{r},\boldsymbol{p},t)}{\mathrm{d}t} &= \frac{\partial f}{\partial t} + \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\cdot\nabla_r f + \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t}\cdot\nabla_p f \\ &= \frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m}\cdot\nabla_r f - [\nabla_r V(\boldsymbol{r})]\cdot\nabla_p f = \frac{\partial f}{\partial t}\Big|_{\mathrm{coll}} , \qquad (1.1)\end{aligned}$$

where $V(\boldsymbol{r})$ is a single-particle potential. The left-hand side of (1.1) describes the dynamics of a single particle. The influence of the other particles will give rise to a further change of the distribution function $\partial f/\partial t|_{\mathrm{coll}}$ which describes the effect of the collisions in the gas. We will not proceed historically, but include directly the proper quantum statistics for quantum gases, so that we are not limited to nondegenerate gases. This extension is necessary for the application of the Boltzmann kinetics to electron gases in semiconductors which are often degenerate, whether they are produced by doping, injection, or optical excitation. Fermi's golden rule gives us the transition probability per unit time and thus the wanted change of f due to collisions. For an interacting Fermi gas we calculate this change by considering approximately free-particle collisions in which the particle is scattered from a momentum state $\boldsymbol{p}$ to a momentum state $\boldsymbol{p}'$ and simultaneously another particle is scattered from state $\boldsymbol{p}_1$ to $\boldsymbol{p}_1'$, as well as the inverse process

$$\begin{aligned}\frac{\partial f(\boldsymbol{p})}{\partial t}\Big|_{\mathrm{coll}} = -\sum_{\boldsymbol{p}',\boldsymbol{p}_1,\boldsymbol{p}_1'} w(\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}',\boldsymbol{p}_1')\Big\{&f(\boldsymbol{p})f(\boldsymbol{p}_1)[1-f(\boldsymbol{p}')][1-f(\boldsymbol{p}_1')] \\ &-[1-f(\boldsymbol{p})][1-f(\boldsymbol{p}_1)]f(\boldsymbol{p}')f(\boldsymbol{p}_1')\Big\} , \qquad (1.2)\end{aligned}$$

where the intrinsic transition probalility per unit time is given by

$$\begin{aligned}w(\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}',\boldsymbol{p}_1') &= \tfrac{1}{2}|W_{\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}',\boldsymbol{p}_1'} - W_{\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}_1',\boldsymbol{p}'}|^2 \\ &\quad\times \delta_{\boldsymbol{p}+\boldsymbol{p}_1,\boldsymbol{p}'+\boldsymbol{p}_1'}\frac{2\pi}{\hbar}\delta(\varepsilon_p+\varepsilon_{p_1}-\varepsilon_{p'}-\varepsilon_{p_1'}) . \qquad (1.3)\end{aligned}$$

Here

$$W_{\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}',\boldsymbol{p}_1'} = \langle\boldsymbol{p}\boldsymbol{p}_1|W|\boldsymbol{p}'\boldsymbol{p}_1'\rangle \qquad (1.4)$$

is the interaction matrix element and ε_p is the energy of the particle. The second matrix element in (1.3) is the exchange term in which $\boldsymbol{p}_1'$ and $\boldsymbol{p}'$ are interchanged. This form of the intrinsic transition probability is called the first Born approximation. The population factors take care that the initial states in the scattering event are populated and that the final states are empty in accordance with the Pauli principle. The scattering $\boldsymbol{p}+\boldsymbol{p}_1 \to \boldsymbol{p}'+\boldsymbol{p}_1'$ is a loss term which reduces $f(\boldsymbol{p})$, while the inverse process $\boldsymbol{p}'+\boldsymbol{p}_1' \to \boldsymbol{p}+\boldsymbol{p}_1$ increases the distribution function. For shortness of notation, the parametric dependencies on the spatial coordinate $\boldsymbol{r}$ and time t are not shown in the collision integral. The form of the collision integral leads to five conservation laws for: (a) the number of particles, (b) the vector of the total momentum, and (c) the total energy. In a dilute, nondegenerate gas the final state population can be neglected, so that (1.2) can be simplified by the approximation $1 - f(\boldsymbol{p}) \simeq 1$.

A second important scattering rate for an electron gas in a perfect crystal is the scattering by emission or absorption of a phonon. Its form is

$$\begin{aligned}\left.\frac{\partial f(\boldsymbol{p})}{\partial t}\right|_{\mathrm{coll}} = -\sum_{\boldsymbol{p}',\boldsymbol{q}} w(\boldsymbol{p},\boldsymbol{p}';\pm\boldsymbol{q}) \times \Big\{ & f(\boldsymbol{p})[1-f(\boldsymbol{p}')]\big[\tfrac{1}{2} + n(\boldsymbol{q}) \pm \tfrac{1}{2}\big] \\ & - \big[1-f(\boldsymbol{p})\big] f(\boldsymbol{p}')\big[\tfrac{1}{2} + n(\boldsymbol{q}) \mp \tfrac{1}{2}\big]\Big\}\ ,\end{aligned} \tag{1.5}$$

where the intrinsic transition probabilty per unit time is given by

$$w(\boldsymbol{p},\boldsymbol{p}';\pm\boldsymbol{q}) = |M_q|^2 \delta_{\boldsymbol{p},\boldsymbol{p}'\pm\boldsymbol{q}} \frac{2\pi}{\hbar} \delta\big(\varepsilon_{p'} \pm \hbar\omega_q - \varepsilon_p\big)\ . \tag{1.6}$$

Here, M_q is the electron–phonon interaction matrix element, and $n(\boldsymbol{q})$ and ω_q are the phonon distribution and frequency, respectively. Consider the upper sign first, then the first term in (1.5) describes a scattering of an electron from $\boldsymbol{p}$ into the state $\boldsymbol{p}'$ accompanied with an emission of a phonon. The final state boson population factor $[1+n(\boldsymbol{q})]$ shows that the emission can be spontaneous or stimulated. The energy conservation also shows that the energy ε_p of the initially populated state is shared between the particle in the final state and the phonon. The contribution of the lower sign in (1.5) describes a scattering from $\boldsymbol{p}$ to $\boldsymbol{p}'$ via absorption of a phonon with an occupation factor $n(\boldsymbol{q})$. The form of (1.5) shows that for the electron–phonon scattering rate only the electron particle number is conserved, but no longer the total momentum and the total energy of the electron gas which both can be transferred to the phonon system. The phonon distribution in turn is also governed by a similar Boltzmann equation which we will not give explicitly here.

Obviously the semiclassical Boltzmann equation cannot be used on very short timescales because the assumption that the energy is conserved in an isolated collision (1.2), (1.5) breaks down. In a short time interval δt the energy remains undetermined due to the uncertainty relation $\delta t \delta E \geq \hbar$. Therefore the strict energy conservation in an individual collision is not an inherent property of the quantum kinetic description.

The mathematical properties of the Boltzmann kinetics contained in (1.1), (1.2), and (1.5) have been thoroughly investigated. Its full theory is a wide subject in its own; we will discuss only a few properties here. For a much more complete treatment and for studies of its applications we have to refer to such excellent books as Ziman [380], Cercignani [76], and Smith and Jensen [327].

1.2 Approach to Equilibrium: H-Theorem

It is easy to convince oneself that the semiclassical Boltzmann equation (1.2) describes indeed an evolution toward the thermal equilibrium in the absence of external fields. We introduce first an arbitrary function $F(\boldsymbol{p}, f_{\boldsymbol{p}})$ which depends on the momentum and the distribution $f(\boldsymbol{r}, \boldsymbol{p}, t)$. Its local density is

$$\langle F(\boldsymbol{r}, t)\rangle = \sum_{\boldsymbol{p}} F(\boldsymbol{p}, f_{\boldsymbol{p}}) f_{\boldsymbol{p}} \ . \tag{1.7}$$

The change of this function due to the collisions is [here we consider explicitly the collision operator (1.2)]

$$\begin{aligned} \frac{\partial\langle F(\boldsymbol{r}, t)\rangle}{\partial t}\Big|_{\text{coll}} &= \sum_{\boldsymbol{p}} \left[\frac{\partial F(\boldsymbol{p})}{\partial f(\boldsymbol{p})} + F(\boldsymbol{p})\right] \frac{\partial f(\boldsymbol{p})}{\partial t}\Big|_{\text{coll}} \\ &= - \sum_{\boldsymbol{p}\boldsymbol{p}', \boldsymbol{p}_1, \boldsymbol{p}_1'} w(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}'\boldsymbol{p}_1') \frac{\partial[F(\boldsymbol{p}) f(\boldsymbol{p})]}{\partial f(\boldsymbol{p})} \\ &\quad \times \Big\{ f(\boldsymbol{p}) f(\boldsymbol{p}_1)[1 - f(\boldsymbol{p}')][1 - f(\boldsymbol{p}_1')] \\ &\quad - [1 - f(\boldsymbol{p})][1 - f(\boldsymbol{p}')] f(\boldsymbol{p}_1) f(\boldsymbol{p}_1') \Big\} \ . \end{aligned} \tag{1.8}$$

Exploiting the symmetry of the intrinsic transition probability $w(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}_1'\boldsymbol{p}')$ with respect to the exchange of particle coordinates

$$\begin{aligned} w(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}_1') &= w(\boldsymbol{p}_1, \boldsymbol{p}; \boldsymbol{p}_1', \boldsymbol{p}') \\ &= w(\boldsymbol{p}', \boldsymbol{p}_1'; \boldsymbol{p}, \boldsymbol{p}_1) = w(\boldsymbol{p}_1', \boldsymbol{p}'; \boldsymbol{p}_1, \boldsymbol{p}) \ , \end{aligned} \tag{1.9}$$

one finds that

$$\begin{aligned} \frac{\partial\langle F(\boldsymbol{r}, t)\rangle}{\partial t}\Big|_{\text{coll}} &= -\frac{1}{4} \sum_{\boldsymbol{p}\boldsymbol{p}', \boldsymbol{p}_1, \boldsymbol{p}_1'} w(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}_1') \\ &\quad \times \left[\frac{\partial(Ff)}{\partial f} + \frac{\partial(Ff)}{\partial f_1} - \frac{\partial(Ff)}{\partial f'} - \frac{\partial(Ff)}{\partial f_1'}\right] \\ &\quad \times \Big[f f_1 (1 - f')(1 - f_1') - (1 - f)(1 - f_1) f' f_1' \Big] \ . \end{aligned} \tag{1.10}$$

In (1.10) we have introduced a shorthand notation, for example in $\partial(Ff)/\partial f$ all involved functions are evaluated at the argument $\boldsymbol{p}$. Now consider the following choice for F:

$$f(\boldsymbol{p}) F(\boldsymbol{p}, f_{\boldsymbol{p}}) = f(\boldsymbol{p}) \ln f(\boldsymbol{p}) + [1 - f(\boldsymbol{p})] \ln[1 - f(\boldsymbol{p})] \ . \tag{1.11}$$

The partial derivative with repect to f yields

$$\frac{\partial(Ff)}{\partial f(\boldsymbol{p})} = \ln \frac{f(\boldsymbol{p})}{1 - f(\boldsymbol{p})} \ . \tag{1.12}$$

Equation (1.10) becomes

$$\begin{aligned}
\frac{\partial}{\partial t}\Big|_{\text{coll}} \sum_{\boldsymbol{p}} f(\boldsymbol{p}) \ln f(\boldsymbol{p}) + [1-f(\boldsymbol{p})] \ln[1-f(\boldsymbol{p})] &= \frac{\partial}{\partial t} H(\boldsymbol{r},t)\Big|_{\text{coll}} \\
= -\frac{1}{4} \sum_{\boldsymbol{p}\boldsymbol{p}',\boldsymbol{p}_1,\boldsymbol{p}_1'} w(\boldsymbol{p},\boldsymbol{p}_1;\boldsymbol{p}',\boldsymbol{p}_1') \ln\left[\frac{f f_1(1-f')(1-f_1')}{(1-f)(1-f_1)f'f_1'}\right] \\
\times \left[f f_1(1-f')(1-f_1') - (1-f)(1-f_1)f'f_1'\right] . \qquad (1.13)
\end{aligned}$$

The integrand is of the form $(x-y)\ln(x/y)$, and hence nonnegative, because $x-y$ and $\ln(x/y)$ have the same sign. Thus the H-function (called "eta"-function, the capital greek eta looks like a latin H) always decreases in the approach to equilibrium. This is the content of Boltzmann's famous eta-theorem, generalized to a Fermi gas.

The eta-theorem shows that the entropy density, which for a Fermi gas is given by [226]

$$\begin{aligned}
s(\boldsymbol{r},t) &= -k_{\mathrm{B}} H(\boldsymbol{r},t) \\
&= -k_{\mathrm{B}} \sum_{\boldsymbol{p}} \big\{ f(\boldsymbol{p}) \ln f(\boldsymbol{p}) + [1-f(\boldsymbol{p})] \ln[1-f(\boldsymbol{p})] \big\}, \qquad (1.14)
\end{aligned}$$

reaches a maximum in the equilibrium. Here, k_{B} is Boltzmann's constant.

Finally, we will show that the Boltzmann equation (1.2) describes indeed an approach to the well-known Fermi equilibrium function. For this purpose we formalize the already mentioned conservation laws. We define the functions $F_i(\boldsymbol{p})$ with $i = 1, \ldots, 5$ as

$$F_1 = 1, \quad F_i = p_i, \quad i = 2,3,4, \quad F_5 = \varepsilon_p , \qquad (1.15)$$

we see immediately from (1.10) that the corresponding $\langle F_i \rangle$ are not changed by the collisions. In equilibrium the term in curly brackets in (1.2) has to vanish:

$$\left[f^0 f_1^0 (1-f^{0\prime})(1-f_1^{0\prime}) - (1-f^0)(1-f_1^0) f^{0\prime} f_1^{0\prime}\right] = 0 . \qquad (1.16)$$

From this relation one sees that

$$\ln \frac{f^0}{(1-f^0)} + \ln \frac{f_1^0}{(1-f_1^0)} = \ln \frac{f^{0\prime}}{(1-f^{0\prime})} + \ln \frac{f_1^{0\prime}}{(1-f_1^{0\prime})} . \qquad (1.17)$$

In other words, $\ln[f^0/(1-f^0)]$ is also a conserved quantity. Because we have only five basic conservation laws, this quantity can be expressed as a linear combination of $1, \boldsymbol{p}$, and ε_p:

$$\ln \frac{f^0}{(1-f^0)} = A + \boldsymbol{B} \cdot \boldsymbol{p} + C\varepsilon_p \qquad (1.18)$$

with

$$A = \beta\mu, \quad \boldsymbol{B} = \beta\boldsymbol{u}, \quad C = -\beta \; , \tag{1.19}$$

where $\beta = 1/(k_B T)$, μ is the chemical potential and $\boldsymbol{u}$ is the drift velocity. All the expressions in (1.19) can still be – slowly varying – functions of $\boldsymbol{r}$ and t. Such a situation is called a local equilibrium. Equation (1.18) has the solution

$$f^0(\boldsymbol{p}) = \frac{1}{\mathrm{e}^{\beta(\varepsilon_p - \boldsymbol{p}\cdot\boldsymbol{u} - \mu)} + 1} \; , \tag{1.20}$$

which is the Fermi distribution function. A similar derivation for the Boltzmann equation with electron–phonon scattering results in an equilibrium phonon distribution function of the form

$$n^0(\boldsymbol{p}) = \frac{1}{\mathrm{e}^{\beta(\hbar\omega_p - \boldsymbol{p}\cdot\boldsymbol{u})} - 1} \; , \tag{1.21}$$

because the chemical potential of bosons, whose total number is not conserved, is identical to zero.

1.3 Linearization: Eigenfunction Expansion

Close to thermal equilibrium the nonlinear Boltzmann equation, e.g., (1.2), can be linearized with respect to the deviation $\delta f \equiv f - f^0$ from the thermal equilibrium solution (1.20). For simplicity we consider here a spatially homogeneous electron gas without drift. It turns out that it is advantageous to use a normalized deviation $\phi(\boldsymbol{p}, t)$ which is introduced by writing

$$f(\boldsymbol{p}, t) = \frac{1}{\mathrm{e}^{\beta(\varepsilon_p - \mu) - \phi(\boldsymbol{p}, t)} + 1} \; . \tag{1.22}$$

Expanding this function with respect to $\phi(\boldsymbol{p}, t)$ yields

$$\delta f(\boldsymbol{p}, t) = f^0(\boldsymbol{p})[1 - f^0(\boldsymbol{p})]\phi(\boldsymbol{p}, t) \; . \tag{1.23}$$

The linearized Boltzmann equation yields the following net scattering rate for the state $\boldsymbol{p}$:

$$\begin{aligned} \frac{\partial\phi(\boldsymbol{p}, t)}{\partial t} &= -\frac{2}{f^0(\boldsymbol{p})[1 - f^0(\boldsymbol{p})]} \sum_{\boldsymbol{p}_1, \boldsymbol{p}', \boldsymbol{p}'_1} w(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}'_1) \\ &\quad \times \Big\{ \phi(\boldsymbol{p}, t) \big[f^0(1 - f^0) f_1^0 (1 - f^{0\prime})(1 - f_1^{0\prime}) \\ &\quad + f^0(1 - f^0)(1 - f_1^0) f^{0\prime} f_1^{0\prime} \big] + \cdots \Big\} \; . \end{aligned} \tag{1.24}$$

The dots indicate terms of similar structure proportional to $\phi(\boldsymbol{p}_1, t)$, $\phi(\boldsymbol{p}', t)$, and $\phi(\boldsymbol{p}'_1, t)$. In equilibrium

$$f^0 f_1^0 (1 - f^{0\prime})(1 - f_1^{0\prime}) = (1 - f^0)(1 - f_1^0) f^{0\prime} f_1^{0\prime} \; . \tag{1.25}$$

Using relation (1.25), the linearized Boltzmann equation (1.24) reduces to

$$\frac{\partial \phi(\boldsymbol{p}, t)}{\partial t} = -\frac{2}{f^0(\boldsymbol{p})[1 - f^0(\boldsymbol{p})]} \sum_{\boldsymbol{p}_1, \boldsymbol{p}', \boldsymbol{p}_1'} \mathcal{W}(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}_1') \tag{1.26}$$

$$\times \left[\phi(\boldsymbol{p}, t) + \phi(\boldsymbol{p}_1, t) - \phi(\boldsymbol{p}', t) - \phi(\boldsymbol{p}_1', t) \right] = -\mathcal{L} \; \phi(\boldsymbol{p}, t), \tag{1.27}$$

with

$$\mathcal{W}(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}_1') = w(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}_1') f^0 f_1^0 (1 - f^{0\prime})(1 - f_1^{0\prime}) \; . \tag{1.28}$$

The transition matrix $\mathcal{W}$ of the linearized Boltzmann equation has the following symmetry properties:

$$\begin{aligned} \mathcal{W}(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}', \boldsymbol{p}_1') &= \mathcal{W}(\boldsymbol{p}_1, \boldsymbol{p}; \boldsymbol{p}', \boldsymbol{p}_1') \\ &= \mathcal{W}(\boldsymbol{p}', \boldsymbol{p}_1'; \boldsymbol{p}, \boldsymbol{p}_1) = \mathcal{W}(\boldsymbol{p}, \boldsymbol{p}_1; \boldsymbol{p}_1', \boldsymbol{p}') \; . \end{aligned} \tag{1.29}$$

The linearized Boltzmann equation also conserves the total particle number, the total momentum, and the total energy. If one chooses a $\phi(\boldsymbol{p}, t)$ which is proportional to either $1, \boldsymbol{p}$, or ε_p, the r.h.s of the Boltzmann equation (1.26) vanishes. Thus, these particular forms of $\phi(\boldsymbol{p})$ are eigenfunctions to the collision operator $\mathcal{L}$ with a vanishing eigenvalue. The collision operator is an integral operator

$$\mathcal{L}\phi(\boldsymbol{p}) = \sum_{\boldsymbol{p}'} \mathcal{L}(\boldsymbol{p}, \boldsymbol{p}') \phi(\boldsymbol{p}') \; . \tag{1.30}$$

In general the eigenfunctions $\phi_\lambda(\boldsymbol{p})$ are solutions of the stationary equation

$$\mathcal{L}\phi_\lambda(\boldsymbol{p}) = \lambda \phi_\lambda(\boldsymbol{p}) \; . \tag{1.31}$$

One can define a scalar product $\langle \sigma | \phi \rangle$ and a norm $|\phi|$ by

$$\langle \sigma | \phi \rangle = \sum_{\boldsymbol{p}} f^0(\boldsymbol{p})[1 - f^0(\boldsymbol{p})] \sigma^*(\boldsymbol{p}) \phi(\boldsymbol{p}) \; , \quad |\phi|^2 = \langle \phi | \phi \rangle \; , \tag{1.32}$$

and span a Hilbert space by the eigenfunctions of $\mathcal{L}$. Using the symmetry relations of $\mathcal{W}$, one shows that $\mathcal{L}$ is a hermitian, real, and positive semidefinite operator in this Hilbert space, i.e.,

$$\langle \sigma | \mathcal{L}\phi \rangle = \langle \mathcal{L}\sigma | \phi \rangle ; \quad \langle \phi | \mathcal{L}\phi \rangle \geq 0 \; . \tag{1.33}$$

The equality sign holds, if ϕ is one of the five collision invariants. With these definitions the solution of the time-dependent linearized Boltzmann equation with a given initial deviation $\phi(t = 0) = \phi_0$ can be found by expanding ϕ_0 in terms of the set of eigenfunctions ϕ_λ of $\mathcal{L}$. The solution is then of the form

$$\phi(\boldsymbol{p}, t) = \sum_\lambda A_\lambda \mathrm{e}^{-\lambda t} \phi_\lambda(\boldsymbol{p}) \; . \tag{1.34}$$

The eigenvalues λ are true relaxation frequencies for deviations ϕ_λ. However, it is obvious from (1.34) that, in general, a description of the Boltzmann relaxation kinetics with only one relaxation time is not possible. Therefore the most frequently used linear approximation to the collision rate, the so-called relaxation-time approximation,

$$\left.\frac{\partial f(\boldsymbol{p})}{\partial t}\right|_{\mathrm{coll}} \simeq -\frac{\delta f(\boldsymbol{p})}{\tau} \tag{1.35}$$

is only a very crude description of the relaxation kinetics toward equilibrium. The effective relaxation time τ in the resulting exponential decay of a deviation from the thermal equilibrium distribution has, in general, no well-defined meaning, and is known not to describe adequately the experimentally observed transport properties (e.g., viscosities and thermal conductivity of simple mono- and diatomic gases) [327]. Since the linearized collision operator commutes with the operator for the angular momentum in $\boldsymbol{p}$-space, the normalized deviation $\phi(\boldsymbol{p})$ can be factorized into a radial function and an angular part. Unfortunately, the eigenfunctions have to be evaluated numerically. Only for a nondegenerate system of Maxwell molecules with a repulsive interaction potential $\propto r^{-4}$ analytical eigenfunctions have been found. In the case of degenerate Fermi systems, where all momenta are confined to the neighborhood of p_{F}, the eigenfunction expansions have provided rapidly converging series for various transport coefficients [60, 190].

We will illustrate in Chap. 2 the use of the eigenfunction expansion for the numerical evaluation of the relaxation kinetics due to Coulomb scattering in a quasi-two-dimensional (2D) electron gas. Such a 2D electron gas can be, for example, realized in a semiconductor quantum well structure. This example simultaneously addresses an important relaxation process of hot electrons in semiconductors, because in a dense electron gas in semiconductors the Coulomb scattering provides the fastest relaxation process.

2

Numerical Solutions of the Boltzmann Equation

Summary. Various concepts for the numerical solution of the semiclassical Boltzmann equation are discussed, including an illustration of the use of a linearized Boltzmann equation and its eigenfunction expansion for a 2D electron gas. The numerical results for the linearized Boltzmann equation are compared with those of an ensemble Monte Carlo simulation of the Master equation. Finally the Boltzmann equation together with the Poisson equation is solved self-consistently for a spatially inhomogeneous electron gas in the relaxation time approximation.

2.1 Introduction

In general, the solution of the Boltzmann equation requires numerical methods. One possibility, which has been applied to the study of the Boltzmann kinetics for electron systems in semiconductors, is the direct numerical integration [85, 317, 329]. Several examples of such direct numerical integrations will be discussed in Part IV of this book as limiting cases of the treatment of the more general quantum kinetics, and we postpone the further discussion of this method up to that point.

If one studies only the relaxation of a small deviation from an equilibrium distribution, one can linearize the Boltzmann equation as discussed in Chap. 1. Powerful mathematical solution methods are available for linear integral equations. We will illustrate the use of the eigenfunction expansion by treating the relaxation kinetics due to Coulomb collisions in a dense electron gas in a quasi-two-dimensional quantum well structure in Sect. 2.2. If one can make, in addition to the linearization, an expansion in the small momentum change in the collision, the Boltzmann integral equation can be approximated by the Fokker–Planck equation [241, 295] which is a second-order differential equation and describes the relaxation in terms of a drift and a diffusion of the distribution in momentum space. The Fokker–Planck approximation is particularly useful for electron–phonon scattering, while the additional momentum and energy conservation laws of the Coulomb scattering lead to a more complicated integro-differential equation [144].

Finally, the collision kinetics can be simulated by stochastic methods, called Monte Carlo simulation [42]. Many simulations make use of the semiclassical concept of the population of small phase space volume elements $\Delta^3 x \Delta^3 p$ [109,126,168,169,188,213,277,334]. These methods allow one to treat very naturally spatially inhomogeneous systems and they are very important in the simulation of actual semiconductor devices. Due to the semiclassical nature of the method, the treatment of degenerate electron gases is less accurate. In this respect the ensemble Monte Carlo simulations for homogeneous systems in $\boldsymbol{k}$-space [102] are more accurate because they simulate the underlying Master equation rather than the Boltzmann equation. For spatially homogeneous systems, one studies directly the stochastic time development of the occupation of momentum states, and obtains Boltzmann distribution probabilities from averaging over many microscopic realizations. The algorithm for the ensemble Monte Carlo simulation can be derived rather explicitly from the corresponding Master equation, and we will describe this method in Sect. 2.3, and demonstrate its use again in Sect. 2.4 in the case of Coulomb relaxation kinetics of a dense electron gas in a semiconductor quantum well structure.

2.2 Linearized Coulomb Boltzmann Kinetics of a 2D Electron Gas

The Boltzmann relaxation kinetics of an electron gas in semiconductors can be studied experimentally by time-resolved pump and probe spectroscopy. Therefore we will illustrate the eigenfunction expansion technique for the example of an electron gas in a quantum well structure following [102]. We assume that the quantum well is so narrow, that we can consider only the two-dimensional motion of the electrons in the lowest subband [31, 146]. The 2D electron momentum is $\boldsymbol{p} = \hbar \boldsymbol{k}$, where $\boldsymbol{k}$ is the wavevector, the effective electron mass is m. The field lines of the Coulomb forces also enter the barrier material which often has very similar dielectric properties as the well material. Therefore, the Coulomb potential retains its three-dimensional $1/r$ form in these mesoscopic microstructures in real space. Its 2D Fourier transform is [146]

$$V_q = \frac{2\pi e^2}{\varepsilon_0 L^2 q} , \tag{2.1}$$

where q is the wavenumber, L^2 the 2D volume, and ε_0 is the background dielectric constant. In Coulomb systems the bare Coulomb potential in the collision integral has to be replaced by its screened counterpart [191, 380]. In the simplest approximation the statically screened 2D Coulomb potential $V_{s,q}$ is [146]

$$V_{s,q} = \frac{2\pi e^2}{\varepsilon_0 L^2 (q + \kappa)} , \tag{2.2}$$

where κ is the screening wavenumber [102],

$$\kappa = \frac{2mL^2}{\hbar^2} e^2 f_{k=0} \ . \tag{2.3}$$

Because, in general, the distribution of the lowest k-state changes in time during the relaxation process, the screening wavenumber will depend parametrically on the time. However, in the linearized Boltzmann equation this time dependence does not contribute because $f_0(t) \to f_0^0$.

In the following only isotropic distributions $f_k(t)$ will be considered, thus only the eigenfunctions with angular momentum $l = 0$ are needed. With this restriction only the particle number and the energy remain as collision invariants with eigenvalues $\lambda = 0$. For isotropic deviations an angular integration allows us to write the action of the collision operator (1.26) as that of a matrix with continuous wavenumber indices k:

$$\mathcal{L}\phi_k = \sum_{k'} \mathcal{L}_{k,k'} \phi_{k'} , \tag{2.4}$$

where the integral kernel follows from (1.3), (1.26), and (1.28) as

$$\begin{aligned} \mathcal{L}_{k,k'} = \frac{me^4}{\pi\hbar^3\varepsilon_0^2} \int \mathrm{d}^2p \int \mathrm{d}^2q \frac{\delta[(\boldsymbol{p}-\boldsymbol{k})\cdot\boldsymbol{q}-q^2]}{(q+\kappa)^2} \frac{f_p^0(1-f_{|\boldsymbol{k}+\boldsymbol{q}|}^0)(1-f_{|\boldsymbol{p}-\boldsymbol{q}|}^0)}{(1-f_k^0)} \\ \times \left[\delta(k'-k) + \delta(k'-p) - \delta(k'-|\boldsymbol{k}+\boldsymbol{q}|) - \delta(k'-|\boldsymbol{p}-\boldsymbol{q}|)\right] \ . \end{aligned} \tag{2.5}$$

Here the exchange term of (1.3) has been disregarded for simplicity. In order to determine the eigenfunctions numerically, the integral has to be approximated by a discrete sum on an equidistant grid $k_i = i\varDelta k$ with $i = 0, 1, \ldots, N$. Thus a cutoff wavenumber $k_N > k_\mathrm{F}$ is introduced, which certainly has to be larger than the Fermi wavenumber, defined as $\hbar^2 k_\mathrm{F}^2/2m = \mu$. The diagonal elements of the collision operator are usually called the collision frequencies ν_k. A further simplification of the calculation can be achieved by symmetrizing $\mathcal{L}$ via a similarity transformation,

$$\tilde{\mathcal{L}} = g^{-1}\mathcal{L}g \ , \quad \tilde{\phi} = g^{-1}\phi \text{ with } \tilde{\mathcal{L}}\tilde{\phi}_\lambda = \lambda\tilde{\phi}_\lambda \ , \tag{2.6}$$

where g is a diagonal matrix with the elements

$$g_{k,k'} = \delta_{k,k'} \frac{1}{\sqrt{k f_k^0 (1-f_k^0)}} \ . \tag{2.7}$$

As a first step, the matrix elements $\mathcal{L}_{k,k'}$ are computed for $k, k' \leq k_\mathrm{N}$. Next the eigenfunctions and eigenvalues λ of the symmetric matrix $\tilde{\mathcal{L}}$ are evaluated. The eigenfunctions are finally transformed back by multiplication with the matrix g to get the desired eigenfunctions ϕ_λ. The step width for all calculations is taken to be $\Delta k = k_\mathrm{F}/50$. A further reduction of the step width does not change the results essentially. The dependence of the results on the cutoff wavenumber k_N will be discussed below.

The collision frequency ν_k is sometimes used [249] to get an estimate for the relaxation times due to inelastic carrier–carrier scattering. In Fig. 2.1 the collision frequency ν_k is shown for four different carrier densities. The material parameters are those of the conduction band of GaAs, i.e., $m = 0.0665 m_0$ and $\varepsilon_0 = 13.71$. The collision frequency decreases with increasing density. This effect is caused by the Pauli-blocking of the final scattering states and the enhanced screening of the Coulomb potential. For increasing degeneracy a pronounced dip appears in the vicinity of the Fermi energy. This dip can be understood, if one recalls that ν_k is the sum of the equilibrium scattering rates in and out of the state with energy ε_k. These rates are related by detailed balance, i.e.,

$$\nu_k = \Gamma_k^{\text{in}} + \Gamma_k^{\text{out}}; \quad \Gamma_k^{\text{out}} = \frac{1 - f_k^0}{f_k^0} \Gamma_k^{\text{in}} . \tag{2.8}$$

At low temperatures these rates around k_{F} are very small. Consider, e.g., a state k, above but close to k_{F}; its rate out is small because of the small number of empty final states between k and k_F. For $k \to \infty$ the collision frequency tends to 0. Generally one finds a dense spectrum of eigenvalues λ_n, $n = 1, 2, \ldots, N$, therefore we define a density of eigenstates

$$\varrho(\lambda_n) = \frac{2\Delta k}{\lambda_{n+1} - \lambda_{n-1}} , \tag{2.9}$$

which becomes independent of the step width for small Δk. The density of eigenstates $\varrho(\lambda_n)$ is shown in Fig. 2.2 as a function of λ for two carrier densities

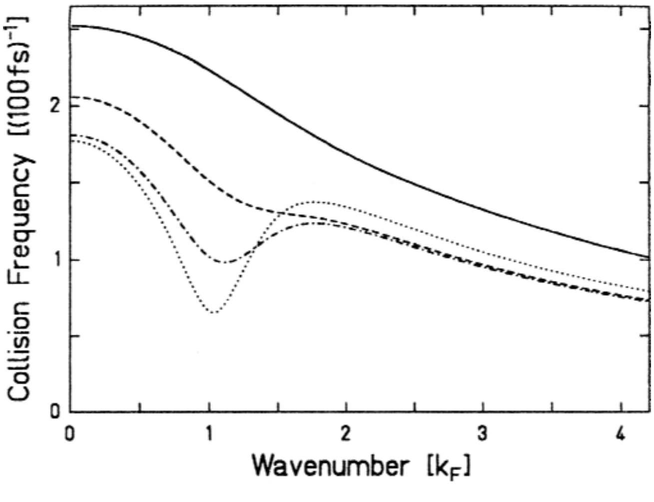

Fig. 2.1. Collision frequency ν_k vs. k/k_{F} for various 2D plasma densities in units of $10^{12}\,\text{cm}^{-2}$: (*Full line*) $n = 0.64$; (*dashed line*) $n = 1.28$; (*dashed-dotted line*) $n = 2.56$; (*dotted line*) $n = 5.12$ according to [102]