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Quantum Kinetic Theory

Second Edition

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Originally published by B.G. Teubner, Leipzig, 1998

ISBN 978-3-319-24119-7 ISBN 978-3-319-24121-0 (eBook)
DOI 10.1007/978-3-319-24121-0

Library of Congress Control Number: 2015950456

Springer Cham Heidelberg New York Dordrecht London

Printed on acid-free paper

Springer International Publishing AG Switzerland is part of Springer Science+Business Media (www.springer.com)

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Preface to the Second Edition

Quite quickly after its publication, this book was unavailable calling for a second edition. However, with my move to Christian-Albrechts-Universität Kiel in 2003 there was no time to tackle this task. The good thing about this time gap is that a critical and a less-biased look at the field and its coverage in the book became possible. It is satisfactory to realize that the (very enthusiastic) perspectives for the subject of field–matter interaction and nonequilibrium many-body theory expressed in the first edition turned out to be completely justified. Certainly, some of the fields that were in the focus before, such as semiconductor optics or laser–plasma interaction, have reached some maturity. At the same time, new fields that are facing very similar problems have undergone a rapid development that is driven by the amazing progress in attosecond laser technology [1, 2]. This includes the fields of attosecond atomic and molecular physics and the dynamics of ultracold atoms in traps and optical lattices, to name just two.

The challenges for many-body physics in general and short-time approaches, in particular, have not faded. The opposite is true: The need for a time-dependent description of correlated quantum systes has grown steadily. Fortunately, the rapid growth in computational resources, combined with brilliant young scientists including K. Balzer, N.E. Dahlen, M. Garny, S. Hermanns, F. Jahnke, R. van Leeuwen, G. Stefanucci, C. Verdozzi, and many others entering the field, has allowed for an unexpected burst of activity in computational studies of ultrafast quantum dynamics. In fact, non-Markovian quantum kinetic equations and, even more, nonequilibrium Green's functions have now become not just nice theoretical concepts but standard practical tools in many fields.[1] Some of the progress can be seen in recent text books by Kremp et al. [8], Rammer [9], Stefanucci et al. [10], and Balzer et al. [11]. Some overview on the numerical activity can be found in [12].

[1]The developments in nonequilibrium Green's functions are also reflected in the proceedings of the conferences "Progress in Nonequilibrium Green Functions" that have been taking place since 1999 [3–7].

In this active environment this book still seems to have its place. The central topics—the methods of nonequilibrium density operators and nonequilibrium Green's functions—have not lost their importance. An analysis of the connections of both has become even more important. This issue is now presented in more detail. Also, to improve the understandability, introductory discussions have been extended, in particular, in Chaps. 1, 6 and 13. In this spirit, a new chapter "Properties of the quantum kinetic equation" has been included. Obviously, many other approaches to the nonequilibrium quantum dynamics have appeared or grown to importance since the first edition was published. This includes density matrix renormalization group approaches, time-dependent density functional theory or wavefunction-based approaches of quantum chemistry. Here only brief comments have been found appropriate, together with references to the dedicated literature.

Over the last 15 years, this book has been used actively in my lectures in Rostock and Kiel on short-time physics and quantum statistical theory. This practical test has led not only to the correction of errors but also to many improvements, such as the inclusion of more and better examples. Some technical details and derivations have been taken out of the main text and moved to new problems and solutions section. I thank Karsten Balzer, Alfred Leitenstorfer, Hauke Thomsen, and Torben Ott for providing figures. I am grateful to many students and colleagues, in particular to Karsten Balzer, Sebastian Bauch, Tobias Dornheim, Jim Dufty, Alexei Filinov, Frank Graziani, Simon Groth, Sebastian Hermanns, Christopher Hinz, David Hochstuhl, Frank Jahnke, Hanno Kählert, Nai-Hang Kwong, Denis Lacroix, Patrick Ludwig, Torben Ott, Hartmut Ruhl, Niclas Schlünzen, Tim Schoof, Dirk Semkat, Gianlucca Stefanucci, Robert van Leeuwen, Claudio Verdozzi, and Jan Vorberger for valuable feedback. Finally, I thank Hauke Thomsen for assistence with editing the final version.

Kiel Michael Bonitz

Preface to the First Edition

We are at the beginning of a new revolution in science and technology, which is fueled by the tremendous progress in short-pulse laser technology over the last 10–15 years. Fundamental physical principles which have been known before only from abstract theory, are suddenly becoming accessible to direct experimental observation. This includes the quantum states of single atoms, Heisenberg's uncertainty principle, low temperature phenomena such as Bose condensation and Wigner crystallization, as well as ultraintense electromagnetic fields, and the possibility to create, in small university facilities, relativistic electrons or hot dense plasmas which eventually will lead to thermonuclear fusion. In the view of technological applications promised by these developments, many countries have established special research projects, including, the National Ignition Facility in the U.S. or the new Schwerpunkt "Laserfelder" of the Deutsche Forschungsgemeinschaft in Germany.

These developments are a major challenge for Theoretical Physics—to understand and predict the interaction of matter with electromagnetic fields ranging from milliwatt to petawatt ($10^{-3}-10^{15}$ W) powers and lasting from seconds to femtoseconds (10^{-15} s). Within this very complex frame, the current monograph is devoted to *quantum many-particle systems* under *extreme nonequilibrium* conditions. It attempts to answer the question how these systems behave immediately after and also during their creation, thereby focusing on a general approach.

The statistical description of many-particle systems in nonequilibrium began with L. Boltzmann's famous kinetic equation [13]. Since then, numerous theoretical methods have been developed to describe nonequilibrium processes in various fields, including fluids, dense plasmas, solids, and nuclear matter, which are often very efficient but, at the same time, so specialized that they are understood only by a few immediate specialists. And this, despite the fact that the underlying physics is often very similar if it is uncovered from the shell of (certainly needed) field-specific jargon and notation as well as system-inherent details and parameters. Moreover, many of these specialized theories have common roots, and a return to them, from time to time, can be extremely fruitful, even for an experienced

specialist, and lead to new ideas. On the other hand, for students or researchers new in the field, the best choice is to start from the roots.

This is particularly true for the problems related to ultrafast relaxation. Here exist three main branches of the theory: the two *statistical methods* based on density operators and nonequilibrium Green's functions, respectively, and the *mechanical approach* of molecular dynamics. All three of them are discussed and compared in this book. The simplest and the most intuitive one is the *density operator theory* which, for this reason, is chosen as the basic concept. A very general and comprehensive introduction to this approach is given in Chaps. 2 and 3. First, applications to many-particle effects are given in Chaps. 4–6, to collective phenomena (plasmons and instabilities) and to correlations. Students with *basic knowledge in quantum mechanics and statistical physics* will have no problems in following this treatment.[2]

More advanced applications follow in Chaps. 7–11. It is demonstrated that the density operator approach is very efficient in deriving generalized non-Markovian *quantum kinetic equations* with *memory* and *initial correlations*, and that it further allows to incorporate self-energy, dynamical screening, strong coupling effects, as well as the interaction with electromagnetic fields.

An introduction to the method of *nonequilibrium Green's functions* is given in Chap. 12, starting from a fully relativistic formulation. Here, the main results are coupled *Kadanoff–Baym equations for carriers and photons* for which various approximations are considered, including the nonrelativistic limit and the extension to multi-band systems. Moreover, *recent numerical results* are presented which will be of interest also for experienced readers. Finally, Chap. 13 is devoted to the *molecular dynamics* approach, where the modern developments in the field quantum MD are also discussed. Furthermore, a detailed comparison of the concepts of quantum statistics and molecular dynamics is performed, and the idea of numerical comparisons of the two is developed.

For illustration of the theoretical methods, a variety of recent numerical results on quantum kinetic equations, non-Markovian effects, and correlation phenomena have been included. *Numerical analysis* is an important part of modern kinetic theory. Therefore, throughout this book, the theoretical results are cast in a form best suitable for numerical evaluation. Furthermore, to enable the reader to do numerical work by himself, an extensive introduction to the concepts of numerical solution of quantum kinetic equations is supplied in Appendix F.

Thus, I hope the reader will *gain broad fundamental knowledge* in quantum kinetic theory in general, and on the theoretical description of ultrafast relaxation in particular, which should allow him to creatively adapt these concepts to any field of many-particle physics.

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[2]Sections which are not necessary for the understanding of the basic concepts and which may be skipped on the first reading are marked with an asterisk. Readers interested in derivations and details beyond the basic material can find the main ideas outlined in footnotes and appendices. Extensive references are provided to the specialized literature of various fields and to classical works as well.

Physics would not even be half as exciting and rewarding without continuous discussions and sharing of ideas with colleagues—so I am grateful to Martin Axt, Lazi Banyai, Karim ElSayed, Hartmut Haug, Klaus Henneberger, Frank Jahnke, Tilman Kuhn, Günter Manzke, Klaus Morawetz, Ronald Redmer, Hartmut Ruhl, Wilfried Schäfer, Chris Stanton, Heinrich Stolz, and Günter Zwicknagel. I very much enjoyed working together with Rolf Binder, Thomas Bornath, Jim Dufty, Andreas Förster, Dirk Gericke, Yuri L'vovich Klimontovich, Stephan Koch, Sigurd Köhler, Sylvio Kosse, Wolf Kraeft, Dietrich Kremp, Nai Kwong, Thomas Ohde, Manfred Schlanges, Don Scott, and Dirk Semkat. It is my great pleasure to thank my remarkable teachers Yuri L'vovich Klimontovich, Dietrich Kremp, and Stephan Koch, who guided me through various fields of physics and life, and Werner Ebeling and Wilfried Schäfer for continuous encouragement of my work.

The results which are the basis for this book would not have been possible without the generous support from the Deutscher Akademischer Austauschdienst, grants from the Deutsche Forschungsgemeinschaft and grants for CPU–time at the HLRZ Jülich and the CCIT of the University of Arizona. This book greatly benefited from comments of Nai Kwong and Dirk Semkat who also assisted me in preparing several figures for Chap. 12, as did Renate Nareyka and my wife.

Finally, I thank my father for raising my interest in physics, Christine for her tremendous patience and encouragement, and Sebastian and Martin for their willingness to give up our PC for this book.

Rostock
June 1998

Michael Bonitz

Symbols

$\mathcal{E}$	Electric field
$\epsilon^{\pm}$	Retarded/advanced dielectric function (4.21)
$\epsilon_{\alpha\beta}$	Dielectric tensor (4.36)
$f_{1\ldots s}$	s-particle Wigner distribution (2.53)
$F_{1\ldots s}$	Reduced s-particle density operator (2.13)
$F_a^{\gtrless}$	One-particle/hole operator (3.19)
$g_{1\ldots s}$	s-particle correlation operator (2.92)
$H_{1\ldots s}$	s-particle Hamilton operator (2.3)
H_i	One-particle Hamilton operator of particle i (2.4)
$\bar{H}_i$	Effective one-particle Hamiltonian (contains U^{H}) (2.94)
H_i^{HF}	Hartree–Fock potential (3.10)
$\langle H \rangle$	Total energy (2.42)
$\Lambda^{\pm}_{1\ldots s}$	s-particle (anti-)symmetrization operator (3.7)
μ	Chemical potential
n	Number density
$\Omega^{\pm}$	Retarded/advanced Møller operator (9.30)
PDF	Pair distribution function Fig. 1.1
$P_{1\ldots s}$	s-particle permutation operator Chap. 3
$\Pi^{\pm}, \Pi^{R/A}$	Retarded/advanced polarization function (4.18)
$\rho_{1\ldots N}$	N-particle density operator (2.8)
$\Sigma_i^{\pm}$	Retarded/advanced one-particle self-energy (7.80)
$T^{\pm}$	Retarded/advanced T-operator (9.33)
$\langle T \rangle$	Mean kinetic energy (2.32)
$\mathcal{U}_i$	External potential acting on particle i (2.4)
$U^{\pm}$	Retarded/advanced propagator Appendix D
$U^{0\pm}$	Retarded/advanced quasi-particle propagator Appendix D
U_i^{H}	Hartree field (2.97)

$\mathcal{V}$	System volume
V_{ij}	Binary interaction potential (2.5)
$V_{ij}^{\pm}$	Potential with exchange contribution (3.10)
$\langle V \rangle$	Mean potential energy (2.33)

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