NONEQUILIBRIUM MANY-BODY THEORY OF QUANTUM SYSTEMS

The Green's function method is among the most powerful and versatile formalisms in physics, and its nonequilibrium version has proved invaluable in many research fields. With entirely new chapters and updated example problems, the second edition of this popular text continues to provide an ideal introduction to nonequilibrium many-body quantum systems and ultrafast phenomena in modern science. Retaining the unique and self-contained style of the original, this new edition has been thoroughly revised to address interacting systems of fermions and bosons, simplified many-body approaches like the GKBA, the Bloch equations, and the Boltzmann equations, and the connection between Green's functions and newly developed time-resolved spectroscopy techniques. Small gaps in the theory have been filled, and frequently overlooked subtleties have been systematically highlighted and clarified. With an abundance of illustrative examples, insightful discussions, and modern applications, this book remains the definitive guide for students and researchers alike.

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NONEQUILIBRIUM MANY-BODY THEORY OF QUANTUM SYSTEMS

A Modern Introduction

Second Edition

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To my wife Marina
GS

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Preface to the Second Edition

During the past decade, research in physics has considerably drifted toward the nonequilibrium properties of quantum matter. Many different time-resolved spectroscopy techniques (angle-resolved photoemission, streaking, fragmentation chronoscopy, absorption, reflectivity, transport, etc.) have been developed and further refined. It is today possible to "film" the motion of electrons and nuclei with high temporal resolution (about one-billionth of one-millionth of a second) and to investigate a large variety of ultrafast quantum phenomena. The nonequilibrium Green's function formalism remains the most versatile theoretical technique to address the new emerging physics. We therefore felt it necessary to integrate the material of the first edition with a textbook introduction on the connection between Green's functions and the outcomes of the newly developed time-resolved spectroscopy techniques.

We have taken the opportunity of writing this second edition to improve the presentation of the existing material. We have optimized the presentation by rearranging some of the topics and by grouping related topics together. An example is the new chapter on the electron gas, which combines sections that were previously scattered throughout different chapters.

The first edition also lacked a fundamental topic, namely the Green's function treatment of multi-component systems, such as electrons and photons or electrons and phonons. The second edition contains an entirely new chapter entitled "Green's Functions for Nonequilibrium Fermion–Boson Systems" devoted to this topic. Here we also provide a pedagogical introduction to the recently developed ab initio theory of electrons and phonons. Finally, we have included one additional chapter entitled "From Green's Functions to Simplified Many-Body Approaches," where we discuss popular approaches like the Generalized Kadanoff–Baym Ansatz, the semiconductor Bloch equations, the Boltzmann equations, the Redfield equation, and the Lindblad equation. Starting from the nonequilibrium Green's function formalism, we derive all these approaches step by step, highlighting the underlying approximations and limitations.

This second edition maintains the same pedagogical style as the first edition. The book remains a self-contained and self-learning book for masters and PhD students and a textbook for undergraduate courses. As in the first edition, *there is not a single result which is not derived.*

Lastly but not least importantly, we want to express our gratitude to our students over the past 10 years, particularly Simone Latini, Fabio Covito, Francesco Fantini, Simone Manti, Paolo Gazzaneo, Silvia Bianchi, Tommaso Mazzocchi, Kai Wu, Zhenlin Zhang, and Alessandro Moreci, for their valuable suggestions and observations. Their input has greatly contributed to refining the presentation of various topics year after year. Any errors that may remain are solely the responsibility of the authors.

Preface to the First Edition

This textbook contains a pedagogical introduction to the theory of Green's functions *in* and *out* of equilibrium, and is accessible to students with a standard background in basic quantum mechanics and complex analysis. Two main motivations prompted us to write a monograph for beginners on this topic.

The first motivation is research-oriented. With the advent of nanoscale physics and ultrafast lasers it became possible to probe the correlation between particles in excited quantum states. New fields of research (e.g., molecular transport, nanoelectronics, Josephson nanojunctions, attosecond physics, nonequilibrium phase transitions, ultracold atomic gases in optical traps, optimal control theory, kinetics of Bose condensates, quantum computation) added up to the already existing fields in mesoscopic physics and nuclear physics. The Green's function method is probably one of the most powerful and versatile formalisms in physics, and its nonequilibrium version has already proven to be extremely useful in several of the aforementioned contexts. Extending the method to deal with the new emerging nonequilibrium phenomena holds promise to facilitate and quicken our comprehension of the excited state properties of matter. At present, unfortunately, to learn the nonequilibrium Green's function formalism requires more effort than learning the equilibrium (zero-temperature or Matsubara) formalism, despite the fact that *nonequilibrium Green's functions are not more difficult*. This brings us to the second motivation.

The second motivation is educational in nature. As students we had to learn the method of Green's functions at zero temperature, with the normal-orderings and contractions of Wick's theorem, the adiabatic switching-on of the interaction, the Gell–Mann–Low theorem, the Feynman diagrams, etc. Then we had to learn the finite-temperature or Matsubara formalism where there is no need of normal-orderings to prove Wick's theorem, and where it is possible to prove a diagrammatic expansion without the adiabatic switching-on and the Gell–Mann–Low theorem. The Matsubara formalism is often taught as a disconnected topic but the diagrammatic expansion is exactly the same as that of the zero-temperature formalism. Why do the two formalisms look the same? Why do we need more "assumptions" in the zero-temperature formalism? And isn't it enough to study the finite-temperature formalism? After all, zero-temperature is just one possible temperature. When we became postdocs we bumped into yet another version of Green's functions, the nonequilibrium Green's functions or the so-called Keldysh formalism. And again another different way to prove Wick's theorem and the diagrammatic expansion. Furthermore, while several excellent textbooks on the equilibrium formalisms are available, here the learning process is considerably slowed down by the absence of introductory textbooks. There exist a few review articles on the

Keldysh formalism, but they are scattered over the years and the journals. Students have to face different jargon and different notation, dig out original papers (not all downloadable from the web), and have to find the answer to lots of typical newcomer questions: Why is the diagrammatic expansion of the Keldysh formalism again the same as that of the zero-temperature and Matsubara formalisms? How do we see that the Keldysh formalism reduces to the zero-temperature formalism in equilibrium? How to introduce the temperature in the Keldysh formalism? It is easy to imagine the frustration of many students during their early days of study of nonequilibrium Green's functions. In this book we will introduce only *one* formalism, which we can call the *contour formalism*, and we will do it using a very pedagogical style. The contour formalism is not more difficult than the zero-temperature, Matsubara or Keldysh formalisms and we will explicitly show how it reduces to those under special conditions. Furthermore, the contour formalism provides a natural answer to all previous questions. Thus, the message is: *There is no need to learn the same thing three times*.

Starting from basic quantum mechanics, we introduce the contour Green's function formalism step by step. The physical content of the Green's function is discussed with particular attention to the time-dependent aspect and applied to different physical systems ranging from molecules and nanostructures to metals and insulators. With this powerful tool at our disposal we then go through the Feynman diagrams, the theory of conserving approximations, the Kadanoff–Baym equations, the Luttinger–Ward variational functionals, the Bethe–Salpeter equation, and the Hedin equations.

This book is not a collection of chapters on different applications, but a self-contained introduction to mathematical and physical concepts of general use. We made a serious effort in organizing apparently disconnected topics in a *logical* instead of *chronological* way, and in filling up many small gaps. The adjective "modern" in the title refers to the presentation more than to specific applications. The overall goal of the present book is to derive a set of kinetic equations governing the quantum dynamics of many identical particles and to develop perturbative as well as nonperturbative approximation schemes for their solution.

About 600 pages may seem too many for a textbook on Green's functions, so let us justify this voluminousness. First of all, *there is not a single result which is not derived*. This means that we inserted several intermediate steps to guide the reader through every calculation. Second, for every formal development or new mathematical quantity we present carefully selected examples which illustrate the physical content of what we are doing. Without examples and illustrations (more than 250 figures) this book would be half the size but the actual understanding would probably be much less. The large number of examples compensates for the moderate number of exercises. Third, in the effort of writing a comprehensive presentation of the various topics, we came across several small subtleties which, if not addressed and properly explained, could give rise to serious misunderstandings. We therefore added many remarks and clarifying discussions throughout the text.

The structure of the book is illustrated in Fig. 1 and can be roughly partitioned in three parts: mathematical tools, approximation schemes, and applications. For the detailed list of topics the reader can have a look at the table of contents. Of course, the choice of topics reflects our personal background and preferences. However, we feel reasonably confident to have covered all fundamental aspects of Green's function theory in and out of equilibrium. We tried to create a self-contained and self-study book capable of bringing

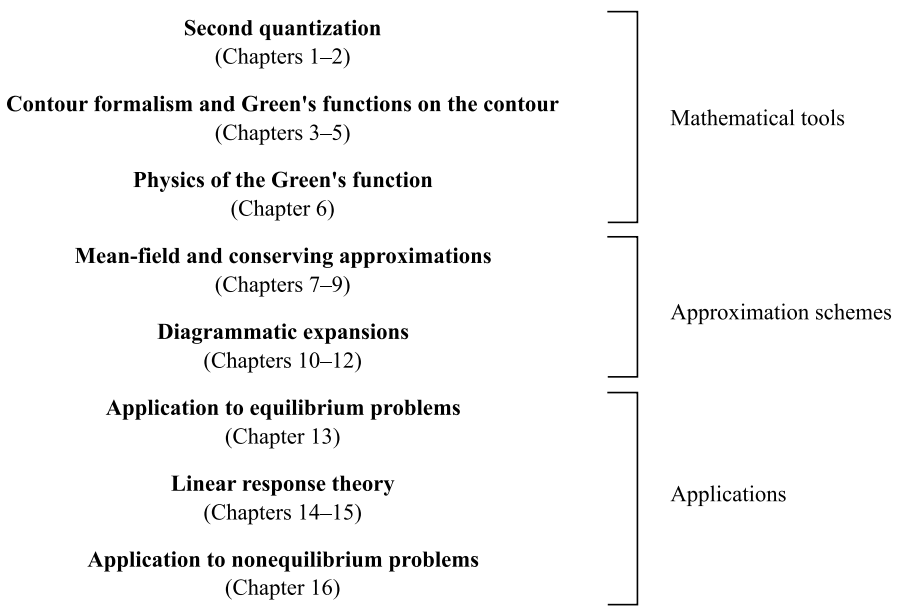

Figure 1 Structure of the book.

the undergraduate or PhD student to the level of approaching the modern literature and enabling him/her to model or solve new problems with physically justified approximations. If we are successful in this endeavor, it will be due to the enthusiastic and motivated students in Rome and Jyväskylä to whom we had the privilege to teach part of this book. We thank them for their feedback, from which we indeed benefited enormously.

Speaking of thanks: Our first and biggest thanks goes to Carl-Olof Almbladh and Ulf von Barth, who introduced us to the wonderful world of many-body perturbation theory and Green's function theory during our postdoc years in Lund. Only now that we were forced to deepen our understanding in order to explain these methods could we fully appreciate all their "of-course-I-don't-need-to-tell-you" or "you-probably-already-know" answers to our questions. We are also thankful to Evert Jan Baerends, Michele Cini, and Hardy Gross, from whom we learned a large part of what today is our background in physics and chemistry and with whom we undertook many exciting research projects. We wish to express our gratitude to our PhD students, postdocs, and local colleagues Klaas Giesbertz, Petri Myöhänen, Enrico Perfetto, Michael Ruggenthaler, Niko Säkkinen, Adrian Stan, Riku Tuovinen, and Anna-Maija Uimonen, for providing us with many valuable suggestions and for helping out in generating several figures. The research on the Kadanoff–Baym equations and their implementation which forms the last chapter of the book would not have been possible without the enthusiasm and the excellent numerical work of Nils Erik Dahlen. We are indebted to Heiko Appel, Karsten Balzer, Michael Bonitz, Raffaele Filosofi, Ari Harju, Maria Hellgren, Stefan Kurth, Matti Manninen, Kristian Thygesen, and Claudio Verdozzi, with whom we had many inspiring

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Abbreviations and Acronyms

ARPES	angle-resolved photoemission spectroscopy
a.u.	atomic units
BvK	Born–von Karman
GKBA	Generalized Kadanoff–Baym Ansatz
h.c.	Hermitian conjugate
HF	Hartree–Fock
HOMO	highest occupied molecular orbital
HSEX	Hartree plus screened exchange
KMS	Kubo–Martin–Schwinger
LUMO	lowest unoccupied molecular orbital
LW	Luttinger–Ward
MBPT	many-body perturbation theory
NEGF	nonequilibrium Green's function
PES	photoemission spectroscopy
ph	particle–hole
PPP	Pariser–Parr–Pople
QMC	Quantum Monte Carlo
RPA	Random Phase Approximation
Tph	T-matrix approximation in the particle–hole channel
Tpp	T-matrix approximation in the particle–particle channel
WBLA	Wide-Band Limit Approximation
XC	exchange-correlation

Fundamental Constants and Basic Relations

Fundamental Constants

Electron charge: $e = -1$ a.u. $= 1.60217646 \times 10^{-19}$ coulomb

Electron mass: $m_e = 1$ a.u. $= 9.10938188 \times 10^{-31}$ kg

Planck constant: $\hbar = 1$ a.u. $= 1.054571 \times 10^{-34}$ J s = 6.58211×10^{-16} eV s

Speed of light: $c = 137$ a.u. $= 3 \times 10^5$ km/s

Boltzmann constant: $K_{\rm B} = 8.3 \times 10^{-5}$ eV/K

Basic Quantities and Relations

Bohr radius: $a_{\rm B} = \frac{\hbar^2}{m_e e^2} = 1$ a.u. $= 0.5$ Å

Electron gas density: $n = \frac{(\hbar p_{\rm F})^3}{3\pi^2} =$ ($p_{\rm F}$ being the Fermi momentum)

Electron gas radius: $\frac{1}{n} = \frac{4\pi}{3}(a_{\rm B} r_s)^3$, $r_s = \frac{(9\pi/4)^{1/3}}{\hbar a_{\rm B} p_{\rm F}}$

Plasma frequency: $\omega_{\rm p} = \sqrt{\frac{4\pi e^2 n}{m_e}}$ (n being the electron gas density)

Rydberg $R = \frac{e^2}{2a_{\rm B}} = 0.5$ a.u. $\simeq 13.6$ eV

Bohr magneton $\mu_{\rm B} = \frac{e\hbar}{2m_e c} = 3.649 \times 10^{-3}$ a.u. $= 5.788 \times 10^{-5}$ eV/T

Room temperature ($T \sim 300$ K) energy: $K_B T \sim \frac{1}{40}$ eV

$\hbar c \sim 197$ MeV fm (1 fm = 10^{-15} m)

$m_e c^2 = 0.5447$ MeV