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978-0-521-76617-3 - Nonequilibrium Many-Body Theory of Quantum Systems: A Modern Introduction

Gianluca Stefanucci and Robert Van Leeuwen

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NONEQUILIBRIUM MANY-BODY THEORY OF QUANTUM SYSTEMS

The Green's function method is one of the most powerful and versatile formalisms in physics, and its nonequilibrium version has proved invaluable in many research fields. This book provides a unique, self-contained introduction to nonequilibrium many-body theory.

Starting with basic quantum mechanics, the authors introduce the equilibrium and nonequilibrium Green's function formalisms within a unified framework called the contour formalism. The physical content of the contour Green's functions and the diagrammatic expansions are explained with a focus on the time-dependent aspect. Every result is derived step-by-step, critically discussed and then applied to different physical systems, ranging from molecules and nanostructures to metals and insulators. With an abundance of illustrative examples, this accessible book is ideal for graduate students and researchers who are interested in excited state properties of matter and nonequilibrium physics.

GIANLUCA STEFANUCCI is a Researcher at the Physics Department of the University of Rome Tor Vergata, Italy. His current research interests are in quantum transport through nanostructures and nonequilibrium open systems.

ROBERT VAN LEEUWEN is Professor of Physics at the University of Jyväskylä in Finland. His main areas of research are time-dependent quantum systems, many-body theory, and quantum transport through nanostructures.

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A Modern Introduction

GIANLUCA STEFANUCCI

University of Rome Tor Vergata

ROBERT VAN LEEUWEN

University of Jyväskylä



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CAMBRIDGE UNIVERSITY PRESS

Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org

Information on this title: www.cambridge.org/9780521766173

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First published 2013

Printed and bound in the United Kingdom by the MPG Books Group

A catalog record for this publication is available from the British Library

ISBN 978-0-521-76617-3 Hardback

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Preface

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 like, 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, etc. added 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 post-docs we bumped into yet another version of Green's functions, the nonequilibrium Green's functions or the so called Keldysh formalism. And again this was 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 few review

articles on the Keldysh formalism and they are scattered over the years and the journals. Students have to face different jargons and different notations, dig out original papers (not all downloadable from the web), and have to find the answer to lots of typical newcomer questions like, e.g., 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 do we 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 introduce only *one* formalism, which we call the *contour formalism*, and we do it using a very pedagogical style. The contour formalism is not more difficult than the zero-temperature, Matsubara or Keldysh formalism and we 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. As such, we have preferred to refer to books, reviews and classical articles rather than to recent research papers whenever this was possible. We have made a serious effort in organizing apparently disconnected topics in a *logical* instead of *chronological* way, and in filling 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 have inserted several intermediate steps to guide the reader through every calculation. Secondly, for every formal development or new mathematical quantity we present carefully selected examples which illustrate the physical content of what we are doing. Sometimes the reader will find further supplementary discussion or explanations printed in smaller type; these can be skipped at a first reading. 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. Thirdly, 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 have 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 a detailed list of

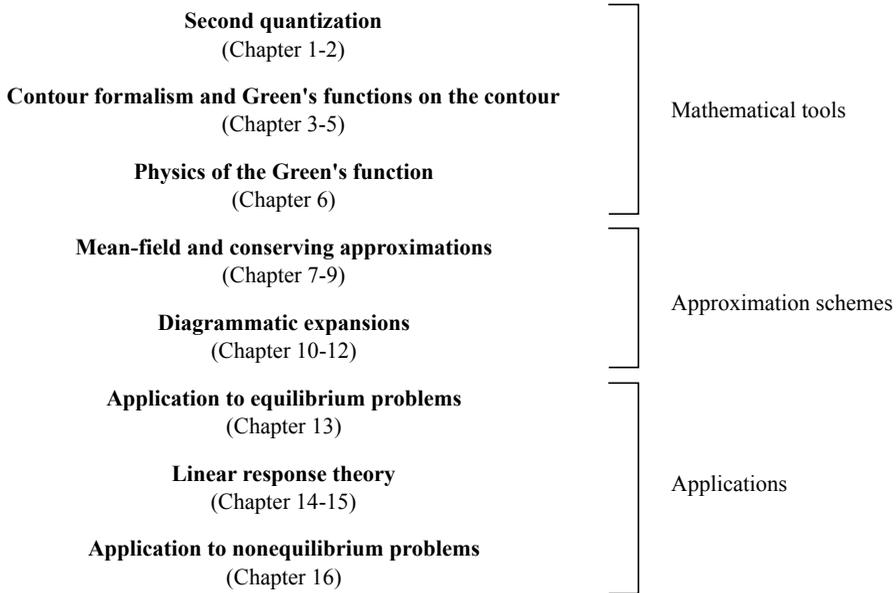


Figure 1 Structure of the book

topics the reader can 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 have tried to create a self-contained and self-study book capable of bringing the undergraduate or PhD student to the level of approaching 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 thank you goes to Carl-Olof Almladh and Ulf von Barth who introduced us to the wonderful world of many-body perturbation theory and Green's function theory during our post-doc years in Lund. Only now that we have been forced to deepen our understanding in order to explain these methods can 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, post-docs 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

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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 Filofofi, Ari Harju, Maria Hellgren, Stefan Kurth, Matti Manninen, Kristian Thygesen, and Claudio Verdozzi with whom we had many inspiring and insightful discussions which either directly or indirectly influenced part of the contents of the book. We further thank the Department of Physics and the Nanoscience Center of the University of Jyväskylä and the Department of Physics of the University of Rome Tor Vergata for creating a very pleasant and supportive environment for the writing of the book. Finally we would like to thank a large number of people, too numerous to mention, in the research community who have shaped our view on many scientific topics in and outside of many-body theory.

Abbreviations and acronyms

a.u. : atomic units

BvK : Born-von Karman

e.g. : exempli gratia

HOMO : highest occupied molecular orbital

i.e. : id est

KMS : Kubo–Martin–Schwinger

l.h.s. : left hand side

LUMO : lowest unoccupied molecular orbital

LW : Luttinger–Ward

MBPT : Many-body perturbation theory

PPP : Pariser–Parr–Pople

QMC : Quantum Monte Carlo

r.h.s. : right hand side

RPA : Random Phase Approximation

WBLA : Wide Band Limit Approximation

XC : Exchange-Correlation

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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. = 1.054571×10^{-34} Js = 6.58211×10^{-16} eVs

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

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

Basic quantities and relations

Bohr radius: $a_B = \frac{\hbar^2}{m_e e^2} = 1$ a.u. = 0.5 \AA

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

Electron gas radius: $\frac{1}{n} = \frac{4\pi}{3} (a_B r_s)^3$, $r_s = \frac{(9\pi/4)^{1/3}}{\hbar a_B p_F}$

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

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

Bohr magneton $\mu_B = \frac{e\hbar}{2m_e c} = 3.649 \times 10^{-3}$ a.u. = 5.788×10^{-5} eVT

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