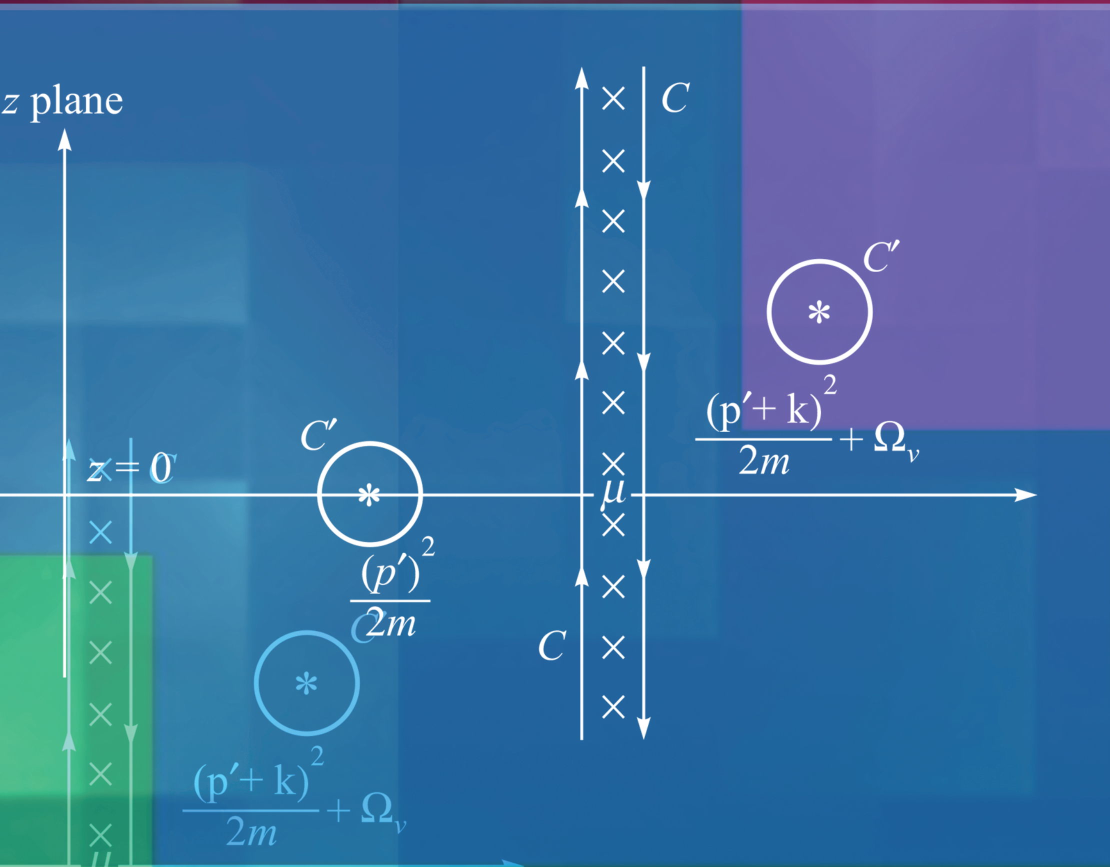
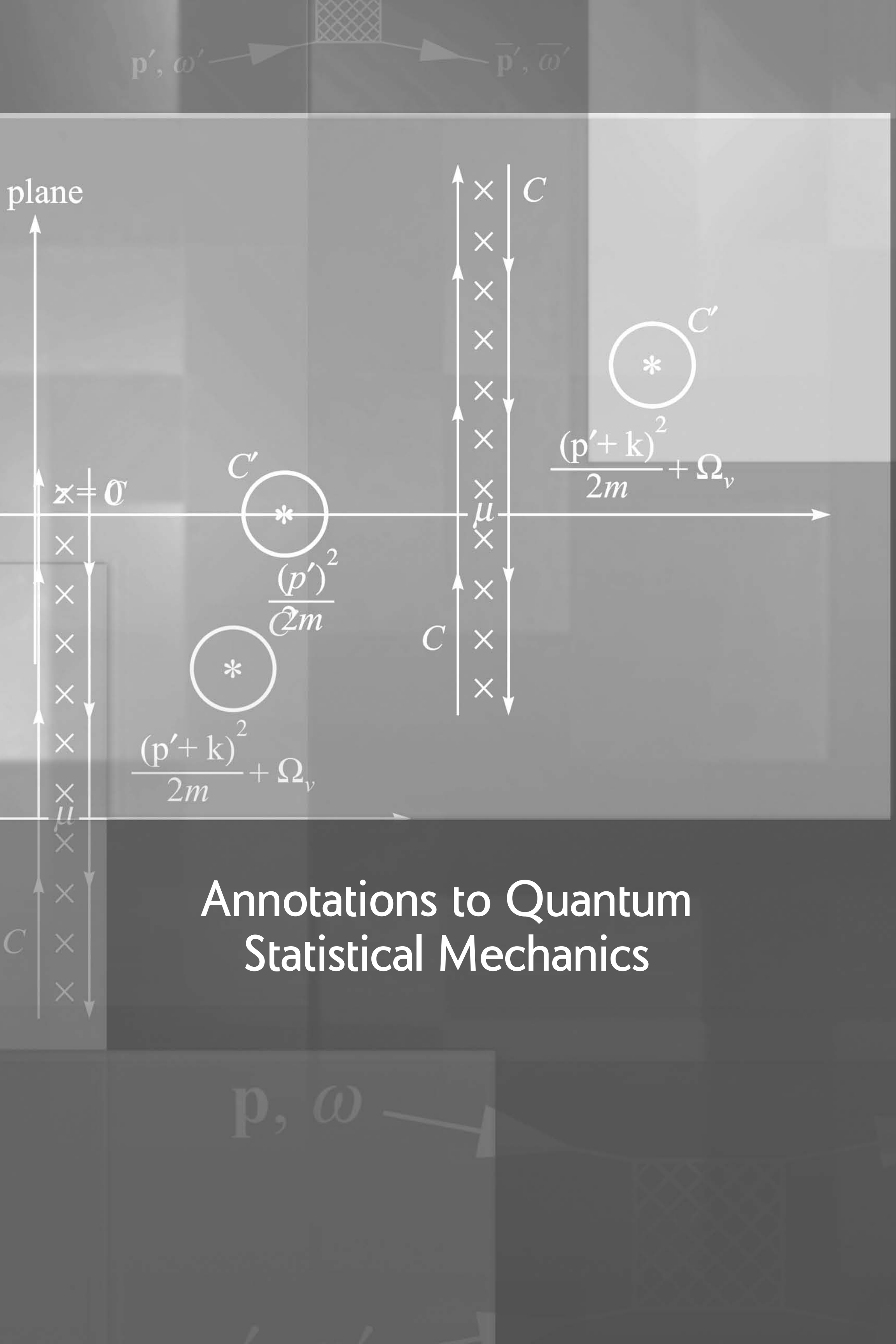


Annotations to Quantum Statistical Mechanics

In-Gee Kim



Annotations to Quantum Statistical Mechanics

Annotations to Quantum Statistical Mechanics

In-Gee Kim

Pan Stanford Publishing

Published by

Pan Stanford Publishing Pte. Ltd.
Penthouse Level, Suntec Tower 3
8 Temasek Boulevard
Singapore 038988

Email: editorial@panstanford.com
Web: www.panstanford.com

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

Annotations to Quantum Statistical Mechanics

ISBN 978-981-4774-15-4 (Hardback)
ISBN 978-1-315-19659-6 (eBook)

To my wife Gajean
and
my daughter Eugenie

Contents

Preface

Physicists around the world received the sad news of the demise of Professor Leo P. Kadanoff in October 2015. I had no personal interaction with him. I heard about him during my first statistical physics class when I was a college junior while I studied Kadanoff's block spin procedure that provides an insight into the renormalization group theory. Since my professional career has long been dedicated to investigating the electronic structure problems in solids, I usually studied the density functional theory, which is conventionally on top of the zero-temperature or the finite-temperature quantum many-body theory in equilibrium.

My first professional touch on the nonequilibrium statistical physics was during my post-doctoral experience at Northwestern University, Illinois, USA, in 2005, when I was struggling to develop a computer code, under the guidance of Miyoung Kim and Art Freeman, for calculating the Seebeck coefficients from the electronic structures of solids. The transport coefficients, such as electric conductivity, thermal conductivity, and thermoelectric power, are defined by the assumption that a system is in a near-equilibrium state, i.e., essentially in a nonequilibrium state close to equilibrium; this leads to a completely different physical formalism from the equilibrium physics with what I usually had dealt. At that time, I adapted a branch of Boltzmann equation, the so-called Bhatnagar–Gross–Krook (BGK) model in which the collision term is replaced by a simple parametric function of the distribution function. The BGK model has been known, erroneously in many textbooks for solid state physicists, as the Boltzmann equation. The code for the Seebeck coefficients based on the BGK model was written incompletely, so the remaining numerical problems were fixed by my friend Jung-Hwan Song, who unexpectedly passed away on June

15, 2011, and its first realistic application was done by Min Sik Park and Julia Medvedeva, who wrote the first draft of the manuscript for publishing in *Physical Review B* in 2010.

During my POSTECH period, I faced a bunch of problems on nonequilibrium statistical physics, but they are full of phenomenological and empirical treatments dedicated for metallurgical applications. I have had spent most of my efforts to build a research framework, the so-called multiscale simulation method, by organizing a research team consisting of Korean experts from the vast disciplines of electronic structure modeling, molecular dynamics modeling, phase field modeling, phase thermodynamics with databases, and dislocation dynamics modeling. Struggling to understand those theories, I realized that we need a rather smoothly unified theoretical framework derived from first principles. To this end, it is necessary to eliminate structural complications by arranging atoms to form crystals and solids. Such a system is nothing more than a very cold and dense plasma. In 2014, I decided to move to the New Mexico Consortium, Los Alamos, New Mexico, where I studied the two-component equilibrium quantum plasma physics, the classical and quantum kinetic theories for multicomponent systems, and the two-temperature molecular dynamics for calculating transport coefficients.

In the meantime, I carefully read Leo P. Kadanoff and Gordon Baym's book *Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems* (Benjamin, New York, 1962). Like many other classic books, especially *Frontiers in Physics: A Lecture Note and Reprint Series*, this book also explains nonequilibrium statistical physics in a systematic way. It contains essential concepts on statistical physics in terms of Green's functions with sufficient and rigorous details. However, as my friends agree with me, a lack of effort at the publisher's end reduced the readability of this book. The book was printed as a photocopy of the original manuscript, which was prepared with the help of a typewriter. In my humble opinion, a book prepared with careful typesetting helps a reader's brain to work smoothly because it does not have to work hard to interpolate text from bad printing. I have rewritten the text in the LaTeX2e format, fixed some typographical errors, corrected mistakes in equation numbers, drawn figures with modern computer programs, added my own footnotes to the text, and saved in my laptop. This rather tedious work was extremely helpful for me to understand the formalism of nonequilibrium quantum statistical mechanics.

During this rewriting and annotating, I felt the necessity to provide a short note on the second quantization chapter in front of the original text. Although there are no substantial paradigm shifts after the publication of the original text, the curricula of graduate schools have evolved since the 1960s. Graduate students of modern physics now learn relativistic quantum field theory and quantum many-body physics and have to work on their own research topics. It, therefore, becomes necessary for them to spend time on consistent study to make the knowledge of a topic concrete in their minds in addition to passing relevant examinations. My experience tells me that a systematically prepared summary is extremely useful for settling down the key knowledge of a subject.

I would like to appreciate Mr. Stanford Chong, Pan Stanford Publishing, for encouraging me to publish this rewritten text, which was prepared purely for personal purposes, in the form of a book, so that graduate students as well as senior researchers may benefit from these annotations on the classical text.

In-Gee Kim
Winter 2017

Preface of
Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems

These lectures are devoted to a discussion of the use of thermodynamic Green's functions in describing the properties of many-particle systems. These functions provide a method for discussing finite-temperature problems with no more conceptual difficulty than ground-state (e.g., zero-temperature) problems; the method is equally applicable to boson and fermion systems, equilibrium and nonequilibrium problems.

The first four chapters develop the equilibrium Green's function theory along the lines of the work of Martin and Schwinger. We use the grand-canonical ensemble of statistical mechanics to define thermodynamic Green's functions. These functions have a direct physical interpretation as particle propagates. The one-particle Green's function describes the motion of one particle added to the many-particle system; the two-particle Green's function describes the correlation motion of two added particles. Because they are propagators they contain much detailed dynamic information, and because they are expectation values in the grand-canonical ensemble they contain all statistical mechanical information. Several methods of obtaining the partition function from the Green's functions are discussed. We determine the one-particle Green's function from its equation of motion, supplemented by the boundary conditions appropriate to the grand-canonical ensemble. This equation of motion, which is essentially a matrix element of the second-quantized Schrödinger equation, gives the time derivative of the one-particle Green's function G in terms of the two-particle Green's function G_2. We physically motivate simple approximations, which express G_2 in terms of G, by making use of the propagator interpretation of the Green's functions.

Chapter 6 presents a formal method for generating Green's function approximations. This method is based on a consideration of the system in the presence of an external scalar potential. We also discuss here the relation between our equation of motion method and the more standard perturbative expansions.

Chapters 7, 8, and 9 outline a theory of nonequilibrium phenomena. We consider the deviations from equilibrium arising from the application of an external time- and space-dependent force field to the system. By making use of the results of Chapter 6 we show that every Green's function approximation for an equilibrium system can be generalized to describe nonequilibrium phenomena. In this way the Green's function equations of motion can be transformed into approximate quantum mechanical equations of transport. These are used, in Chapter 10, to derive generalizations of the Boltzmann equation. As examples of the nonequilibrium theory, we then discuss ordinary sound propagation and also the Landau theory of the low-temperature Fermi liquid.

Chapters 13 and 14 describe two approximations that have been extensively applied in the recent literature. A dynamically shielded potential is employed to discuss the properties of a Coulomb gas; the two-body scattering matrix approximation is developed for application to systems with short-range interactions.

An appendix and a list of references and supplementary reading are included at the end.

We should like to express our gratitude for the hospitality offered us at the Institutes for Theoretical Physics in Warsaw and Krakow, Poland, and Uppsala, Sweden, where these lectures were given in part. Special thanks are due Professor Niels Bohr of the Institute for Theoretical Physics in Copenhagen, where lectures were first delivered and finally written.

Leo P. Kadanoff
Gordon Baym
March 1962