Statistical Mechanics and the Physics of Many-Particle Model Systems

This page intentionally left blank

Statistical Mechanics and the Physics of Many-Particle Model Systems

Alexander Leonidovich Kuzemsky
Joint Institute for Nuclear Research, Russia

World Scientific
NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI • TOKYO

Published by

World Scientific Publishing Co. Pte. Ltd.
5 Toh Tuck Link, Singapore 596224
USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601
UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

Library of Congress Cataloging-in-Publication Data
Names: Kuzemskiĭ, A. L. (Aleksandr Leonidovich), author.
Title: Statistical mechanics and the physics of many-particle model systems /
by Alexander Leonidovich Kuzemsky (Joint Institute for Nuclear Research, Russia).
Description: Singapore ; Hackensack, NJ : World Scientific [2017] |
Includes bibliographical references and index.
Identifiers: LCCN 2016053884| ISBN 9789813145627 (hard cover ; alk. paper) |
ISBN 9813145625 (hard cover ; alk. paper) | ISBN 9789813145634 (pbk ; alk. paper) |
ISBN 9813145633 (pbk ; alk. paper)
Subjects: LCSH: Quantum statistics. | Statistical mechanics. | Many-body problem--
Approximation methods. | Quantum theory. | Solid state physics.
Classification: LCC QC174.4 .K84 2017 | DDC 530.13/3--dc23
LC record available at https://lccn.loc.gov/2016053884

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

Desk Editor: Ng Kah Fee

Typeset by Stallion Press
Email: enquiries@stallionpress.com

Printed in Singapore

Dedicated to the memory of my teachers
N. N. Bogoliubov and D. N. Zubarev

This page intentionally left blank

Preface

We may say that equilibrium statistical mechanics is mainly statistical, whereas the nonequilibrium statistical mechanics is mainly mechanical.
Radu Balescu

"Statistical Mechanics and the Physics of Many-Particle Model Systems" is devoted to the study of correlation effects in many-particle systems from a unified standpoint. The book is a self-contained and thorough treatment of the long-term researches that have been carried out in quantum-statistical mechanics since 1969 by author and some other researchers belonging to the N. N. Bogoliubov's school. The book includes description of the fundamental concepts and techniques of analysis, including recent developments. It also provides an overview that introduces main notions of the quantum many-particle physics with the emphasis on concepts and models. It treats various actual systems having big significance in condensed matter physics and quantum theory of magnetism. In addition, the book introduces basic concepts and analytical methods for weakly interacting systems, and then extends concepts and methods to strongly interacting systems. This book combines the features of textbook and research monograph and was written with intention as a *treatise*. Most of this material cannot be found in any other text. The book also contains an extensive bibliography.

The primary aim of this book is to provide a detailed account of a selected group of results and developments in statistical mechanics and quantum many-particle physics in the approach of the N. N. Bogoliubov's school. The emphasis is on concepts and models and methods which are used in quantum-statistical physics. The fundamental works of N. N. Bogoliubov on statistical mechanics, many-body theory and quantum field theory [1–4], on the theory of phase transitions, and on the general theory of interacting systems provided a new perspective in various fields of mathematics and physics. The purpose of this book is to present the development of some advanced methods of quantum statistical mechanics (equilibrium and nonequilibrium), and also to show their effectiveness in applications to problems of quantum solid-state theory, and especially to problems of quantum theory of magnetism. The backbone of the entire book is the notion of thermodynamic two-time (Bogoliubov–Tyablikov) Green functions [5, 6].

Hence, the present text reflects the various techniques and developments in statistical mechanics in the approach of the N. N. Bogoliubov's school, covering a variety of concepts and topics. The book is devoted to the investigation of a series of problems of the strongly correlated electronic systems such as Hubbard, Anderson, spin–fermion models, model of disordered alloys, etc. A microscopic approach is developed to determine the quasiparticles excitation spectra of highly correlated electronic systems. For this purpose, the Green functions method is generalized to describe the excitation energetics in a self-consistent way within the irreducible Green functions method. The scheme was verified for a variety of systems and models of condensed matter physics. Many topics presented here are usually not well covered in standard textbooks, therefore the aims of the present book were to provide foundations and highlights on a variety of aspects in these fields with emphasis on the thorough discussion of the self-consistent approximations for suitable models.

The book contains introductory pedagogical chapters 1–14 with a hope to make the presentation more coherent and self-contained. Many chapters also include varied additional information and discuss many complex research areas which are not often discussed in other places.

Thus, those chapters 1–14 are intended as a brief summary and short survey of the most important notions and concepts of quantum dynamics and statistical mechanics for the sake of a self-contained formulation. We tried to describe those concepts which have proven to be of value, and those notions which will be of use in clarifying subtle points.

The book is intended as a general course on the quantum many-body physics at graduate and postgraduate levels for all-purpose physicists. The text is based mainly on my numerous lectures which were given in about 50 Universities and Research Centers in nine countries. When preparing my lectures, I made numerous notes. It was designed to acquaint readers with key concepts and their applications, to stimulate their own researches and to give in their hands a powerful and workable technique for doing that. Those notes (extended and rewritten in a coherent way) constituted the basis of the present book.

Thus, this text provides conceptual, technical, and factual guidance on advanced topics of modern quantum solid-state theory and quantum-statistical physics. In addition, this book offers a unique and informative overview of various aspects of quantum many-particle physics and quantum theory of condensed matter physics. The main part of the text is centered around the application of methods of the quantum field theory to study of the many-particle model systems, including the Green functions technique. We attempted to present both basic and more advanced topics of quantum many-particle physics in a mathematically consistent way, focusing on its operational ability as well as on physical consistency of the considered models and methods.

It is necessary to stress that the path to understanding the foundations of the modern statistical mechanics and the development of efficient methods for computing different physical characteristics of many-particle systems was quite complex. The main postulates of the modern thermodynamics and statistical physics [7, 8] were formulated by J. P. Joule (1818–1889), R. Clausius (1822–1888), W. Thomson (1824–1907), J. C. Maxwell (1831–1879), L. Boltzmann (1844–1906), and, especially, by J. W. Gibbs (1839–1903). The foundational monograph by Gibbs "Elementary Principles in Statistical Mechanics Developed with Special Reference to the Rational Foundations of Thermodynamics" [9–11] remains one of the highest peaks of modern theoretical science. A significant contribution to the development of modern methods of equilibrium and nonequilibrium statistical mechanics was made by academician N. N. Bogoliubov (1909–1992) [1–4].

In the present book, selected short biographies of the key scientists are included at the end of some chapters to remind for readers (rather schematically) the significant persons who contributed innovative ideas and methods in the matter discussed.

It should be emphasized that specialists in theoretical physics, as well as experimentalists, must be able to find their way through theoretical problems of the modern physics of many-particle systems because of the following reasons. Firstly, the statistical mechanics is filled with concepts, which widen the physical horizon and general world outlook. Secondly, statistical mechanics and, especially, quantum statistical mechanics demonstrate remarkable efficiency and predictive ability achieved by constructing and applying fairly simple (and at times even crude) many-particle models. Quite surprisingly, these simplified models allow one to describe a wide diversity of real substances, materials, and the most nontrivial many-particle systems, such as quark-gluon plasma, the DNA molecule, and interstellar matter. In systems of many interacting particles, an important role is played by the so-called correlation effects [12], which determine specific features in the behavior of most diverse objects, from cosmic systems to atomic nuclei. This is especially true in the case of solid-state physics.

Indeed, the last few decades have witnessed an enormous development of condensed matter physics. A large number of data have accumulated and many experimental facts are known. Investigations of systems with strong inter-electron correlations, complicated character of quasiparticle states, and strong potential scattering are extremely important and topical problems of the modern theory of condensed matter. In addition, our time is marked by a rapid advancement in design and application of new materials, which not only find a wide range of applications in different areas of engineering, but they are also connected with the most fundamental problems in physics, physical chemistry, molecular biology, and other branches of science. The quantum cooperative effects, such as magnetism and superconductivity, frequently determine the unusual properties of these new materials. The same can also be said about other nontrivial quantum effects like, for instance, the quantum Hall effect, topological insulators, Bose–Einstein condensation, quantum tunneling, and others. The further development of our understanding of the new materials and complex substances and even some biological systems has depended, and still depend, on the development of more powerful experimental techniques for measuring physical properties and more powerful theoretical techniques for describing and interpreting these properties. These research directions are developing very rapidly, setting a fast pace for widening the domain where the methods of quantum-statistical mechanics are applied. The material of this book will support the above statements by concrete examples. The book also describes the resources and techniques necessary to realize those opportunities.

This book is devoted in its entirety to the following tasks. Its subject matter is theoretical condensed matter physics, by which we mean the theoretical concepts, methods and models, and considerations which have been devised in order to interpret the experimental material and to advance our ability to predict and control solid-state phenomena. Special attention was paid to the unifying ideas and methods of the quantum-statistical mechanics. Obviously, this book does not pretend to cover all aspects of theoretical condensed matter physics. We were forced to omit many details and special developments. The omissions are due partly to the lack of space and partly to the author's personal preferences.

It is worth mentioning that the author belongs to the N. N. Bogoliubov's school of theoretical physics. Thus, the methods formulated by N. N. Bogoliubov and his pupils were presented and elaborated in this book in the most detailed way.

Chapters 15–29 are devoted to equilibrium quantum-statistical physics. The aim of Chapters 30–35 devoted to nonequilibrium statistical mechanics was to provide better understanding of a few approaches that have been proposed for treating nonequilibrium (time-dependent) processes in statistical mechanics with the emphasis on the inter-relation between theories. The ensemble method, as it was formulated by J. W. Gibbs, has the great generality and the broad applicability to equilibrium statistical mechanics. Different macroscopic environmental constraints lead to different types of ensembles with particular statistical characteristics. In the present book, the statistical theory of nonequilibrium processes, which is based on nonequilibrium ensemble formalism, is discussed. We also outlined the reasoning leading to some other useful approaches to the description of the irreversible processes. The kinetic approach to dynamic many-body problems, which is important from the point of view of the fundamental theory of irreversibility, was alluded to.

The emphasis is on the method of the nonequilibrium statistical operator (NSO) developed by D. N. Zubarev [6]. The NSO method permits one to generalize the Gibbs ensemble method to the nonequilibrium case and to construct an NSO which enables one to obtain the transport equations and calculate the transport coefficients in terms of correlation functions, and which, in the case of equilibrium, goes over to the Gibbs distribution. Although some space was devoted to the formal structure of the NSO method, the emphasis is on its utility. Applications to specific problems such as the generalized transport and kinetic equations, and a few examples of the relaxation and dissipative processes, which manifest the operational ability of the method, are considered.

Hence, the book presents a broad selection of important topics, including basic models of many-particle interacting systems on a lattice and various advanced methods of equilibrium and nonequilibrium statistical mechanics. Throughout, emphasis has been placed on the logical structure of the theory and consistent character of approximations. The course of study is aimed at under-graduate, graduate, and post-graduate students and various researches who have had prior expose to the subject matter at a more elementary level or have used other many-particle techniques. The part of the material is discussed at the level of an advanced course on quantum-statistical physics, highlighting a number of applications and useful examples, which in many cases goes beyond the material covered in many advanced undergraduate courses. The material of this book can also be of use in other contexts such as mathematical physics and physics of materials.

Author profited greatly from fundamental insights offered in the Refs. [3–6]. Also, he found very useful many other texts and monographs on statistical and many-body physics which he tried to cite in appropriate sections. However, author took care to avoid duplication of information covered in other books.

It is the hope of the author that the present book will serve as an introduction to the subject and a reference book and will help reader to appreciate vividly a beauty and elegance of statistical mechanics as an actual and developing branch of contemporary science.

This book is dedicated to the memory of our common teacher academician N. N. Bogoliubov (21.08.1909–13.02.1992). His inspiration, support and kind attention to author's work are most gratefully acknowledged. I am grateful to my teacher Prof. D. N. Zubarev (30.11.1917–16.07.1992). The book contains many marks of our numerous and sometimes hot discussions on statistical mechanics. I am also indebted for discussions and cooperation with my friends Dr. L. A. Pokrovski, Prof. A. Holas, and Prof. K. Walasek (deceased). I am grateful to Prof. R. A. Minlos for the useful and clarifying discussions on mathematical statistical mechanics topics. I also wish to thank my collaborators for fruitful cooperation and to thank numerous other colleagues of mine who in various ways contributed much to my understanding of the phenomena discussed.

A. L. KUZEMSKY
Bogoliubov Laboratory of Theoretical Physics,
Joint Institute for Nuclear Research,
141980 Dubna, Moscow Region, Russia.
http://theor.jinr.ru/˜kuzemsky
e-mail: kuzemsky@theor.jinr.ru

Contents