Cambridge University Press
978-0-521-84198-6 - Elements of Statistical Mechanics: With an Introduction to Quantum Field Theory and Numerical Simulation
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Frontmatter
More information

ELEMENTS OF STATISTICAL MECHANICS

With an Introduction to Quantum Field Theory and Numerical Simulation

Elements of Statistical Mechanics provides a concise, self-contained introduction to the key concepts and tools of statistical mechanics including advanced topics such as numerical methods and non-relativistic quantum field theory.

Beginning with an introduction to classical thermodynamics and statistical mechanics the reader is exposed to simple, exactly soluble models and their application to biological systems. Analytic and numerical tools are then developed and applied to realistic systems such as magnetism and fluids.

The authors discuss quantum statistical mechanics in detail with applications to problems in condensed matter as well as a selection of topics in astrophysics and cosmology. The book concludes with a presentation of emergent phenomena such as phase transitions, their critical exponents and the renormalization group.

Combining their extensive experience in research and teaching in this field, the authors have produced a comprehensive textbook accessible to advanced undergraduate and graduate students in physics, chemistry and mathematics.

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CAMBRIDGE
UNIVERSITY PRESS

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/9780521841986

First published 2006

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

ISBN 978-0-521-84198-6 Hardback
ISBN 978-0-521-14364-6 Paperback

Contents

Preface

Statistical mechanics is a fundamental part of theoretical physics. Not only does it provide the basic tools for analyzing the behavior of complex systems in thermal equilibrium, but also hints at, and is fully compatible with, quantum mechanics as the theory underlying the laws of nature. In the process one encounters such complex emergent phenomena as phase transitions, superfluidity, and superconductivity which are highly non-trivial consequences of the microscopic dynamics. At the same time statistical mechanics poses conceptual problems such as how irreversibilty can appear from an underlying microscopic system governed by reversible laws.

Historically, statistical mechanics grew out of classical thermodynamics with the aim of providing a dynamical foundation for this phenomenological theory. It thus deals with many-body problems starting from a microscopic model which is typically described by a simple Hamiltonian. The power of statistical mechanics lies in both its simplicity and universality. Indeed the same concept can be applied to a wide variety of systems both classical and quantum mechanical. These include non-interacting and interacting gases, chemical interactions, paramagnetic and spin systems, astrophysics, and solids. On the other hand statistical mechanics brings together a variety of different tools and methods used in theoretical physics, chemistry, and mathematics. Indeed while the basic concepts are easily explained in simple terms a quantitative analysis will quickly involve sophisticated methods.

The purpose of this book is twofold: to provide a concise and self-contained introduction to the key concepts of statistical mechanics and to present the important results from a modern perspective. The book is introductory in character, and should be accessible to advanced undergraduate and graduate students in physics, chemistry, and mathematics. It is a synthesis of a number of distinct undergraduate and graduate courses taught by the authors at the University of Dublin, Trinity College over a number of years.

Chapters 1 to 4 provide an introduction to classical thermodynamics and statistical mechanics beginning with basic concepts such as Carnot cycles and thermodynamic potentials. We then introduce the basic postulates of statistical mechanics which are applied to simple systems. This part then ends with a classical treatment of interactions in terms of a cluster expansion.

Although these techniques can provide us with considerable information about many systems they are in general not sufficient for all purposes. Therefore, in Chapters 5 and 6 we present a short self-contained account of the techniques used in the numerical approach to the statistical mechanics of interacting systems. In particular, Monte Carlo integration is reviewed in Chapter 5, while the powerful method of symplectic integrators is described in Chapter 6.

The second part of the book is devoted mostly to quantum statistical mechanics. In particular, in Chapter 7 Bose–Einstein and Fermi–Dirac systems are explained in detail, including high- and low-temperature expansions, Bose–Einstein condensation as well as blackbody radiation and phonon excitations in solids.

After introducing the basic concepts of classical and quantum statistical mechanics we make a short excursion into astrophysics and cosmology in Chapter 8, where we illustrate the importance of this formalism for a quantitative understanding of important problems such as determining the surface temperature of stars, the stability of compact objects such as white dwarfs and neutron stars, as well as the cosmic background radiation.

We then return to the main focus by systematically including interactions into quantum statistical mechanics. For this, the framework of non-relativistic quantum field theory is developed in Chapter 9, leading to a systematic, perturbative formalism for the evaluation of the partition function for interacting systems. In addition, in Chapter 10, we develop non-perturbative techniques which are used to give a qualitative derivation of the phenomenon of superfluidity.

In Chapter 11 the path integral formulation of quantum mechanics and field theory is described. The purpose of this chapter is to establish an intuitive link between classical and quantum statistical mechanics and also to establish some tools required in the treatment of critical phenomena in the last chapter.

Before that, however, we take another break in Chapter 12 with a critical review of the material presented thus far. Among the issues analyzed in some detail are the question of ergodicity, Poincaré recurrence, negative temperatures, and surface effects.

The final chapter is then devoted to the important subject of phase transitions and critical phenomena. After some general comments, Landau's phenomenological theory for phase transitions is introduced and then generalized, using the path integral formalism, to compute critical exponents which, in turn, play a central role in any quantitative discussion of phase transitions.

For the first half of the book a good knowledge of classical mechanics is assumed. For the second part some practice with quantum mechanics will be necessary. The aim is to present the concepts and methods of statistical mechanics with the help of simple examples. These examples illustrate a variety of phenomena that can be analyzed within statistical mechanics. We have tried, wherever possible, to physically motivate each step and to point out interconnections between different concepts. When appropriate we have included a short paragraph with some historical comments to place the various developments in this context.

We would like to thank Samik Sen for help in preparing the manuscript and Seamus Murphy for help with the figures. Many thanks to Matthew Parry, Mike Peardon, Fabian Sievers and Wolfgang Wieser for their help with the numerical algorithms. Further thanks to Herbert Wagner for helpful comments and to Sean Keating for a careful reading of the manuscript.

Fundamental physical constants

Planck constant	$h = 6.6260755 \cdot 10^{-34}$ J s
	$\hbar = h/2\pi = 1.05457266 \cdot 10^{-34}$ J s
Boltzmann constant	$k = 1.380658 \cdot 10^{-23}$ J/K
Avogadro number	$N_{\mathrm{A}} = 6.0221367 \cdot 10^{23}$ particles/mol
Gas constant	$R = N_{\mathrm{A}}k = 8.31451$ J/K per mol
Speed of light	$c = 2.99792458 \cdot 10^{8}$ m/s
Elementary charge	$e = 1.60217733 \cdot 10^{-19}$ J
Electron rest mass	$m_{\mathrm{e}} = 9.1093897 \cdot 10^{-31}$ kg
Neutron rest mass	$m_{\mathrm{n}} = 1.6749286 \cdot 10^{-27}$ kg
Proton rest mass	$m_{\mathrm{p}} = 1.6726231 \cdot 10^{-27}$ kg
Compton wavelength of the electron	$\lambda_C = \frac{h}{m_e c} = 2.42631 \cdot 10^{-12}$ m
Acceleration due to gravity	$g = 9.80665$ m/s^2
Newton constant	$G = 6.67 \cdot 10^{-11}$m^3/kg $\cdot$ s^2
Bohr radius	$a_0 = 5.29177 \cdot 10^{-11}$ m
Stefan–Boltzmann constant	$\sigma = \frac{\pi^2 k^4}{60\hbar^3 c^2} = 5.6703 \cdot 10^{-8}W/m^2 \cdot$ K^4