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高等统计物理

戴显燾 主编

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PREFACE

Statistical physics establishes a bridge from the macroscopic world to study the microscopic world. All theories in which the Boltzmann constant appears involve statistical physics. This is a theory with the fewest assumptions and the broadest conclusions. Up to now there is no evidence to show that statistical physics itself is responsible for any mistakes, a reflection of the natural beauty of this science.

Statistical physics has become an important branch of modern theoretical physics. At the same time it has influenced many fields, so this course has become one of the common fundamental courses of graduate students in different majors in physics departments.

Statistical physics is a branch of science engaged in studying the laws of thermal motion of macroscopic systems. It has its own special laws, which cannot be derived from mechanical laws. However mechanical law is one of its foundations. Statistical physics when based on classical mechanics is called classical statistics, while statistical physics based on quantum mechanics is called quantum statistics. Usually statistical physics as taught in fundamental courses for undergraduate students focuses mainly on classical statistics, while advanced statistics for graduate students mainly studies quantum statistics.

Chapter 1 of this book outlines the fundamental principles of statistical physics. Chapter 2, with simple applications of these principles, solves some typical problems in statistical physics, i. e. quantum perfect gases. Chapters 3 and 4 are devoted to the study of second quantization for many-particle systems and fields. Chapter 5 addresses Bose-Einstein condensation. Chapter 6 is devoted to the study of a class of inverse

problems in quantum statistics, their Chen (or Möbius-Chen) exact solution formulas, Dai's exact solution formulas, asymptotic behavior control (ABC) theory, and concrete realizations of the inversion theories, especially obtaining the phonon spectrum from real specific heat data for high T_c superconductors. Chapter 7 is an introduction to the theory of Green's functions in quantum statistics (where double-time Green's functions are the main tool) . Chapter 8 presents the unified diagonalization theorem for Hamiltonians of quadratic form, for both Fermi and Bose systems. Chapter 9 is an introduction to the third formulation of quantum statistics and the functional integral approach. Applying this formalism along with the diagonalization theorem established in chapter 8, an asymptotically exact solution is obtained in the thermodynamic limit for a model of superconductivity. The first four chapters are fundamental, and should be well known. The last five chapters are recent developments.

This course was edited by revising the lecture notes of the author, from courses of quantum statistics and advanced statistics for graduate students in the Department of Physics, Fudan University, since 1978. At the same time, this work contains the research results of some related projects, supported by the National Natural Science Foundation of China (NSFC: Nos. 19975009; 10174016; 19834010.) The author thanks the NSFC for its valued support over many years. I would like to thank my graduate students and students, especially including Dr. T. Wen, D. M. Ming, G. X. Hu, L. Sun, J. P. Ye, Mr. F. M. Ji, Y. He, Miss X. Xiang and etc, who studied these courses in a variety of majors in our and related departments, for their important support and discussions.

I also would like to sincerely thank Prof. C. N. Yang, my teacher, and Prof. Zhou Shixun, for their guidance and encouragement, Prof.

W. E. Evenson for his significant discussions and improving the English. I would like to express my special thanks to Prof. Wang Xun, for his important support and encouragement for this book.

I would like to thank all those who have helped me in writing and editing the book. Because of the limitations of the author, mistakes and errors are unavoidable, so all suggestions and comments which will help to improve the book are sincerely welcome.

Xianxi Dai

February, 2007

Fudan University

前 言

统计物理架起人们由宏观世界研究微观世界的桥梁。凡出现 Boltzmann 常数的理论就涉及统计物理。它是假设最少,结论众多的一门学科。至今还没有任何证据,确认某些错误必须由统计物理本身负责。这反映出该学科自然的美。

它已成为现代理论物理的一个重要部分。同时它又渗透到物理学的众多领域,因此自然成为物理系的多个专业的研究生基础课程。

统计物理是研究体系的热运动规律的学科。它有自己的特殊规律,不能从力学推导出来。但必须以力学为其基础之一。基于经典力学的,称经典统计,基于量子力学的,称量子统计。通常大学生基础课程中的统计物理以研究经典统计为主,而研究生的高等统计,则以量子统计为主。

本书的第一章是统计物理基本原理。第二章作为这些基本原理的简单应用,解决几个典型的统计物理问题:量子理想气体。第三章和第四章分别致力于多粒子体系和场的二次量子化。第五章研究玻色-爱因斯坦凝结。第六章研究一批量子统计中的反问题,它们的陈氏(或 Möbius-Chen)严格解公式,戴氏严格解公式及其渐近行为控制理论和反演理论的具体实现,特别是由高温超导体的实际比热数据,直接反演出声子谱。第七章是 Fermi 和 Bose 的二次型哈密顿量的统一的对角化定理。第八章是量子统计中的 Green 函数(以双时 Green 函数理论为主线)引论。第九章则介绍

量子统计第三种表述和泛函积分理论。并运用它和第七章的对角化定理,获得一个超导模型的热力学极限下的渐近严格解。本书的前四章是基础部分,是必须掌握的。后五章是最新发展。

本书是作者依据自 1978 年以来为复旦大学物理系研究生讲课所使用的量子统计课程和高等统计课程的教材修改而成的,同时也是国家自然科学基金的多个有关项目的研究结果。作者对国家自然科学基金委多年来的宝贵支持,对我所指导的多位研究生,以及多年来选读本课程的本系和外系的研究生和部分本科生,特别包括温涛、明灯明、胡光喜、孙磊、叶季平博士及季丰民、何源和相湘同学的讨论与支持,表示衷心的感谢。

作者对杨振宁教授,对我的老师周世勋教授多年来的关心、指导和鼓励表示衷心的感谢。对 Evenson 教授多年来的讨论和对本书的英语方面的修饰表示衷心感谢。作者还特别感谢王迅教授对本书的支持和鼓励。

作者还感谢所有支持和帮助过本书编写和出版的人们。限于作者的水平和时间,错误和不当之处在所难免,如蒙赐教,不胜感激。

戴显熹

2007 年 2 月于复旦大学

CONTENTS

Chapter 1	Fundamental Principles	1
1.1	Introduction: The Characters of Thermodynamics and Statistical Physics and Their Relationship	1
1.2	Basic Thermodynamic Identities	3
1.3	Fundamental Principles and Conclusions of Classical Statistics	7
1.3.1	Microscopic and Macroscopic Descriptions, Statistical Distribution Functions	8
1.3.2	Liouville Theorem	10
1.3.3	Statistical Independence	13
1.3.4	Microscopical Canonical, Canonical and Grand Canonical Ensembles	14
1.4	Boltzmann Gas	16
1.5	Density Matrix	19
1.5.1	Density Matrix	20
1.5.2	Some General Properties of the Density Matrix	22
1.6	Liouville Theorem in Quantum Statistics	25
1.7	Canonical Ensemble	29
1.8	Grand Canonical Ensemble	33
1.8.1	Fundamental Expression of the Grand Canonical Ensemble	33
1.8.2	Derivation of the Fundamental Thermodynamic Identity	34
1.9	Probability Distribution and Slater Sum	36
1.9.1	Meaning of the Diagonal Elements of the Density Matrix	36

1.9.2	Slater Summation	37
1.9.3	Example: Probability of the Harmonic Ensemble	39
1.10	Theory of the Reduced Density Matrix	44
Chapter 2	The Perfect Gas in Quantum Statistics	55
2.1	Indistinguishability Principle for Identical Particles	55
2.2	Bose Distribution and Fermi Distribution	60
2.2.1	Perfect Gases in Quantum Statistics	60
2.2.2	Bose Distribution	61
2.2.3	Fermi Distribution	62
2.2.4	Comparison of Three Distributions; Gibbs Paradox Again	62
2.3	Density of States, Chemical Potential and Equation of State	65
2.3.1	Density of States	65
2.3.2	Virial Equation for Quantum Ideal Gases	66
2.4	Black-body Radiation	69
2.4.1	Thermodynamic Quantities for the Black-body Radia- tion Field	71
2.4.2	Exitance and Variety of Displacement Laws	72
2.4.3	Waveband Radiant Exitance and Waveband Photon Exitance	75
2.5	Bose-Einstein Condensation in Bulk	79
2.5.1	Bose Condensation, Dynamical Quantities with Tem- perature Lower Than the λ Point	79
2.5.2	Discontinuity of the Derivatives of Specific Heat and λ Phenomena	82
2.5.3	Two-Fluid Theory	85

2.5.4	2-D Case	86
2.6	Degenerate Fermi Gases and Fermi Sphere	87
2.6.1	Properties of Fermi Gases at Absolute Zero	87
2.6.2	Specific Heat of Free Electron Gases	89
2.6.3	State Equation, Heat Capacity at Constant Pressure, and Heavy Fermions	93
2.7	Fermi Integrals and their Low Temperature Expansion	95
2.8	Magnetism of Fermi Gases	97
2.8.1	Spin Magnetism: Paramagnetism	98
2.8.2	Energy Spectra and Stationary States of Electrons in a Homogeneous Magnetic Field	100
2.8.3	Diamagnetism of Orbital Motion of Free Electrons	103
2.9	Peierls Perturbation Expansion of Free Energy	106
2.9.1	Classical Case	107
2.9.2	Quantum Case	108
2.9.3	Expansion of Free Energy of an Ideal Gas in an Exter- nal Field	110
2.10	Appendix	114
Chapter 3	Second Quantization and Model Hamiltonians	117
3.1	Necessity of Second Quantization	117
3.2	Second Quantization for Bose System	119
3.3	Second Quantization • Fermi System	128
3.4	Some Conservation Laws	135
3.5	Some Model Hamiltonians	140
3.6	Electron Gases with Coulomb Interaction	145

3.6.1	Completely Ionized Gases — the High Temperature Plasma	146
3.6.2	The Degenerate Electron Gas with Coulomb Interaction (Metal Plasma)	150
3.7	Anderson Model	167
Chapter 4	Least Action Principle, Field Quantization and the Electron-Phonon System	169
4.1	Classical Description of Lattice Vibrations	169
4.2	Continuous Media Model of Lattice Vibration (Classical)	174
4.3	The Least Action Principle, Euler-Lagrange Equation and Hamilton Equation	177
4.4	Lagrangian and Hamiltonian of Continuous Media	188
4.5	Quantization of the Lattice Vibration Field	191
4.6	Debye Theory of Specific Heat of Solids	197
4.7	The Electron-Phonon System and the Fröhlich Hamiltonian	203
Chapter 5	Bose-Einstein Condensation	208
5.1	Spatial and Momentum Distributions of Bose-Einstein Condensation in Harmonic Traps and Bloch Summation	208
5.1.1	Introduction	208
5.1.2	Generalized Expression for Particle Density	209
5.1.3	Distributions for Ideal Systems	211
5.1.4	New Expression with Clear Physical Picture	212
5.1.5	Momentum Distributions	215

5.1.6	Results of Numerical Calculations	216
5.1.7	Discussion and Concluding Remarks	216
5.1.8	Momentum Distribution of BEC	219
5.2	BEC in Confined Geometry and Thermodynamic Mapping	220
5.2.1	Introduction	220
5.2.2	Confinement Effects	222
5.2.3	Thermodynamic Mapping	222
5.2.4	Mapping Relation for Confined BEC	225
5.2.5	Determination of the Critical Temperature	229
5.2.6	Discussion	233
Chapter 6 Some Inverse Problems in Quantum Statistics		
		235
6.1	Introduction	235
6.2	Specific Heat-Phonon Spectrum Inversion	237
6.2.1	Technique for Eliminating Divergences	239
6.2.2	Unique Existence Theorem and Exact SPIE Solution	241
6.2.3	Summary	242
6.3	Concrete Realization of Inversion	244
6.3.1	The Specific Heat-Phonon Spectrum Inversion Problem	244
6.3.2	Results and Concluding Remarks	250
6.4	Möbius Inversion Formula	252
6.4.1	Riemann ζ Function and Möbius Function	252
6.4.2	Möbius Inversion Formula	253
6.4.3	The Modified Möbius Inversion Formula	255

6.4.4	Applications in Physics	256
6.5	Unification of the Theories	258
6.5.1	Introduction	258
6.5.2	Deriving Chen's Formula from Dai's Exact Solution	259
6.5.3	Concluding Remarks	262
6.6	Appendix	263
Chapter 7	An Introduction to Theory of Green's Functions	265
7.1	Temperature-Time Green's Functions	265
7.1.1	Definition of Temperature-Time Green's Functions	265
7.1.2	The Equation of Motion of Double-Time Green's Functions	269
7.1.3	Time Correlation Functions	270
7.2	Spectral Theorem	272
7.2.1	Spectral Representation of Time Correlation Functions	272
7.2.2	Spectral Representations of Retarded and Advanced Green's Functions	274
7.2.3	Spectral Representation of Causal Green's Functions	278
7.3	Example: Ideal Quantum Gases	279
7.4	Theory of Superconductivity with Double-Time Green's Functions	283
7.5	Higher-Order Spectral Theorem, Sum Rules and Uniqueness	290

Chapter 8	A Unified Diagonalization Theorem for Quadratic Hamiltonian	291
8.1	A Model Hamiltonian	293
8.2	Diagonalization Theorem for Fermi Quadratic Forms	296
8.3	Conclusion: A Unified Diagonalization Theorem	305
Chapter 9	Functional Integral Approach: A Third Formulation of Quantum Statistical Mechanics	308
9.1	Introduction	308
9.1.1	Hubbard's Method	309
9.1.2	Difficulties	310
9.2	An Operator Identity	311
9.3	Functional Integral Formulation of Quantum Statistical Mechanics	311
9.4	Reality and Method of Steepest Descents	314
9.5	Discussion and Concluding Remarks	318
9.6	Some Recent Developments	318
9.7	Application: An Exact Solution	319
References	324
Index	330

Fundamental Principles

1.1 Introduction: The Characters of Thermodynamics and Statistical Physics and Their Relationship

Thermodynamics and statistical physics have the same focus of study: the laws of thermodynamic motion of macroscopic systems, consisting of huge numbers of particles (such as molecules, atoms, etc.). However, their starting points and methods are different. They have their own merits and deficiencies and supplement each other.

Thermodynamics is a macroscopic phenomenological theory. From a huge number of direct observations of phenomena and experiences, scientists summarized and induced some fundamental laws of thermal motion, i. e. the zeroth, first, second and third laws of thermodynamics. These fundamental laws can be applied to theoretically deduce and explain the equilibrium properties of macroscopic systems. The merit of the theory of thermodynamics is that it is built upon a sound and broad experimental background. Its conclusions have high reliability and universality. Its general conclusions are independent of internal structures of systems. Its limitations are also due to its phenomenological nature, without microscopically taking into account the structures of atoms and molecules. Thus it cannot be used to study fluctuation phenomena and to obtain parameters related to material properties. However, the achievements of thermodynamics in non-equilibrium problems are rather limited.

The essential achievements of thermodynamic theory lie in setting up the three thermodynamic laws, from which one can deduce universal

internal relations for various thermodynamic quantities and attribute the concrete characteristics of macroscopic systems to their **equations of state and specific heats**, both of which can be directly measured or established by experiment. Thermodynamics can also relate the concrete properties of macroscopic systems to **one characteristic function of the system**, then all the properties of the equilibrium states of the system can be derived from this characteristic function and its derivatives with respect to the corresponding characteristic variables. In other words, one attributes the thermodynamic properties to the problem of the differential geometry of the characteristic functions. Some important characteristic functions, such as **the internal energy, Helmholtz free energy, Gibbs free energy, thermodynamic potential, etc.**, can be calculated by statistical physics.

Thermodynamics allows statistical physics to concentrate on the calculation of a single characteristic function, and other thermodynamic quantities can then be derived using the universal thermodynamic relations.

Statistical physics is a microscopic theory. Its starting point is different from that of thermodynamics. (1) It assumes or accepts the fact that all macroscopic systems consist of molecules and atoms. (2) It assumes the properties of the particles making up the system and the interactions between them. These assumptions can be demonstrated or analyzed by other experiments. (3) It assumes that the motion of these particles obey mechanical laws, i. e. the macroscopic observed value is taken to be the statistical average value. Statistical physics does not hold that thermodynamic laws are mechanical laws, but it takes mechanics as the foundation of statistical physics. The statistical laws are new special laws which cannot be reduced to mechanical laws. As the number of particles increases, statistical laws reveal themselves in the collective average properties of many-particle systems. As the number of particles decreases, the statistical properties disappear. For example, for a single particle, there are no concepts of temperature and entropy.

The main achievements of statistical physics lie in the derivation of the three fundamental laws of thermodynamics based on the fundamental principles of statistics. Given some assumptions for concrete microscopic structures, statistical physics can be used to derive the characteristic functions, or state equations and specific heats. This theory can also be used to calculate statistical fluctuations and various non-equilibrium processes. Its limitations lie in lack of universality because it requires

concrete assumptions about specific systems. Its strength lies in respecting the individuality and the internal structures of the systems studied. It is thus possible to understand the microscopic structures of these systems. An important historical contribution of statistical physics is in studies of black-body radiation, which led to quantum theory.

Since one of the basic assumptions of statistical physics is that particle motions in a macroscopic system obey mechanical laws, then it is necessary to distinguish what kind of mechanics: classical or quantum mechanics? Statistical physics based on classical mechanics is called classical statistics, while that based on quantum mechanics is called quantum statistics.

Before the 1950's, quantum statistics was primarily used to treat the so-called perfect Fermi and Bose gas, i. e. the quantum gases without interactions. Due to difficulties in the theory and limited mathematical skills, practical systems with interactions could not be treated during that period. Since the 1950's, quantum field theory, developed in particle physics, has progressively matured. Although problems remain in its applications in particle physics, the methods of quantum field theory, such as perturbation theory, Feynman diagram techniques, Green's function methods, etc., poured into quantum statistics. After solving some important difficult problems, such as the mechanism of superconductivity which has been unsolved for 40 years, quantum statistics rapidly developed and quickly formed into an important branch of theoretical physics. This theory also provides a vast and practical testing field for studies of fundamental theories. Major parts of modern quantum statistics are devoted to study the quantum statistics based on quantum field theory.

1.2 Basic Thermodynamic Identities

In general studies of thermodynamics, one primarily studies the thermodynamic equilibrium properties of systems containing a fixed number of particles. However, in studies of quantum statistics, one usually needs to consider systems with variable numbers of particles, because these kind of models can be applied to more general cases. Sometimes their treatment is more convenient than that for fixed particle numbers in mathematical calculations. In addition, there are physical systems where the variable number of particles is an essential feature, rather than a mathematical convenience. For example, the macroscopic condensate in superconductors or superfluid liquid helium acts as a particle bath which