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Advanced Statistical Mechanics

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高等统计力学
影 印 版 序

Barry M. McCoy 先生是著名的理论物理学家，纽约州立大学石溪分校杨振宁理论物理研究所教授，主要从事统计物理，特别是精确可解模型方面的研究工作. 本书是作者在纽约州立大学石溪分校讲授高等统计力学课程的基础上撰写的一本统计力学著作.

该著作是面向从事统计力学或相关学科研究的研究生或研究人员的，它的选材和处理过程因而不同于通常的统计力学教材，也不同于一般的专著. 诚如作者在前言中所指出的，该书主要关注正在研究中的课题，也就是并非所有讨论的问题均有明确的结论，几乎所有涉及这些问题的专题讨论最终将引向那些未解决的问题. 为了充分体现这一特点，几乎在每一章中作者均设专节论及未解决的问题. 在讨论中，作者给出了相关的计算过程和重要结果的证明，对文献也作了仔细地梳理和充分地详述.

该著作分为三部分内容，一般理论，级数和数值方法以及精确可解模型，其中第一和第二部分分别约占总篇幅的四分之一，第三部分占一半. 第一部分主要讨论了统计物理的基本原理，热力学现象，模型，各类热力学性质(如稳定性，唯一性，序)以及它们的描述和处理方法(如系综理论，标度理论等)，是后两部分讨论的基础. 第二部分则专注于级数展开和数值计算方法这两种重要的处理统计模型的方法. 它们对于理解模型的性质是必不可少的，因为能够得到某些性质的解析表示式的那类所谓精确可解模型是非常稀少的. 这一部分集中讨论了位力展开方法，高密度展开和高温展开等几种级数方法. 数值方法包括 Monte-Carlo 方法，分子动力学方法等.

第三部分系统讨论精确可解模型，这是近几十年以来数学物理、统计物理、凝聚态物理等学科中广泛研究的一个课题，围绕与杨振宁-巴克斯特(Baxter)方程相关的研究取得了许多重要的成果，1990 年的菲尔兹奖中有三位得奖者的工作是与此相关的. 该书作者也是研究精确可解问题的专家. 所以第三部分篇幅大的原因一方面是这类问题本身的重要性，另一方面当然也与作者的研究背景密不可分.

精确可解模型主要是 2 维系统，对它们的处理包含了许多方法性和技巧性的内容. 第三部分选择了 Ising 模型，8-顶角模型，XYZ 模型，硬六边形模型，RSOS 模型和手征 Potts 模型等几类重要的有代表性的模型，分别就可解性、可积性、配分函

数的求解，关联函数的确定，边界条件与可积性的关系，对热力学性质的影响等多个方面进行了系统的讨论.

自 1982 年巴克斯特出版《统计力学中的精确可解模型》专著以来，基本上再未出版过系统讨论这些模型和相关进展的著作，因此许多重要的结果仍然分散在研究文章中. McCoy 先生的这本著作很大程度上弥补了这种缺陷，建立了通向阅读相关研究文献的重要桥梁. 因此，无论是对于研究人员还是对于将进入该领域的年轻学子而言，该著作均是值得深入研读的必备参考书.

南京大学物理学院教授　鞠国兴

2012-5-15

前　言

了解一个学科的最佳途径就是撰写一本关于它的书。

Benjamin Disraeli(本杰明·迪斯雷利)[①]

统计力学这个学科可以追溯到19世纪，它有丰富的历史.在所有本科生和研究生的物理教学计划中均要求讲授统计力学的基础.因此，有许多著作解释这个学科的基础内容，这些内容构成凝聚物质系统所有热性质的基础.这些书的内容相当类似，这在于它们均包括热力学，系综理论，单体问题，理想 Bose 和 Fermi 气体等内容.这些专题全部被视为是已透彻理解的成定论的问题.

本书是作者讲授高等统计力学课程的产物，该课程包含超出基础课程的一些专题，并力图向读者介绍正在研究中的一些专题.与一门基础课程中的材料相比，本书中几乎所有专题均引导至一些未解决的问题，本书的目的是向尽可能广泛的读者介绍这些正在研究中的专题.因此，在几乎所有章中设有关于未解决问题的节，并且我所称的缺失定理是那些人的物理直觉暗示结果应该是正确的、但是还没有给予证明的定理.通过明示许多地方存在未解决的问题，希望本书能促进本领域的发展.

在对一个学科的任何高等处理中，专题的选择往往受到作者兴趣风格的影响，故此有关我对专题的选择作几点评述.我已确定将统计力学这个学科有点任意地分为三个部分：一般理论；级数和数值方法；精确可解模型.每一部分均有大量的文献.在一本书的容量范围内不可能陈述所有结果，证明所有已知的定理.为此，我采用了这样的处理方法——陈述并解释许多结果，但是仅对所陈述定理中的一部分给予证明.没有其他可行的选择，因为许多重要的定理，它们在文献中的证明过程就需要 40～50 页的篇幅.例如，物质稳定性的证明本身就是 Elliot Lieb 的一本著作的主题.Rodney Baxter 专门用整本书讨论六顶点模型，八顶点模型和硬六角模型的自由能以及序参数；吴大峻和本书作者则用整本书专注于 Ising 模型.在这种意义上，可以将本书视为对过去 50 多年的文献的一个介绍和引导，但是很难将其作为对文献的一种替代.

读者将会立刻注意到，有几个统计物理中非常著名的专题并没有包含在本书中，即重正化群和平均场理论.这种省略是刻意的，因为这两个专题很好地包含在

① Benjamin Disraeli，1804－1881，小说家，英国保守党领袖，曾两度出任英国首相.——译注

许多著作中，并且按照我的意见，再多一次来说明这些方法完全是多余的.

统计力学不断地取得进展，可以肯定的是，即使在出版的当时，一些专题的进展已超出这里所呈现的. 特别地，我提请读者注意近期研究工作中的几个例子：第 4 章讨论的 Kepler 猜想的证明(该猜想是，在三维中硬球的堆积不会比面心立方晶格更稠密)以及也在第 4 章介绍的一个发现(椭球可以有比面心立方晶格更密的堆积). 有几个所介绍的计算(最初是部分地出于希望澄清并更好理解已有的文献)，尤其是第 7 章中关于第十阶位力系数的计算，第 10 章和第 12 章中 Ising 模型的对角磁化率以及形状因子积分的求值，第 14 章中八顶点模型 TQ 方程的处理.

有许多有趣而又非常重要的问题仅因为篇幅的限制而省略了. 特别是，有许多可解模型没有提及. 此外，没有讨论坐标 Bethe 拟设方法，代数 Bethe 拟设方法以及量子群和共性场论的数学. 这些专题需要比本书所允许的更多篇幅，并且它们已被其他作者进行了广泛地论述.

然而，尽管有许多必要的省略，作者已经尽力包含了足够大量的专题，读者将能由此欣赏到这个学科的广博，领略到在过去 40～50 年中已经取得的进展的众多方面以及领悟到将来可能取得进展的许多地方.

我非常喜欢这个说法："直到你推广了一篇文章，你才能说你理解了它."当然，这导致一个逻辑推论"没有作者可以被认为他或她理解了他或她最近的文章". 这本书是这个推论的真实性以及含义的最佳显示. 每一章中均有未解决的问题和专题，它们需要进一步的研究和解释. 这些问题中的一些更为明显和无法回避的问题已经被挑选出来用作讨论. 但是，即使不是大多数，还是有许多问题静静地隐藏起来等待读者去发现它们. 书中呈现了许多推导和计算过程，除非包括打印错误，证明过程应该足以证明结论. 但是，没有地方曾经表明，所给出的证明对结论实际上是必要的，所展示的步骤实际上揭示了正在讨论的现象的机制. 这个问题最突出的例子是第 12 章中用 MAPLE 进行的积分求值，在本书写作的时侯，它是没有解析推导过程的.

本书中有许多地方，我是需要感谢合作者和朋友的帮助和建议的：Nathan Clisby 对第 7 章中位力系数的计算；Jean-Marie Maillard 教我如何在计算机上进行第 12 章中的积分的符号求值；与 Klaus Fabricius 关于第 14 章中八顶点模型的 Q 矩阵所进行的合作；以及与 Jacques Perk 和 Helen Au-Yang 关于第 15 章中手征 Potts 模型以及图 15.4 和图 15.5 所开展的合作. 在第 6 章中证明 Mayer 展开所使用的方法来自 Hans Groeneveld 在 20 世纪 60 年代后期所作的一系列讲座，在准备这章时他也给予我许多宝贵的建议.

我要非常感谢国家自然科学基金会在我写作这本书的许多时间里给予的部分资助，非常感谢洛克菲勒基金会提供的在其贝拉吉奥(Bellagio)会议和研究中心的

一个月居住项目的资助，在那里修改和完善了本书的几章内容.

最后，我必须感谢两位不平凡的人物，我深深地感谢他们，没有他们的鼓励和启发，这本书就不可能完成. 第一位是我的已故夫人 Tun-Hsu Martha McCoy(汤敦序)，在我投入于写作的许多年月中，她在每一个阶段帮助我，并且忍受了其间我所经历的无数次的挫折. 另一位是我 51 年前亚利桑那州图森市卡塔利娜高中的同班同学 Margaret Hagen Wright，感谢她在非常需要之时所给予我的深厚友谊.

巴里 M. 麦科伊

纽约　石溪

2009 年

Preface

The best way to become acquainted with a subject is to write a book about it.

Benjamin Disraeli

The subject of statistical mechanics dates back to the 19th century. It has a rich history, and the basics of the subject are taught in all undergraduate and graduate physics programs. Consequently there is a wealth of books that explain the elementary aspects of the subject which form the foundation for all thermal properties of condensed matter systems. The content of these books is all rather similar in that they cover thermodynamics, ensemble theory, one-body problems and the perfect Bose and Fermi gases. These topics are all considered to be closed subjects which are thoroughly understood.

This book is an outgrowth of the author's teaching of advanced courses in statistical mechanics which go beyond the topics covered in elementary courses and is aimed at introducing the reader to topics in which there is ongoing research. In contrast to the material in an elementary course almost all topics lead to open questions, and the aim of this book is to present these topics of ongoing research to as wide an audience as possible. Consequently in almost all chapters there are sections on open questions and what I call missing theorems where one's physical intuition suggests that results should be true but for which no proof yet exists. It is hoped that, by highlighting the many places where there are unresolved questions, this book can stimulate progress in the field.

The selection of topics in any advanced treatment of a subject is affected by the tastes of the author and so several comments about my selection of topics are in order. I have chosen to divide the subject somewhat arbitrarily into three parts: exact general theorems; series expansions and numerical results; and solvable models. Each of these divisions has an immense literature and within the confines of one book it is not possible to state all results and prove all known theorems. I have therefore adopted the procedure of stating and explaining many results but have only given the proofs of a selection of the theorems stated. There is no other alternative since there are many important theorems whose proof in the literature requires papers of 40–50 pages. For example the proof of the stability of matter is the subject of a book in its own right by Elliot Lieb; Rodney Baxter devotes an entire book to the free energy and order parameters of the six-vertex, eight-vertex and hard hexagon models; T.T. Wu and the present author devote an entire book to the Ising model. In this sense this present book can be considered to be an introduction and guide to, but is hardly a substitute for, the literature of the past 50 years.

The reader will almost instantly note that there are several well-known topics in statistical physics which are not covered in this book: namely the renormalization group and mean field theory. This omission is deliberate since both of these topics are well covered in many books and it is, in my opinion, superfluous to give one more account of these methods.

Constant progress is being made in statistical mechanics and it is certain that even at the time of publication some topics will have advanced beyond what is presented here. In particular I draw the reader's attention to several examples of recent work: the proof discussed in chapter 4 of Kepler's conjecture that no packing of hard spheres in three dimensions can be more dense than the face centered cubic lattice, and the discovery also presented in chapter 4 that for ellipsoids there are packings denser than the fcc lattice. There are several computations presented which were initiated in part by the desire to clarify and better understand the existing literature, in particular the computation of the tenth order virial coefficients in chapter 7, the diagonal susceptibility and the evaluation of the form factor integrals of the Ising model in chapter 10 and 12 and the treatment of the TQ equation of the eight-vertex model in chapter 14.

There are also many interesting and important problems which are omitted merely for lack of space. In particular there are many solvable models which have not been mentioned. Furthermore there is no discussion of the methods of the coordinate and algebraic Bethe's ansatz and the mathematics of quantum groups and conformal field theory. These topics require much more space than this book allows and are treated extensively by other authors.

However, it is hoped that in spite of the many necessary omissions that this book covers a sufficiently large number of topics so that the reader will gain an appreciation of the great breadth of the subject; the many areas of progress which have been made in the past 40–50 years, and the places where future advances will be made.

I am fond of saying that "you cannot say that you understand a paper until you generalize it." This, of course, leads to the logical corollary that "no author can be said to understand his/her most recent paper." This book is an excellent demonstration of the truth and meaning of this corollary. In every chapter there are open questions and topics that need further research and explanation. Some of the more obvious and unavoidable of these questions have been singled out for discussion but many, if not most, are quietly hidden away waiting for the reader to discover them. There are many derivations and computations presented and, barring misprints, the proofs should be sufficient to prove the conclusions. But in no place is it ever shown that the given proof is actually necessary for the conclusion and that the steps exhibited actually reveal the mechanism for the phenomena being discussed. The most glaring example of this problem is the evaluation of integrals done in chapter 12 by the use of MAPLE for which, at the time of writing, no analytic derivation exists.

There are many places in this book where I need to thank collaborators and friends for their help and suggestions: Nathan Clisby for the evaluations of virial coefficients in chapter 7; Jean-Marie Maillard for teaching me how to do the symbolic evaluation of integrals on the computer in chapter 12; Klaus Fabricius for collaboration on the Q matrices of the eight-vertex model of chapter 14; and Jacques Perk and Helen Au-Yang for collaboration on chiral Potts models and for figures 4 and 5 of chapter 15. The

method used in chapter 6 to prove the Mayer expansion comes from a set of lectures given by Hans Groeneveld in the late 1960s who has given me much valuable advice in the preparation of that chapter.

I am most grateful to the National Science Foundation for partial support during much of the time when I was writing this book and to the Rockefeller Foundation for a one-month residency at their Bellagio Conference and Study Center where several chapters were revised and perfected.

In conclusion I must thank and acknowledge two remarkable people to whom I am deeply indebted and without whose encouragement and inspiration this book would never have been completed. The first is my late wife, Tun-Hsu Martha McCoy , who helped me every step of the way and put up with the innumerable frustrations I have had during the far too many years I have spent in writing. The other is my classmate of 51 years ago from Catalina High School in Tucson, Arizona, Margaret Hagen Wright, who has given me profound friendship in a time of great need.

Stony Brook, New York
2009

目　　录

第一部分　一般理论

第三部分 精确可解模型