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Computational Statistical Physics

From Billiards to Monte Carlo



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Computational Statistical Physics

From Billiards to Monte Carlo

With 141 Figures



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Preface

Physics deals with systems ranging from one or a few elementary particles and elementary interactions to large scale systems like the climate or even stars. Although in principle each of the macroscopic systems can be described on a microscopic level, that would lead to a huge number of variables and make a detailed treatment hopeless.

However, in many cases, if not in most cases, a very small number of variables suffice to describe the system reasonably well. The reason is that many degrees of freedom are not individually relevant, but only their overall behavior is of significance at the macroscopic level. Statistical physics provides a conceptual answer to the problem of handling the majority of the degrees of freedom, namely by treating them in a statistical way. This reduction in the number of degrees of freedom has made it possible to gain a deep understanding of many different physical systems such as radiation, gases, or granular matter.

The power of statistical physics has increased significantly with the advent of computers. The possibility of simulating physical systems, rather than just describing them, has opened up a whole new range of methods and allows us nowadays to analyze the properties of large systems quantitatively.

Hence with the advance of computational resources, the area of application of today's statistical physics has grown wider than ever. New methods have been developed enabling us to treat systems which were previously not open to analysis owing to the limited power of available analytical methods. Nowadays systems can be analyzed which allow no solution in closed form, i.e., over-complicated terms which are interesting and important need no longer be omitted from the defining equations of the model. In addition to the available solutions, the advent of computers and their graphics capabilities has allowed the visualization of many phenomena. This in turn has improved insight into the physics and demonstrated its beauty in many cases.

While there are certainly several good textbooks for the field of statistical physics as a whole, and for parts of it, numerical methods and topical developments which are impossible without the massive use of computers are usually inadequately presented in textbooks, if they are presented at all. On the other hand, available review articles usually concentrate on one particular field of research. In this book, we try to fill this gap by covering a large number of topics in computational statistical physics on an introductory level, as well as leading the reader to related research problems currently under investigation.

The book is aimed at graduate students and researchers and tries to reveal broad areas in which methods of statistical physics are now applied. It is espe-

cially devoted to computational approaches. In addition, the book demonstrates that the powerful methods developed in computational statistical physics are now successfully used in neighbouring areas and even in several rather different fields. Subjects range from the application of statistical methods in solid state physics to their application in financial modelling, from neural networks to billiards and from traffic modelling to game theory.

The easy-to-read articles emphasize topical computational methods and give readers ready access to the most advanced methods used today in these fields. Contributions by the various authors, experts in the relevant fields, are arranged in such a way that this percolation of important physical methods into other areas becomes apparent, showing how interdisciplinary science is progressing today. One example is provided by methods developed to analyse chaotic motion in billiards, which are then used in the optimization of combinatorial problems. Another example is the application of Monte Carlo methods such as the Metropolis algorithm, which is then used in simulated annealing to solve important industrial optimization problems. The analysis of time series is a further example which shows how methods developed in statistical physics, e.g., to analyse temperature profiles, can be used in the description of financial time series. Likewise, random matrix theory and the statistical analysis of eigenvalue distributions has become a powerful tool, not only in statistical physics, but also in semiconductor physics and metal physics, describing metal–insulator transitions, electrons in quantum dots and quasicrystals.

Several authors have provided simple programs for training purposes. These programs are not included in this book, but we have archived them at

<http://www.tu-chemnitz.de/physik/HERAEUS/2000/Springer.html>

so that they can be downloaded. In this way it is also possible to update the programs and data, and offer new links to topical developments for the various subjects.

The articles are based on topics which were presented to about 50 students who took part in a Heraeus Physics School, organized at the Chemnitz University of Technology in the fall of 2000. We thank all the lecturers for their contributions, which made it possible for us to provide our students with this wide overview of the field of computational statistical physics. Knowing the shortage of time and the many obligations our coauthors have, we would like to express our gratitude to our colleagues who have found time among many administrative, research, and teaching duties to prepare the high quality articles presented here. Finally, we would like to thank Peter Blaudeck, Angelique Gaida, Karin Nerger and Steffen Seeger for their technical help, and Springer-Verlag for making this volume a reality. Last, but not least, we thank the Wilhelm und Else Heraeus-Stiftung for the generous financial support which has made the school possible and which has also helped to make this book available.

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