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7

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Volumes 1–38 are listed on the back inside cover

Monte Carlo Methods

in Statistical Physics

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Second Edition

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Preface to the Second Edition

In the seven years since this volume first appeared, there has been an enormous expansion of the range of problems to which Monte Carlo computer simulation methods have been applied. This fact has already led to the addition of a companion volume ("Applications of the Monte Carlo Method in Statistical Physics", Topics in Current Physics, Vol. 36), edited in 1984, to this book. But the field continues to develop further; rapid progress is being made with respect to the implementation of Monte Carlo algorithms, the construction of special-purpose computers dedicated to execute Monte Carlo programs, and new methods to analyze the "data" generated by these programs.

Brief descriptions of these and other developments, together with numerous additional references, are included in a new chapter, "Recent Trends in Monte Carlo Simulations", which has been written for this second edition. Typographical corrections have been made and fuller references given where appropriate, but otherwise the layout and contents of the other chapters are left unchanged. Thus this book, together with its companion volume mentioned above, gives a fairly complete and up-to-date review of the field. It is hoped that the reduced price of this paperback edition will make it accessible to a wide range of scientists and students in the fields to which it is relevant: theoretical physics and physical chemistry, condensed-matter physics and materials science, computational physics and applied mathematics, etc.

The editor is grateful to his colleagues for their valuable contributions to this book and he thanks them, as well as many other colleagues, for stimulating comments and advice.

Mainz, February 1986 *Kurt Binder*

Preface to the First Edition

The "Monte Carlo method" is a method of computer simulation of a system with many degrees of freedom, and thus has widespread applications in science. It has its name from the use of "random numbers" to simulate statistical fluctuations in order to numerically generate probability distributions (which otherwise may not be known explicitly since the considered systems are so complex). While the method would work in principle also with random numbers generated at a roulette table, an effective and economic use of this method requires the use of high-speed digital computers. Thus the first successful application of this method to a problem of statistical thermodynamics dates back only to 1953, when Metropolis and co-workers studied a "fluid" consisting of hard disks. Since then this technique has experienced an impetuous development which is likely to even speed up in the future, since better computers now available allow many fascinating applications.

What are then the specific advantages of Monte Carlo "computer experiments"? To answer that question, one first notes that Monte Carlo methods yield information on "model systems" (where specific assumption about the effective forces between the atoms have been made) which in principle is numerically exact, i.e., the results are accurate apart from statistical erros which can be made as small as desired if only enough computing time is invested. Thus the purpose of the Monte Carlo method is twofold: comparing the results with data from experiments on real systems, one checks the extent to which a model system approximates a real system; and comparing the results to analytic theories starting with the same model, one checks the validity of various approximations made in the analytic treatment. In direct comparisons of theory and experiment it is often hard to separate the influence of errors due to inappropriate models and errors due to inappropriate approximations. It is one of the main purposes of the present book to clearly bring out this interplay between computer simulation and experiment on the one side and theory on the other side, and the progress which thereby is obtained. One more advantage then is that one obtains a microscopic information on the system both in space and in time; this information can be much more detailed than what is available from experiments on real systems, and hence it gives insight into some problems which cannot be obtained else. This insight may stimulate new theoretical descriptions as well as new experiments. For all these reasons, Monte Carlo computer experiments

are a valuable tool for many branches of statistical physics, and since their application is relatively simple they will become a standard method of scientific research in the near future.

In the present book, first the theoretical background and the efficient practical implementation of this method are described, and then an up-to-date review of widespread applications is given: calculation of thermal properties and scattering functions for dense gases, fluids and plasmas; short- and long-range order properties of metallic alloys and various magnetic systems including the behavior near "critical points"; ground state properties of quantum fluids; thermal properties and structure of microscopically small liquid droplets and solid "clusters" of molecules; relaxation phenomena and diffusion in solids; kinetics of crystal growth and of other phase transformations; structural and magnetic properties of surfaces and adsorbed layers, and the kinetics of adsorption on surfaces; structural and thermal properties of disordered systems like glasses and amorphous magnets, etc. So far, these applications have been scattered throughout the literature, and it was necessary to bring together from several countries a team of leading experts in this field to accomplish such a review for the first time: D. Ceperley and M.H. Kalos from New York University, D.P. Landau from the University of Georgia, D. Levesque, J.P. Hansen, and J.J. Weis from Orsay, H. Müller-Krumbhaar from Jülich and D. Stauffer from Cologne. It is a pleasure to thank them for their fruitful collaboration.

Jülich, September 1978 *Kurt Binder*

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