Numerical investigations of phase transitions and critical phenomena

M. I. Tribel'skiĭ

Usp. Fiz. Nauk **154**, 174 (January 1988)

O. G. Mouritsen. *Computer Studies of Phase Transitions and Critical Phenomena.* Springer-Verlag, Berlin; Heidelberg; New York; Tokyo, 1984. pp. 200 (Springer Series in Computational Physics).

The book being reviewed belongs to the series "Computational Physics" and was written by the well-known specialist in this field—Danish physicist, O. Mouritsen. The material of the book is based to a large extent on the author's own work, and this is at the same time both its merit (a deep understanding of the problems being discussed, a clear presentation of the material), and also its defficiency (due to the relatively narrow range of problems being discussed it is impossible to acquire an overall view that is in some measure complete concerning the state of affairs in this field of physics).

The book can tentatively be divided into two parts. In the first part a brief presentation is provided of the basic information from the modern theory of phase transitions and critical phenomena: definitions are given of the order parameter, critical indices etc. The Monte Carlo method is also presented here in detail—from general principles on which the method is based to its different specific realizations in carrying out numerical calculations. The difficulties of numerical investigation of phase transitions are discussed (slow convergence of the modelling process in the neighborhood of the point of transition due to the increase in the relaxation time; the effect of the finite dimensions of the system; the statistical dependence of the fluctuations due to an increase in the correlation radius etc.) and also the methods of overcoming them. This part of the book also contains a brief characterization of the technical possibilities of modern computers, including the latest models of computers for specific applications, such as the computer of the University of Santa Barbara constructed specially for research on the Ising model. In addition to the direct simulation of phase transitions by the Monte Carlo method semianalytic methods of research are also discussed, in which the computer is used to calculate the coefficients of a series, the summation of diagrams, etc.

The second part of the book is devoted to a discussion of specific examples of using numerical methods in the theory of phase transitions. In this part in turn one can distinguish three sections:

1. Numerical study of different variants of the Ising and Heisenberg models which also admit to some degree an analytic investigation in order to compare the numerical and analytic results.

2. Numerical checking of the principal hypotheses of modern theory of phase transitions and critical phenomena.

3. Direct numerical experiments on the study of complex physical objects (phase transitions in a double layer of lipid molecules, simulating biological membranes, and the model of nuclear spin systems with a dipole interaction, such as CaF_2; LiH; LiF and others, and also the model of a layer of homopolar molecules of the N_2; H_2; D_2, type absorbed on the surface of graphite, for which a study is made of orientational phase transitions and the kinetics of the growth of ordered domains in the case of a discontinuous transition of a system through the temperature of the phase transition).

The book is undoubtedly of interest for specialists working in this field of computational physics, but for a first acquaintance with the subject it is too fragmentary.

Translated by G. M. Volkoff