THEORY OF CRITICAL PHENOMENA IN FINITE-SIZE SYSTEMS

Scaling and Quantum Effects

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Scaling and Quantum Effects

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To our children

Milena and Valentin,
Marin,
Ivailo and Rossen

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Preface

It is hard to find a field in theoretical physics which can compete with the theory of phase transitions and critical phenomena with respect to the number of written textbooks, reviews and monographs. In our opinion, writing a new book can be justified only by treating in a different manner new trends existing in the area. What do we have in mind in our case? There are just a few books on critical phenomena in systems with confined geometry: a collection of reprints [Cardy, ed. (1988)], a collection of reviews [Privman, ed. (1990)], and the monograph [Krech (1994)] on the Casimir effect. Indeed, in some modern texbooks on critical phenomena one can find special chapters devoted to this topic, see, e.g., [Cardy (1996)], [Domb (1996)], [Zinn-Justin (1996)], [Henkel (1999)]. Against the background of the numerous papers that appear annually, the gap in the monographic literature on the subject is obvious. The present book attempts to partially fill up this gap. We hope also to give our modest contribution in spreading the scaling ideas for fruitful interpretation and analysis of phase transitions in classical and quantum systems of finite volume.

It is a well known fact that the volume is an irrelevant parameter for the local properties of a macroscopic system and, therefore, can be chosen arbitrary large. The conventional statistical mechanical theory studies abstract systems, consisting of infinitely many particles in an infinite volume, due to the essential simplifications that occur in their description. Moreover, it becomes possible to describe phase transitions mathematically in terms of discontinuous or singular behavior of some thermodynamic functions. In constructing the above, so called thermodynamic limit [Van Hove (1949)], [Fisher (1964)], one has to keep constant values of some intensive quantities. For example, in the canonical Gibbs ensemble the increase in the number of particles N has to be accompanied by a proportional increase in the volume V, so that the density $\rho = N/V$ be constant. Any intensive quantity a_V of a finite system can be written in the form $a_V = a_\infty + \delta a_V$, where a_∞ is the bulk value and δa_V is a finite-size correction which tends to zero as $V \to \infty$. The finite-size correction δa_V contains a more detailed information about the shape of the system and the boundary conditions. Usually, the correction term becomes essential under rather special conditions, e.g., in the vicinity of a second-order phase transition. When the relevant thermodynamic parameters approach a critical point, the correlation length ξ of an infinite system will grow unboundedly. Therefore, if we apply the theory of infinite (bulk) systems for the description of a large but finite system, very close to the critical point the bulk correlation length will become comparable with the smallest size of the system and deviations from the real critical behaviour will set in.

In the beginning of the 70's, M. Fisher and his followers developed a comprehensive theory of finite-size scaling. As in the bulk case, this theory of critical behaviour of finite systems is based on renormalization group properties and offers a universal description depending, in addition, on the shape of the system and the type of boundary conditions.

During the last two decades, the study of finite-size effects has undergone an extensive development and gained still growing importance for the theory of phase transitions and critical phenomena. The factors stimulating the interest in these studies may be classified in three groups.

1. On the one side, singularities in intensive thermodynamic functions may appear only in the limit of an infinitely large system. On the other side, all the experimental observations pertain to finite samples. As mentioned above, finite-size effects necessarily become essential near a critical point. This fact, combined with the traditional difficulties in the description of strongly interacting many-particle systems, poses a serious challenge to the theory. The study of the universal features of finite-size effects, which arise due to large-scale collective behaviour (highly correlated classical or quantum fluctuations), is a subject of the modern theory of finite-size scaling. The latter theory reveals the intimate mechanism of how the critical singularities build up in the thermodynamic limit, as well as the role of boundary and shape effects.

2. The interpretation of experimental results on finite-size effects in real systems is not a simple task for several reasons. First of all, they are de-

tectable only in samples of a rather small size (in all, or at least one spatial dimension), and are generally mixed up with strong effects due to gravity, impurities, or other inhomogeneities. In practice, the divergence of the correlation length is limited also by the finite temperature resolution. Nevertheless, the high precision of some modern experimental techniques makes finite-size effects accessible. Correlation lengths of the order of hundreds of nanometers have been achieved. A number of successful measurements have been performed and substantial progress has been made in overcoming most of the standing problems. There are various types of experimental results, for which the theory of finite-size effects seems relevant. Such are the specific heat and superfluid density measurements near the superfluid ("lambda") transition of liquid helium in small pores and thin films [Gasparini and Rhee (1992)], [Nissen et. al. (1993)]; or the direct measurements of magnetization in nanoscale ferrimagnetic particles [Tang et. al. (1991)], [Kulkarni et. al. (1994)]. In some binary fluids (2.6-lutidine and water) demixed between narrowly spaced plates [Scheiber et. al. (1979)], shifts in the critical temperature T_c as large as 100 mK have been observed. Magnetic insulators, such as transition metals difluorides, can be epitaxially grown in very thin films. The latter show both finite-size shift in the critical point and rounding of the thermodynamic singularities. It is an experimental observation that the specific heat as a function of temperature shows one or two maxima, depending on the layer thickness [Lederman et. al. (1993a)], [Lederman et. al. (1993b)], in quantitative agreement with the theory of finite-size scaling. Highly precise measurements of magnetic phase transitions in some ultrathin Fe and Ni films exhibit thickness dependence of T_c and crossovers between different regimes which reveal important aspects of the universality hypothesis and finite-size scaling theory [Durr et. al. (1989)], [Li and Baberschke (1992)]. Some layered superconductors (including high-temperature superconductors) also exhibit a pronounced size effect in T_c which has been discussed in [Michielsen et. al. (1991)], [Schneider (1991)].

3. Along with the development of highly productive computer systems, the numerical methods of modelling took a prominent place between the laboratory experiment and theory in the study of phase transitions and critical phenomena. Since, due to technical limitations, one works with rather small systems consisting of, say, up to 10^6 particles, the finite-size effects in the numerical data are essential. It is the finite-size scaling theory

which is the most reliable tool for extrapolation to the thermodynamic limit of data obtained by Monte Carlo and Molecular Dynamics simulations, as well as by transfer-matrix calculations, or exact diagonalization of the Hamiltonian for small lattice systems.

The aim of the present book is to familiarize the reader with the rich collection of ideas, methods and results relevant to the theory of critical phenomena in systems with confined geometry. At that the authors believe in the instructive role of the simple models approach towards the better understanding of complex physical systems. Thus, by following a tradition which exists from the very beginning of the theory of phase transition, we put the accent on the derivation of rigorous and exact results. We have confined ourselves to the investigation of few exactly solved models which allow one to derive analytical expressions for the physical quantities of interest, preferably at any space dimensionality.

Here it is in place to emphasize that the thermodynamic limit leads to great simplifications in the analytical results. In the case of finite systems, the derivation of exact results (valid for any finite number of particles) is a much more complicated task. Hence, the number of models subject to rigorous finite-size analysis is extremely limited. For example, even in the case of ideal gases, see [Ziff et. al. (1977)], one has to avoid taking the usual limit (as $V \to \infty$)

$$\frac{1}{V}\sum_{\mathbf{k}} \to \frac{1}{(2\pi)^d}\int \mathrm{d}^d\mathbf{k},$$

where d is the space dimensionality, and the sum runs over the set of normal modes which depends on the shape of the system and the boundary conditions. Obviously, the starting expressions one usually has at hand for finite systems are very cumbersome. Moreover, one has to derive their asymptotic form in special regimes, when the values of the temperature and the relevant external fields tend to the critical point together with $L \to \infty$, so that the ratio L/ξ remains of the order of unity. Such a finite-size scaling analysis requires specific analytical techniques, the description of which takes a due place in the present book. Some of the calculations are performed rather circumstantially, so that the reader could master the mathematical tools, the details of which are usually lacking in the specialized papers on the subject.

Of course, the selection of the material in a monograph depends on the taste and professional interests of its authors. The present case is not an exception. Attention is paid to some specific problems and mathematical tools characteristic of the case of long-range interactions with power-law decay. Another example is the probabilistic point of view on finite-size scaling which makes close connection with the concept of limit Gibbs states. Of special interest to the reader could be the investigation of systems in which the quantum fluctuations play an essential role together with the thermal ones. The extension of the finite-size scaling theory to such systems is based on the observation that the Gibbs weight $\exp(-\beta\mathcal{H})$, where $\beta = (kT)^{-1}$ is the inverse temperature, and $\mathcal{H}$ is the Hamiltonian, is formally identical with the time evolution operator $\exp(it\mathcal{H}/h)$ upon replacement of time t by the imaginary quantity $ih\beta$. Hence, the partition function of a quantum system looks like a classical partition function with an additional dimension, except that this extra dimension is of finite extent βh in units of time. When the temperature goes to zero and the quantum effects become important, the size in this "imaginary time direction" tends to infinity. This observation provides an useful interpretation of quantum effects as finite-size effects.

Confined critical systems, due to the presence of strong fluctuations, exhibit appearance of long-range forces between the walls - a phenomenon which is the direct analogue of the well-known Casimir effect in electromagnetism. There are different model approaches for obtaining the universal scaling functions that govern the Casimir forces. In this book a detailed, pedagogical account is given of the exact results obtained in the spherical approximation for both classical and quantum systems. Finally, we present a survey of the theoretical results known for other models, make comments and give reference to experimental results.

Unfortunately, many important topics are omitted due to the lack of space and expertize on the part of the authors.

The exposition of the main issues is given in a self-contained form which presumes the reader's knowledge in the framework of standard courses on the theory of phase transitions and critical phenomena. The authors experience in the preparation of one-semester courses for students at the Catholic University of Leuven (JGB) and the University of Wuppertal (DMD) is taken into account.

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