Finite Size Scaling and Numerical Simulation of Statistical Systems

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PREFACE

This book presents a collection of review articles providing both an introduction and a survey of recent advances in the field of *Finite Size Scaling* in phase transitions and related disciplines. Both theoretical foundations and numerical methods are covered. This includes scaling theory, the renormalization group approach, Monte Carlo and transfer matrix numerical applications, and recent uses of finite size scaling in Lattice Gauge Theory and for random systems.

Finite size scaling theory attempts to describe how *long-scale, collective phenomena* associated with the onset of large fluctuations near critical points, at first order phase transitions, in polymer systems, etc., manifest themselves in small samples (capillaries, pores), and in *numerical computer simulations* which are always done on limited-size lattice or continuum models. The latter application of finite size scaling theory has grown in importance in the last decade. Indeed, the advances in large-scale computing, based largely on the Monte Carlo method, have allowed accurate evaluation of bulk, surface, and interfacial properties of statistical mechanical models, as well as applications in particle physics, polymers, and random systems. All these studies employ finite size scaling ideas and also provide stimuli for theoretical advances, suggesting new emphases, topics, and testing the existing theoretical predictions.

Reviews in this book offer convenient reference sources, introductions, and guides to current research, with an emphasis on various numerical methods and their relations to finite size effects. Each review has a substantial introductory component, and the book as a whole should be accessible to readers with no special prior knowledge of finite size scaling theory or details of its applications in conjunction with numerical methods. However, a general background in phase transitions or a related field is assumed.

The first three reviews (Chapters I-III), by Privman, Jasnow, and Rudnick, are theoretical. They provide an introduction to the modern theory of finite-size effects. Chapter I summarizes *scaling theory* and related approaches, for critical points, for interfacial properties, and also for first-order transitions. In Chapter II, field-theoretical techniques are surveyed, culminating in the formulation of the renormalization group method for finite systems. Then, Chapter III presents results for spherical models which serve to illustrate and test the general theoretical predictions.

The next three chapters (Chapters IV-VI), by Binder, Landau, and Mon, review applications of the finite size scaling theory in *Monte Carlo numerical studies* of critical phenomena. All three reviews describe quantities, geometries, and scaling results in the formulation appropriate for Monte Carlo data analyses. Specific results for selected models and details of their numerical derivation followed by finite-size analysis are described, illustrating the general versatility and growing importance of the Monte Carlo method. The emphasis in Chapter IV is on general definitions, anisotropic systems, and other recent results. Chapter V presents diverse examples of applications of Monte Carlo methods to critical points and first-order transitions. The focus of Chapter VI is on universal finite-size amplitudes and associated geometry related properties such as surface and corner free energies, etc.

Recent theoretical developments related to conformal invariance and other new exact results obtained for *two-dimensional models* have generated further interest in *numerical techniques based on the transfer matrix method.* In two dimensions, the transfer matrix approach, termed phenomenological renormalization, is among the most powerful methods of estimating critical-point quantities. Foundations of the phenomenological renormalization method, selected results, and their finite size scaling analyses are reviewed in Chapters VII and VIII by Nightingale and Henkel. Chapter VII is centered on more conventional isotropic model results, as well as on a general overview of the field. Chapter VIII is devoted to the quantum Hamiltonian variant of the method. Both chapters discuss connections with conformal invariance and other exact results in two dimensions, and also recent applications of the phenomenological renormalization method to three-dimensional systems.

The last three chapters of the book (Chapters IX-XI), by Bhanot, Young, and Schulman, are devoted to finite size effects in systems for which the theoretical framework, and the appropriate nomenclature, are outside the more "traditional" uses of finite size scaling ideas in phase transitions. Thus, Chapter IX describes applications of finite size scaling, including a survey of recent numerical results, in Lattice Gauge Theories of *particle physics.* Chapter X is devoted to spin glasses. Generally, for *random systems*, new aspects of the finite size behavior enter, related to long equilibration times, and to averaging over randomness. Finally, Chapter XI introduces finite size effects associated with metastable phases.

The editor wishes to express his thanks to C.R. Doering and M.E. Fisher for their interest in this project and valuable suggestions, and to the contributing authors for a job well done. He hopes that in addition to being a comprehensive summary/introduction, this book will convey the excitement and dynamics of a rapidly growing and developing field of science.

Vladimir Privman

October 1989

Potsdam, New York

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*Each review has a separate, detailed table of contents.

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FINITE-SIZE SCALING THEORY

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1. INTRODUCTION

1.1. *Opening Remarks*

In this chapter we review the finite-size scaling theory of continuous phase transitions (critical points), as well as certain results on finite-size effects at first-order transitions, and also for systems with fluctuating interfaces. Studies of finite-size effects are important in interpreting experimental data and numerical results of Monte Carlo (MC) and transfer matrix calculations, and in connection with other theoretical developments, notably, conformal invariance and surface critical phenomena.

Our exposition will be biased towards numerical data analyses where a prototype finite-size system is d-dimensional hypercubic, L^d, or nearly hypercubic-shaped, or cylindrical, $L^{d-1} \times \infty$, (for transfer matrix studies). Much of our discussion will refer to the theoretically most studied case of *periodic boundary conditions* which are a natural choice in many MC and transfer matrix applications. Results for other boundary conditions will be described, when available. While most of the considerations will be quite general, we will use the nomenclature of the ferromagnetic n-vector models on regular d-dimensional lattices. Note that transfer matrix calculations are usually performed in $d = 2$. Only recently, some $d = 3$ studies have been reported. On the other hand, MC calculations can be carried out in dimensionalities as high as $d = 5$ or 6.

1.2. *Outline of the Review*

As previously mentioned, this chapter is devoted to scaling theories of finite-size effects. Other chapters of this book cover calculational methods, *e.g.*, the Renormalization Group (RG) approach, and numerical applications.

Since the introduction of the finite-size scaling ideas by Fisher and co-workers in early seventies, several comprehensive expository and review articles have appeared covering both the original scaling ideas and later advancements, see, *e.g.*, [1-7]. Some of the important contributions have been reprinted in [8]. In the following subsection of the introduction (Sect. 1.3) a simple finite-size scaling ansatz [1] will be explained.

The modern form of the critical-point finite-size scaling [9], reviewed in Sect. 2, incorporates *hyperscaling* ideas and leads to the identification of universal finite-size critical-point amplitudes. Universal amplitudes and, more generally, universal quantities derivable from finite-size scaling functions have been estimated by numerical

MC, exact $2d$ conformal invariance, and numerical transfer matrix calculations. These studies are selectively surveyed in Sect. 3: a more comprehensive review can be found, *e.g.*, in [10].

Sections 4 and 5 are devoted, respectively, to interfacial finite-size properties, and to first-order transitions. Size effects on interfacial fluctuations (Sect. 4) both near T_c and below T_c, are quite diverse and have been studied relatively recently. Finite-size rounding of first-order transitions (Sect. 5) involves an interesting phenomenon of the emergence of characteristic finite-size length scales. Finally, brief summary remarks are given in Sect. 6.

1.3. *Basic Scaling Postulate*

Near the critical point at $t = 0$, $H = 0$, where

$$t \equiv (T - T_c)/T_c \quad , \tag{1.1}$$

and H is the ordering field, various thermodynamic quantities diverge. The bulk ($L = \infty$) zero field critical behavior of, *e.g.*, the specific heat, $C(t, H; L)$, is given by

$$C_s(t, 0; \infty) \approx (A_\pm/\alpha)|t|^{-\alpha}, \tag{1.2}$$

where s denotes "singular part", and the exponent α is included in the amplitudes for historical reasons. The standard scaling expression in nonzero field (see, *e.g.*, a review [11]) is

$$C_s(t,H;\infty) \approx |t|^{-\alpha} \mathcal{C}_{\pm}\left(H|t|^{-\Delta}\right), \tag{1.3}$$

where $\mathcal{C}_{\pm}$ are certain scaling functions. As usual, in the above expressions the $+-$ refer to $t > 0$ and $t < 0$, respectively; the sign $\approx$ indicates that corrections to scaling have been omitted. The exponents α and $\Delta = \beta + \gamma$ are universal, as is the ratio A_+/A_-. The full scaling functions $\mathcal{C}_{\pm}$ can be made universal by introducing proper metric factors for t and H; see Sect. 2.1-2.2 and further below.

For finite-size systems it has been recognized [1,12,13] that the system size L "scales" with the correlation length $\xi(t,H;\infty)$ of the bulk system. (Strictly speaking, this is only true in $d = 2,3$, see Sect. 2.1.) Indeed, if $L >> \xi(t,H;\infty)$, no significant finite-size effects should be observed. On the other hand, for $L \leq \xi(t,H;\infty)$, the system size will cut-off long-distance correlations so that an appreciable finite-size rounding of critical-point singularities is to be expected. Since the bulk correlation length scales similarly to (1.3),

$$\xi(t,H;\infty) \approx |t|^{-\nu} \Xi_{\pm}\left(H|t|^{-\Delta}\right), \tag{1.4}$$

the finite-size scaling combination is naturally $L/|t|^{-\nu}$. Thus one assumes

$$C_s(t,H;L) \approx |t|^{-\alpha} \tilde{\mathcal{C}}_{\pm}\left(H|t|^{-\Delta}; L|t|^{\nu}\right), \tag{1.5}$$

$$\xi(t,H;L) \approx |t|^{-\nu} \tilde{\Xi}_{\pm}\left(H|t|^{-\Delta}; L|t|^{\nu}\right), \tag{1.6}$$

with similar expressions for other quantities [1]. It is interesting to note that no new critical exponents were introduced in (1.5)-(1.6).

Relations (1.5)-(1.6) already yield many useful predictions, for example,

$$C_s(0,0;L) \propto L^{\alpha/\nu} \quad \text{and} \quad \xi(0,0;L) \propto L\,. \tag{1.7}$$

However, it turns out that additional rearrangement is quite useful. It involves four steps. Firstly, we use the so-called L-scaled instead of the t-scaled relations, *i.e.*, we redefine the scaling functions to have L enter in nonanalytic powers, while t and H enter linearly in combinations $tL^{1/\nu}$ and $HL^{\Delta/\nu}$. Secondly, we note that for a finite-size system there is actually no singularity at $t, H = 0$. Therefore, the scaling function will be smooth, analytic at the origin $tL^{1/\nu}, HL^{\Delta/\nu} = 0$. No distinct $\pm$ functions are needed. The third step is to allow for nonuniversal metric factors for t and H, by using scaling combinations $atL^{1/\nu}$ and $bHL^{\Delta/\nu}$. Then the scaling functions will be universal. It turns out that no metric factor is needed for L, see [9]. This issue will be further explored in Sect. 2.1-2.2. The final point is to use *free-energy density*, f, measured per k_BT, instead of the specific heat. Note that in terms of the singular parts, we have a simple relation

$$C_s = -k_B \frac{\partial^2 f_s}{\partial t^2} \quad . \tag{1.8}$$

Various thermodynamic quantities follow from the free energy by differentiation.