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Monte Carlo tests of theoretical predictions for critical phenomena: still a problem?

K. Binder *, E. Luijten

Johannes-Gutenberg-Universität, Institut für Physik, WA 331, D-55099 Mainz, Germany

Abstract

Two Monte Carlo studies of critical behavior in ferromagnetic Ising models are described: the first one deals with the crossover from the Ising class to the mean field class, when the interaction range increases. The second study deals with the finite size behavior at dimensionalities above the marginal dimension where Landau theory applies. The numerical results are compared to pertinent theoretical predictions, and unsolved problems are briefly described. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Since the development of renormalization group methods [1–3] the theory of critical phenomena has seen spectacular progress. However, there are still a number of challenging problems: e.g., while an impressive accuracy in the estimation of critical exponents has been reached (see, e.g., [3–5]), the accuracy of work dealing with the study of crossover phenomena from one universality class to another is much less good. This is true even for the simplest case; crossover from the Ising universality class to Landau mean field behavior as the range of interaction R increases [6–15,19,17]. This problem is experimentally relevant for the understanding of critical phenomena both in small molecule fluids [18] and in polymer mixtures [16,20,21]. Monte Carlo simulations now can provide benchmarks against which various theoretical approaches can be tested [13–15,17].

Another issue where there has been a longstanding controversy between theory and simulation is the question of finite size scaling at dimensionalities d above the marginal dimension d^* where mean field theory becomes valid [22–30]. For systems with short range forces, $d^* = 4$, so in $d = 5$ all critical exponents (including corrections to scaling) are known, and hence finite size scaling methods can be exposed to a stringent test. However, it will be shown that comparison between theory [29] and simulation [30] is still disappointing!

2. Monte Carlo study of crossover for Ising models with medium range interactions

While the (normalized) susceptibility $\hat{\chi} \equiv k_B T_c (\partial m/\partial H)_T$ in the mean field limit obeys a simple Curie–Weiss law, $\hat{\chi} \propto t^{-1}$ where t is the reduced temperature distance from the critical temperature T_c, $t = T/T_c - 1$, a nontrivial exponent (γ) applies in

* Corresponding author. E-mail: kurt.binder@uni-mainz.de.

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the Ising universality class, $\hat{\chi} \propto t^{-\gamma}$, with $\gamma = 7/4$ in $d = 2$ and $\gamma \approx 1.24$ in $d = 3$ [1–5]. Here we consider a model with a large but finite range R of the exchange interactions J_{ij} between spins at sites $\vec{r}_i, \vec{r}_j$, with $J_{ij} = J$ if $r = |\vec{r}_i - \vec{r}_j| \leqslant R_m$ but $J_{ij} = 0$ elsewhere,

$$R^2 = \sum_{j(\neq i)} J_{ij} r^2 / \sum_{j(\neq i)} J_{ij} = z^{-1} \sum_{j(\neq i),\ r \leqslant R_m} r^2,$$
$$z = \sum_{j(\neq i),\ r \leqslant R_m} 1. \qquad (1)$$

Now one expects that in the limit $t \to 0$ Ising exponents are observed, irrespective of R; however, if t is small but still larger than the so-called "Ginzburg number" G [31] one expects to see an "effective exponent" close to the mean field value (1). Such effective exponents are defined as ($\pm$ refers to $T \gtrless T_c$)

$$\gamma_{\text{eff}}^{\pm} \equiv -d \ln \hat{\chi} / d \ln |t|. \qquad (2)$$

Since the variation of γ_{eff} is spread out over many decades in the crossover scaling variable t/G, see Fig. 1, calculation of γ_{eff} by computer simulation has been a particular challenge – only very recently this challenge could be overcome [13–15,17] by combining data taken for a wide range of values of R, noting that $G = G_0 R^{-6}$ in $d = 3$ and $G = G_0 R^{-2}$ in $d = 2$ [11,31]. Of course, simulation of the critical behavior of systems with large R requires the use of huge lattice sizes: this has only become possible due to the invention of a novel cluster algorithm [32] whose efficiency does not deteriorate when R increases. With this algorithm, estimation of $\gamma_{\text{eff}}^{\pm}$ also has been possible in $d = 2$, where predictions of corresponding analytical theory are completely lacking. Note that the variation of γ_{eff}^{-} is nonmonotonic, i.e. $\gamma_{\text{eff}}^{-} \approx 0.85$ for $tR^2 \approx -1$ (Fig. 2) while for $T > T_c$ no such minimum occurs.

Fig. 1 shows that the theoretical curves all disagree with the Monte Carlo data for $t/G \lesssim 10$. However, one does expect that a universal crossover scaling function does exist in the limit $G \to 0, t \to 0, G/t$ finite. A possible interpretation of the discrepancy in Fig. 1 is the idea of Anisimov et al. [12,18], that for not too small G (i.e. not too large R) a second variable is needed to describe the crossover in addition to G, namely the short wavelength cutoff Λ. Thus γ_{eff} in Figs. 1, 2 is not a unique function, but it fans out at the Ising side in a family of curves (each value of R then belongs to a piece of a different curve) [18].

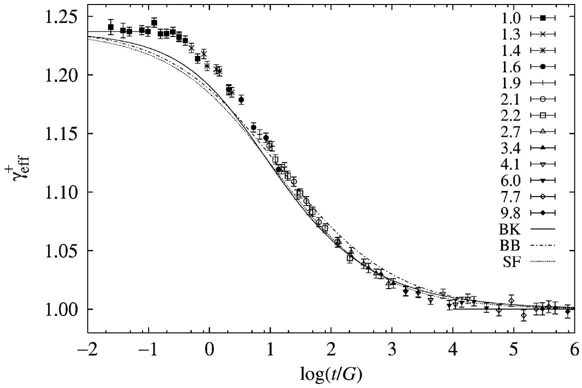

Fig. 1. Effective susceptibility exponent γ_{eff}^{+} for the $d = 3$ variable range Ising model on the simple cubic lattice for $T > T_c$ plotted vs. the logarithm of the crossover scaling variable. Different symbols show various choices of R, as indicated. Three theoretical predictions are included: Belyakov–Kiselev (BK) [9], Bagnuls–Bervillier (BB) [8] and Seglar–Fisher (SF) [6]. From Luijten and Binder [17].

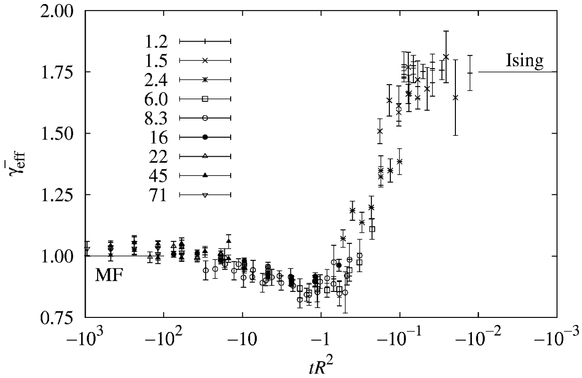

Fig. 2. Effective susceptibility exponent γ_{eff}^{-} for the $d = 2$ variable range Ising model on the square lattice for $T < T_c$ plotted vs. tR^2; different symbols show various choices of R, as indicated. From Luijten et al. [14].

While a description of both experiments [16] and the Ising simulations [18] with this theory [12] is possible, it is not very satisfactory since several adjustable parameters occur. Also the question must be asked how accurate the universal limit of the scaling function in Fig. 1 is known – after all the three analytical results are not in full mutual agreement either, and some are based on somewhat uncontrolled extrapolations of low order renormalization group expansions.

3. Finite size scaling for the five-dimensional Ising model

The theory of finite size scaling [33–35] is one of the standard tools to extract information on critical properties from Monte Carlo simulations on finite lattices. However, since usually neither the leading critical exponents nor the corrections to scaling are known exactly, usually a lot of parameters have to be determined simultaneously, and hence the judgement of accuracy is subtle.

In view of this fact, the Ising model in $d = 5$ is a nice "laboratory" for computer simulation, since the exponents are known precisely. Thus, the singular part of the free energy for a finite hypercubic lattice of volume L^d (and periodic boundary conditions) scales as [34–36]

$$f_L = L^{-d}\tilde{f}\bigl\{t(L/\xi_0)^2, hL^{1+d/2}, uL^{4-d}\bigr\}, \tag{3}$$

where the first argument of the scaling function $\tilde{f}$ could also be written as $(L/\xi)^2$ with $\xi = \xi_0 t^{-1/2}$ the correlation length in mean field. The second term involves the field h conjugate to the order parameter, and the last term the coefficient u of the quartic term in the Landau expansion. Although $uL^{4-d} \to 0$ for $L \to \infty$ in $d > 4$, this term must not be omitted since u is a "dangerous irrelevant variable" [2,36].

Introducing a corresponding length ℓ_0 via $u \propto \ell_0^{d-4}$, we can write the susceptibility and the cumulant ratio $Q \equiv \langle M^2\rangle^2/\langle M^4\rangle$ of the magnetization as follows

$$\chi = -\frac{\partial^2 f_L}{\partial h^2}\bigg|_{h=0} = L^2 P_\chi\bigl\{t(L/\xi_0)^2, (L/\ell_0)^{4-d}\bigr\}, \tag{4}$$

$$Q = P_Q\bigl\{t(L/\xi_0)^2, (L/\ell_0)^{4-d}\bigr\}. \tag{5}$$

Eqs. (4), (5) differ from standard finite size scaling forms for $d < d^*$ [$\chi = L^{\gamma/\nu}P_\chi(tL^{1/\nu})$, $Q = P_Q(tL^{1/\nu})$, where $\xi \propto t^{-\nu}$] by the presence of a second variable.

However, it soon was suggested [22,23] that for $L \to \infty$ Eqs. (4), (5) reduce to a one-variable scaling form, but with ξ being replaced by the "thermodynamic length" $\ell_T \propto t^{-2/d}$,

$$\begin{aligned}
&\chi \to L^{d/2}\widetilde{P}_\chi\bigl\{tL^{d/2}\xi_0^{-2}\ell_0^{(4-d)/2}\bigr\},\\
&Q \to \widetilde{P}_Q\bigl\{tL^{d/2}\xi_0^{-2}\ell_0^{(4-d)/2}\bigr\}\\
&\quad = \widetilde{P}_Q\bigl\{(L/\ell_T)^{d/2}\bigr\}, \quad L \to \infty.
\end{aligned} \tag{6}$$

Brézin and Zinn-Justin [24] then suggested that one could also find the scaling functions $\widetilde{P}_\chi$ and $\widetilde{P}_Q$ explicitly, noting that one should single out from the effective Boltzmann factor the contribution of the uniform magnetization M,

$$\exp\left[-\frac{\mathcal{H}\{S_i\}}{k_B T}\right] = \exp\left[-\frac{(M^2/M_b^2 - 1)^2}{8k_B T\chi_b/M_b^2}L^d + \cdots\right], \tag{7}$$

where M_b, χ_b are the mean field bulk magnetization $\{M_b \propto (-t)^{1/2}\}$ and susceptibility, respectively, and the terms not written represent nonuniform magnetization fluctuations.

Eqs. (6) result from the "zero mode theory" that neglects these fluctuations altogether; i.e. the distribution of the magnetization in the finite system is simply

$$P_L(M) \propto L^{d/2}\exp\bigl\{-\bigl[M^2/M_b^2 - 1\bigr]^2(L/\ell_T)^d/8\bigr\}. \tag{8}$$

In particular, for $t = 0$ ($T = T_c$) one obtains [24] $\widetilde{P}_Q(0) = 8\pi^2/\Gamma^4(1/4) \approx 0.456947$ in $d = 5$, but this seemed to be in conflict with the Monte Carlo results [22,23,25]!

Now recently Chen and Dohm [29,37] criticized all previous work [22–28], claiming that one must not take the step in Eqs. (6), (7) that yields Eq. (8), and suggesting that one always must keep both arguments of P_Q and P_χ.

In view of this criticism, it is clearly appropriate to reanalyze this problem and compare recent very precise Monte Carlo data with the predictions of [29] as well. Fitting the susceptibility for $t > 0$ and large L to the Curie–Weiss law, we obtain the amplitude $\xi_0 \approx 0.549$, taking the lattice spacing as our unit of length [30]. Fitting χ at T_c for $L \to \infty$ to the appropriate power law, $\ell_0 = 0.603$ is found, and hence a comparison with the theory of [29] could be performed without any other adjustable parameters. Fig. 3 shows that both the Monte Carlo data and the theory [29] converge towards the "zero mode" results as L increases: however the Monte Carlo data lie systematically below the asymptotic curve, and the theory of [29] lies above it! An expanded view

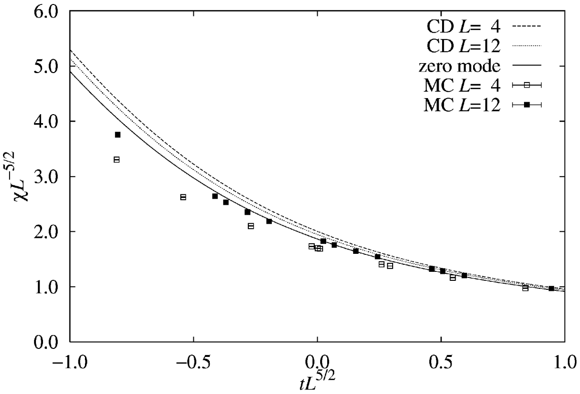

Fig. 3. Plot of $\chi L^{-5/2}$ versus $tL^{5/2}$ including Monte Carlo data for the nearest neighbor Ising lattice in $d = 5$, for $L = 4$ and $L = 12$. Broken curves show the corresponding predictions of Ref. [29], full curve is the zero mode result. From Luijten et al. [30].

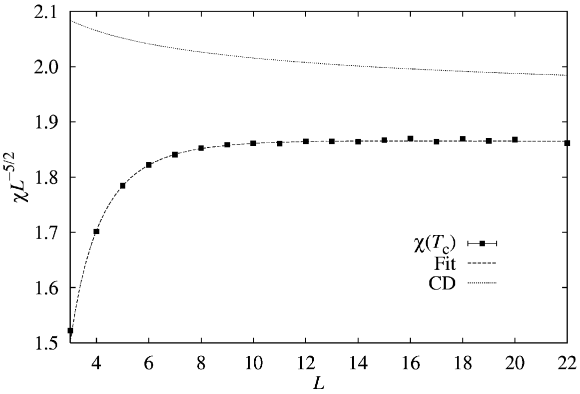

Fig. 4. Plot of $\chi L^{5/2} = p_0 + p_1 L^{-1/2} + p_2 L^{-1} + p_3 L^{-3/2}$, with $p_0 = 1.87 \pm 0.02$. Dotted curve is the result of [29], which converges to the same constant p_0 as $L \to \infty$. From Luijten et al. [30].

of the L-dependence at T_c (Fig. 4) shows that in the accessible range of L ($L \leqslant 22$) there are still pronounced deviations from the asymptotic behavior Eq. (6) present, but the theory of Chen and Dohm [29] clearly is not useful in this range of sizes. This failure may be due either to the neglect of terms of higher order than contained in the first order of the loop expansion, or to the presence of other corrections by which an Ising model might differ from a ϕ^4 theory on a lattice treated in [29].

4. Concluding remarks

In this work two simple aspects of the bulk critical behavior of ferromagnetic Ising models were discussed, and it was shown that both problems (crossover from one universality class to another, and finite size scaling above the marginal dimension) still are incompletely understood. Actually there are still many more problems about critical phenomena that deserve attention – interfacial and wetting phenomena, effects of random quenched disorder, etc., just to name a few. Progress in computer power and new algorithms – such as the cluster algorithm [32] emphasized here – allow to take a new look on these problems with computer simulation methods.

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