Non-perturbative Approaches in Nanoscience and Corrections to Finite-Size Scaling

J. Kaupužs and R. V. N. Melnik

Abstract Non-perturbative approaches in nanoscience are discussed. Traditional applications of these approaches cover description of charge transport and optical phenomena in nano-scale systems. We focus on finite-size effects in spin systems near the critical point, based on Monte Carlo (MC) method and some analytical arguments. We have performed MC simulations of the 3D Ising model for small, as well as large linear lattice sizes up to $L = 2560$, providing a numerical evidence for a recent challenging prediction, according to which the asymptotic decay of corrections to finite-size scaling is remarkably slower than it was expected before. Our approach along with several other non-perturbative approaches, like, e.g., the non-perturbative nonequilibrium Greens functions (NEGF) method, reveals a potential application of non-perturbative methods to nanoscience and nanotechnology through condensed matter physics, including semiconductor physics and physics of disordered systems like spin glasses.

Keywords Ising model · Non-perturbative methods · Finite-size effects Corrections to scaling · Critical exponents · Monte Carlo simulation

J. Kaupužs (✉)
Faculty of Materials Science and Applied Chemistry, Institute of Technical Physics, Riga Technical University, Paula Valdena Str. 3/7, Riga LV–1048, Latvia
e-mail: kaupuzs@latnet.lv

J. Kaupužs
Institute of Mathematical Sciences and Information Technologies, University of Liepaja, 14 Liela Street, Liepaja LV–3401, Latvia

J. Kaupužs · R. V. N. Melnik
The MS2 Discovery Interdisciplinary Research Institute, Wilfrid Laurier University, Waterloo, Ontario N2L 3C5, Canada
e-mail: rmelnik@wlu.ca

R. V. N. Melnik
BCAM - Basque Center for Applied Mathematics, E48009 Bilbao, Spain

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1 Introduction

Non-perturbative approaches like Monte Carlo (MC) simulation [1, 2] and non-perturbative nonequilibrium Greens functions (NEGF) method [3, 4] become increasingly important in nanoscience. Particular applications cover the description of charge transport and optical phenomena in nano-scale systems such as microelectronic devices, graphene layers, etc.

Perturbative approaches not always provide a satisfactory description of physical phenomena in such systems. For example, the recent results of [5] show that the many-body localization (MBL) in translation-invariant systems with two or more very different energy scales is less robust than perturbative arguments suggest. It possibly points to the importance of non-perturbative effects, which induce delocalization in the thermodynamic limit [5]. The importance of non-perturbative effects in laser-illuminated graphene nanoribbons has been demonstrated in [6].

Here we consider another application—behavior of small and large spin systems near the phase transition point, based on non-perturbative analytical evaluation of **k**-space integrals, as well as MC method. Lattice spin models are considered, where certain value of the spin variable is related to each lattice site. In the Ising model, the spin variable σ can take only one of two possible values ± 1. In the scalar φ^4 model, the spin variable φ can take any value within $-\infty < \varphi < \infty$. Such models exhibit second-order phase transition in the thermodynamic limit, where the linear lattice size L tends to infinity. The behavior of these models on finite lattices is described by the finite-size scaling. Moreover, the scaling behavior near the critical point can be remarkably varied depending on whether small or large lattices are considered. This effect is described by corrections to the leading scaling behavior.

Our analytical and MC results serve as a basis for a challenging prediction that the correction-to-scaling exponent ω has a remarkably smaller value $\omega \leq \omega_{\max} \approx 0.38$ than the usually accepted ones of about 0.83 [7] in the 3D φ^4 and Ising models. It implies a much slower decay of corrections to scaling than it was usually expected. We have performed MC simulations of the 3D Ising model for small, as well as large linear lattice sizes up to $L = 2560$, providing a numerical evidence for this challenging prediction.

The vicinity of critical point is not the natural domain of validity of any perturbation theory, therefore one should prefer non–perturbative approaches. Among them are:

- Exact and rigorous analytical solution methods (transfer matrix methods, combinatorial methods, Bethe-ansatz)
- Conformal field theory (CFT) analysis
- Non–perturbative renormalization group (RG) analysis
- Numerical transfer–matrix calculations
- Molecular dynamics simulations
- Monte Carlo (MC) simulations.

Recent study of hierarchical Edwards-Anderson model of spin glasses [8] has shown that non-perturbative effects can be really important in critical phenomena.

Namely, it has been found that the perturbative approach (ε-expansion) correctly predicts the existence of the critical point only in certain mean-field region of parameters. At the same time, non-perturbative calculations show that the critical point exists also in the non-mean-field region, where no phase transition is predicted by the ε-expansion. From the point of view of the renormalization group (RG) theory, the critical behavior in this region is described by certain non-perturbative fixed point [8].

The results of [8] refer to the phase transitions in spin glasses, whereas our analytical and MC arguments, discussed in this paper, allow us to question the validity and/or accuracy of the perturbative treatments even in the apparently very well studied case of the 3D Ising model.

Our approach along with several other non-perturbative approaches reveals a potential application of non-perturbative methods to nanoscience and nanotechnology through condensed matter physics as an example.

2 Finite-Size Effects

Finite-size effects are very important in nano-scaled systems. For example, the charge density in metal nanoparticles after absorption of oxygen shows a very interesting patterns, which essentially depend on the size of these nanoparticles [9]. As another example, the importance of finite-size effects in the many-body localization has been shown in [5].

In our study, it is demonstrated the finite-size effects are pronounced via the finite-size scaling. We consider behavior of spin systems near the phase transition point depending on the lattice size, using the standard arguments of the finite-size scaling theory. For example, magnetic susceptibility χ at the critical temperature scales as $\chi \propto L^{2-\eta}\left(1+\mathscr{O}\left(L^{-\omega}\right)\right)$ at $L \to \infty$, where η is the critical exponent, describing the leading asymptotic behavior, whereas the exponent ω describes the leading correction to scaling.

Finite-size scaling and corrections to scaling are important to understand the difference in the behavior of very small nano-scale systems and large systems in the thermodynamic limit.

3 Non-perturbative Analytical Arguments

First, we consider the continuous φ^4 model as one of the simplest basic models in a hierarchy of spin models. The Hamiltonian $\mathscr{H}$ of this model is given by

$$\frac{\mathscr{H}}{k_B T} = \int \left(r_0 \varphi^2(\mathbf{x}) + c(\nabla\varphi(\mathbf{x}))^2 + u\varphi^4(\mathbf{x})\right) d\mathbf{x}, \tag{1}$$

where k_B is the Boltzmann constant, T is the temperature, $\varphi(\mathbf{x})$ is the local order parameter—an n-component vector, which depends on the coordinate $\mathbf{x}$, and r_0, c, u are Hamiltonian parameters. Configurations of $\varphi(\mathbf{x})$ obey a constraint, represented by certain upper cut-off Λ for its Fourier components. Namely, the Hamiltonian in the Fourier representation reads

$$\frac{\mathscr{H}}{k_B T} = \sum_{i,\mathbf{k}} \left(r_0 + c\,\mathbf{k}^2\right) \mid \varphi_{i,\mathbf{k}} \mid^2 + u V^{-1} \sum_{i,j,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \varphi_{i,\mathbf{k}_1} \varphi_{i,\mathbf{k}_2} \varphi_{j,\mathbf{k}_3} \varphi_{j,-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3} \ , \quad (2)$$

where $\varphi_{j,\mathbf{k}} = V^{-1/2} \int \varphi_j(\mathbf{x}) e^{-i\mathbf{k}\mathbf{x}}\, d\mathbf{x}$ and $\varphi_j(\mathbf{x}) = V^{-1/2} \sum\limits_{k<\Lambda} \varphi_{j,\mathbf{k}} e^{i\mathbf{k}\mathbf{x}}$. Here V is the volume.

The Fourier-transformed two-point correlation function $G(\mathbf{k}) = \langle \mid \varphi_{j,\mathbf{k}} \mid \rangle^2$ is important in our following consideration. The case where r_0 is a linear function of T has been studied in [10], showing that, in this case, the leading singularity of specific heat C_V is given by an integral of $G(\mathbf{k})$ over wave vectors, i.e.,

$$C_V^{sing} = B \xi^{1/\nu} \left(\int\limits_{k<\Lambda} [G(\mathbf{k}) - G^*(\mathbf{k})] d\mathbf{k} \right)^{sing} , \quad (3)$$

where B is a constant, $G^*(\mathbf{k})$ is the critical correlation function, and the superscript "sing" implies the leading singular part, represented in terms of the correlation length ξ. It diverges as $\xi \propto \mid T - T_c \mid^{-\nu}$, approaching the critical temperature T_c.

Non-perturbative analytical calculation of this integral has been performed in [10], based on the well known scaling hypothesis (see, e.g., [11]),

$$G(\mathbf{k}) = \sum_{i \geq 0} \xi^{(\gamma-\theta_i)/\nu} g_i(k\xi) \ , \quad (4)$$

where γ and ν are the critical exponents of susceptibility and correlation length, the term with $i = 0$ (at $\theta_0 = 0$) is the leading term, the terms with $i > 0$ are corrections to scaling with positive correction-to-scaling exponents $\theta_i = \omega_i \nu$, and $g_i(k\xi)$ are scaling functions. The singularity of specific heat in the general form of $C_V^{sing} \propto (\ln \xi)^{\lambda} \xi^{\alpha/\nu}$ has also been accounted for.

In addition, it has been assumed that the contribution of small-k region $k < \Lambda'$ is relevant in the limit $\lim\limits_{\Lambda' \to 0} \lim\limits_{\xi \to \infty}$. It has been verified by MC simulation tests in the lattice φ^4 model [10]. From a physics point of view, this assumption represents the usual statement about the importance of long-wavelength fluctuations in critical phenomena.

Based on these scaling assumptions, a theorem has been formulated and proven in [10], according to which the two–point correlation function contains a correction exponent $\theta_\ell = \gamma + 1 - \alpha - d\nu = \gamma - 1$, provided that $\gamma > 1$ holds. According to the current knowledge, the latter condition is strictly satisfied in two and three

dimensions. The exponent θ_ℓ corresponds to the correction exponent $\omega_\ell = (\gamma - 1)/\nu$ in the finite-size scaling. Since ω_ℓ is not necessarily the leading correction-to-scaling exponent, $\omega \leq (\gamma - 1)/\nu$ is expected for the leading correction exponent. In particular, we have $\omega_\ell = 3/4$ and $\omega \leq 3/4$ for the scalar 2D φ^4 model.

The scalar φ^4 model belongs to the same universality class as the Ising model. Although corrections with $\omega = 3/4$ tend to cancel in the 2D Ising model [10], there is no reason for such a cancellation in general. Hence, corrections with $\omega \leq (\gamma - 1)/\nu$ are expected both in φ^4 and Ising models in three dimensions. Using the widely accepted estimates $\gamma \approx 1.24$ and $\nu \approx 0.63$ [12] for the 3D Ising model, we obtain the upper bound $\omega_{\max} = (\gamma - 1)/\nu \approx 0.38$ for ω. The prediction of the grouping of Feynman diagrams (GFD) theory [13] is $\gamma = 5/4$, $\nu = 2/3$ and, therefore, $\omega_{\max} = 0.375$. Thus, we can state that in any case $\omega_{\max}$ is about 0.38. The value of ω is expected to be $1/8$ according to the GFD theory considered in [13, 14].

The above arguments represent a very challenging prediction, since the currently widely known estimations of ω give essentially larger than 0.38 values, e.g., 0.782(5) [15] and 0.832(6) [7].

4 MC Tests for the 3D Ising Model

We consider the 3D Ising model on a simple cubic lattice with periodic boundary conditions. The Hamiltonian H is given by

$$H/T = -\beta \left(\sum_{\langle ij \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i \right), \tag{5}$$

where T is the temperature in energy units, β is the coupling constant, h is the dimensionless (normalized) external field, and $\langle ij \rangle$ denotes the pairs of neighboring spins $\sigma_i = \pm 1$.

We have performed a detailed MC analysis based on the available simulation data for linear lattice sizes L, ranging from a small value $L = 8$ to a relatively very large value $L = 2560$, with the aim to test the challenging prediction $\omega \leq \omega_{\max} \approx 0.38$, discussed in Sect. 3. These data have been summarized in our papers [16, 17], where the simulations at $h = 0$ have been performed with the Wolff single cluster algorithm [18], using its parallel implementation [19].

The quantities of interest are the magnetization per spin $m = N^{-1} \sum_i \sigma_i$ and the magnetic susceptibility at zero external field, i.e., $\chi = \lim_{h \to 0} \frac{\partial \langle m \rangle}{\partial (\beta h)} = N \langle m^2 \rangle$, where $N = L^3$ is the total number of lattice sites. We consider χ and magnetization moments at certain pseudocritical coupling, i.e., at $\beta = \widetilde{\beta}_c(L)$. This coupling corresponds to a constant value of $\langle m^4 \rangle / \langle m^2 \rangle^2 = U$.

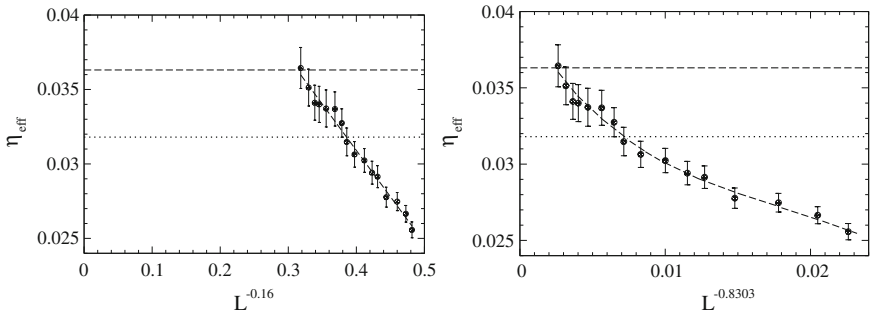

Fig. 1 The effective exponent $\eta_{\text{eff}}(L)$ depending on $L^{-0.16}$ (left) and $L^{-0.8303}$ (right). The dashed straight lines represent the linear fit (left) and a guide to eye (right). The known estimates $\eta = 0.03631(3)$ [20] and $\eta = 0.318(3)$ [15] are shown by dashed and dotted horizontal lines, respectively

The pseudocritical coupling converges to the true critical coupling β_c as $\widetilde{\beta}_c(L) = \beta_c + \mathcal{O}\left(L^{-1/\nu}\right)$ at $L \to \infty$ for $1 < U < 3$ [19]. The constant $U = 1.6$ has been chosen, which is close to the critical value of $\langle m^4\rangle/\langle m^2\rangle^2$ at $\beta = \beta_c$ and $L \to \infty$.

According to the finite-size scaling theory, the susceptibility scales as

$$\chi \propto L^{2-\eta}\left(1 + \mathcal{O}\left(L^{-\omega}\right)\right) \tag{6}$$

at $\beta = \beta_c$ or $\beta = \widetilde{\beta}_c(L)$. It allows to estimate the critical exponent η by fitting the MC data. However, we do not know precisely the correction term, and a fit without this term gives us an effective value of the exponent rather than the true critical exponent.

We define the effective exponent $\eta_{\text{eff}}(L)$ as the average slope of $-\ln\left(\chi/L'^2\right)$ versus $\ln L'$ plot, evaluated by fitting the data within $L' \in [L/2, 2L]$ at $\beta = \widetilde{\beta}_c(L')$. According to (6), it scales as

$$\eta_{\text{eff}}(L) = \eta + \mathcal{O}\left(L^{-\omega}\right) \tag{7}$$

at $L \to \infty$. Hence, the $\eta_{\text{eff}}(L)$ versus $L^{-\omega}$ plot is asymptotically linear at $L \to \infty$. The best linearity of this plot within $L \in [96, 1280]$ (extracted from the susceptibility data within $L \in [48, 2560]$) is observed at $\omega = 0.16(36)$. This plot looks, indeed, much more linear at $\omega = 0.16$ than at $\omega = 0.8303$, as it can be seen from Fig. 1. The latter value comes from the estimate of $\omega = 0.8303(18)$, obtained by the conformal bootstrap method in [20], which agrees with the MC value of 0.832(6) obtained in [7], but is claimed to be more accurate. Other MC values, usually reported in literature, are between 0.82 and 0.87 (see [7, 21]). The perturbative RG estimates are somewhat smaller, e.g., $\omega = 0.799 \pm 0.011$ [12] and $\omega = 0.782(5)$ [15].

The critical exponent $\eta = 0.03631(3)$, estimated in [20], and $\eta = 0.318(3)$, estimated in [15], are also indicated in Fig. 1 for comparison. The MC value of [7], $\eta = 0.03627(10)$, is very similar to that of [20].

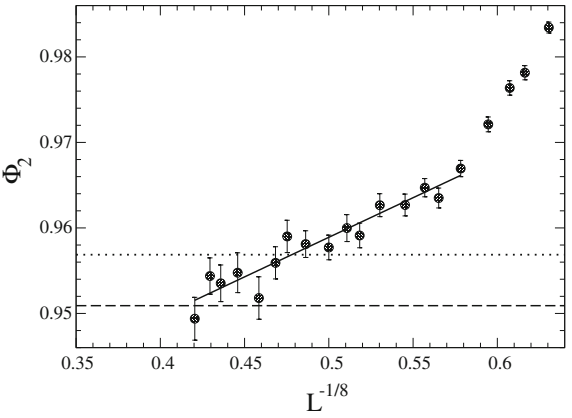

Fig. 2 The ratio $\Phi_2(L) = 2^{-4}\chi(2L)/\chi(L/2)$, evaluated from MC data at $\beta = \widetilde{\beta}_c(L)$, depending on $L^{-1/8}$. The asymptotic values of Φ_2 for $\eta = 0.03631(3)$ [20] and $\eta = 0.318(3)$ [15] are shown by dashed and dotted horizontal lines, respectively

Next, in the following, we consider a more direct method, which gives similar, but slightly more accurate results for ω. We consider the ratio $\Phi_b(L) = b^{-4}\chi(bL)/\chi(L/b)$ at $\beta = \widetilde{\beta}_c(L)$, where b is a constant. According to (6), $\Phi_b(L)$ behaves as

$$\Phi_b(L) = A + BL^{-\omega} \tag{8}$$

at $L \to \infty$, where $A = b^{-2\eta}$ and $B = ab^{-2\eta}\left(b^{-\omega} - b^{\omega}\right)$. The choice $b = 2$ is found to be optimal for the analysis of our data. The $\Phi_2(L)$ versus $L^{-1/8}$ plot can be well approximated by a straight line for large enough lattice sizes $L \in [80, 1280]$, as shown in Fig. 2. It confirms that ω could be as small as $1/8$, in agreement with [13, 14]. Considering ω as a fit parameter in (8), the fit over this region of sizes gives $\omega = 0.21(29)$. Taking into account that the asymptotic value of ω is positive, we can judge from this estimation that ω, most probably, lies between 0 and 0.5. The asymptotic value of Φ_2 is $2^{-2\eta}$. The estimates, corresponding to the same η values as in Fig. 1, are indicated in Fig. 2 for comparison.

Summarizing the results of this section, our MC estimation suggests that $0 < \omega < 0.5$ most probably holds for the correction-to-scaling exponent ω, in agreement with the analytical arguments in Sect. 2. Our values of 0.16(36) and 0.21(29) are remarkably smaller than the earlier estimates, e.g., 0.832(6) [7]. Although the latter MC estimate of [7] is claimed to be very accurate, it has been obtained from relatively small lattice sizes, i.e., $L \leq 360$, as compared to $L \leq 2560$ in our current study. Various estimations from lattice sizes $L \leq 384$ have been discussed in [17], clearly demonstrating that these sizes are still too small for a reliable estimation of ω.

Concerning the exponent η, the plots in Fig. 1 show that η could be similar or larger than the already mentioned estimates of 0.03631(3) [20] and 0.03627(10) [7]. The effective exponent increases well above the perturbative RG value of 0.318(3) obtained in [15] (dotted line).

5 Remarks and Discussion

It should be emphasized that our MC analysis is based on the simulation results for substantially large lattice sizes as compared to those typically considered in literature, e.g., $L \leq 360$ in [7] and even smaller sizes in other studies. It reveals a possibility to explain the inconsistency of our actual findings with earlier numerical results by relating the previous numerical results to a "perturbative" region, whereas our findings—to a "nonperturbative" region, as explained further on.

The "perturbative" region is a region of not–too–small reduced temperatures in the thermodynamic limit and not–too–large lattice sizes in the finite–size scaling regime. It is, very likely, true that the perturbative RG methods describe just only this region, due to the fundamental problems recovered in [22] (see Sect. 5.4.6 there). The "perturbative" region is easily accessible by various numerical methods. It explains the fact why these methods easily produce the results, which are approximately consistent with the estimates of the perturbative RG method and, therefore, also with each other. To the contrary, our findings refer to the "non-perturbative" asymptotic region, which corresponds to substantially larger lattice sizes in the finite–size scaling regime and extremely small reduced temperatures in the thermodynamic limit. This region cannot be easily accessed and is not yet properly investigated by numerical methods.

From the perspective of the non-perturbative RG approach, the "non-perturbative" asymptotic region is described by certain non-perturbative fixed point. We assume that the non-perturbative fixed point is not described by the usual perturbative treatments, just like in the case of spin glasses [8], discussed in Sect. 1. Hence, the critical exponents can be inconsistent with the perturbative RG estimates.

The results of the ε–expansion coincide with a particular treatment of the conformal field theory (CFT) in [20, 23]. This, however, only implies that the perturbative fixed point is, indeed, conformally symmetric and consistent with CFT at specific constraints, assumed in [20, 23].

6 Conclusions

In summary, we conclude the following:

- Non-perturbative approaches become increasingly important in study of critical phenomena, including their applications in nanoscience and nanotechnology.
- Non-perturbative analytical arguments have been provided for the existence of certain correction to scaling with exponent $\omega_\ell = (\gamma - 1)/\nu$ in the φ^4 model, and the leading finite-size correction-to-scaling exponent being $\omega \leq (\gamma - 1)/\nu$.
- The above statement has been supported by MC simulation results for small and very large lattices in 2D φ^4 and 3D Ising models.
- Our results emphasize the importance of corrections to scaling in nano-scale systems, pointing to a slow crossover in finite-size scaling behavior when the

system size is varied from small (nano-scale) to large (thermodynamic limit). This crossover is related to small ω value—remarkably smaller than it was expected before.

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