Monte Carlo test of critical exponents and amplitudes in 3D Ising and $\phi^4$ lattice models

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Abstract

We have tested the leading correction–to–scaling exponent $\omega$ in $O(n)$–symmetric models on a three–dimensional lattice by analysing the recent Monte Carlo (MC) data. We have found that the effective critical exponent, estimated at finite sizes of the system $L$ and $L/2$, decreases remarkably within the range of the simulated $L$ values. This shows the incorrectness of some claims that $\omega$ has a very accurate value 0.845(10) at $n = 1$. A selfconsistent infinite volume extrapolation yields row estimates $\omega \approx 0.547$, $\omega \approx 0.573$, and $\omega \approx 0.625$ at $n = 1$, 2, and 3, respectively, in approximate agreement with the corresponding exact values $1/2$, $5/9$, and $3/5$ predicted by our recently developed GFD (grouping of Feynman diagrams) theory. We have fitted the MC data for the susceptibility of 3D Ising model at criticality showing that the effective critical exponent $\eta$ tends to increase well above the usually accepted values around 0.036. We have fitted the data within $[L; 8L]$, including several terms in the asymptotic expansion with fixed exponents, to obtain the effective amplitudes depending on $L$. This method clearly demonstrates that the critical exponents of GFD theory are correct (the amplitudes converge to certain asymptotic values at $L \to \infty$), whereas those of the perturbative renormalization group (RG) theory are incorrect (the amplitudes diverge). A modification of the standard Ising model by introducing suitable "improved" action (Hamiltonian) does not solve the problem in favour of the perturbative RG theory.

Keywords: $\lambda\phi^4$ model, Ising model, Binder cumulant, Monte Carlo data, critical exponents

1 Introduction

Since the exact solution of two–dimensional Ising model has been found by Onsager [1], a study of various phase transition models is of permanent interest. Nowadays, phase transitions and critical phenomena is one of the most widely investigated fields of physics. Remarkable progress has been reached in exact solution of two–dimensional models [3]. Recently, we have proposed [4] a novel method based on grouping of Feynman diagrams (GFD) in $\phi^4$ model. Our GFD theory allows to
analyse the asymptotic solution for the two-point correlation function at and near
criticality, not cutting the perturbation series. As a result the possible values of
exact critical exponents have been obtained [3] for the Ginzburg–Landau ($\varphi^4$) model
with $O(n)$ symmetry, where $n = 1, 2, 3, \ldots$ is the dimensionality of the order param-
eter. Our predictions completely (exactly) agree with the known exact and rigorous
results in two dimensions [2], and are equally valid also in three dimensions. In [3],
we have compared our results to some Monte Carlo (MC) simulations and exper-
iments [1, 5, 6]. An additional comparison to MC data has been made in [7]. It
has been shown [3, 7] that the actually discussed MC data for 3D Ising [4, 8] and
XY [5] models are fully consistent with our theoretical predictions, but not with
those of the perturbative renormalization group (RG) theory [10, 11, 12]. Some data
for 3D Heisenberg model [9] also have been discussed in [7]. However, these data,
likely, are not accurate enough and here we reconsider the estimation of the critical
point based on more recent MC results. From the theoretical (mathematical) point
of view, the invalidity of the conventional RG expansions has been demonstrated
in [3]. The current paper, dealing with numerical analysis of the three-dimensional
$\lambda \varphi^4$ and Ising models, presents one more confirmation that the correct values of
critical exponents are those predicted by the GFD theory.

2 $\lambda \varphi^4$ model and its crossover to Ising model

Here we discuss a $\varphi^4$ model on a three-dimensional cubic lattice. The Hamiltonian
of this model, further called $\lambda \varphi^4$ model, is given by

$$ H/T = \sum_x \left\{ -2\kappa \sum_{\mu} \varphi_{x+\mu} + \varphi_x^2 + \lambda \left( \varphi_x^2 - 1 \right)^2 \right\} , $$

(1)

where the summation runs over all lattice sites, $T$ is the temperature,
$\varphi_x \in [-\infty; +\infty]$ is the scalar order parameter at the site with coordinate $x$, $\mu$
is a unit vector in the $\mu$-th direction, $\kappa$ and $\lambda$ are coupling constants. Obviously,
the standard 3D Ising model is recovered in the limit $\lambda \to \infty$ where $\varphi_x^2$ fluctuations
are suppressed so that, for a relevant configuration, $\varphi_x^2 \simeq 1$ or $\varphi_x \simeq \pm 1$ holds. The MC data for the Binder cumulant in this $\lambda \varphi^4$ model have been interpreted in accordance with the $\epsilon$-expansion and a perfect agreement with the conventional RG
values of critical exponents has been reported in [13]. According to the definition
in [13], the Binder cumulant $U$ is given by

$$ U = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} , $$

(2)

where $m = L^{-3} \sum_x \varphi_x$ is the magnetization and $L$ is the linear size of the system.
Based on the $\epsilon$-expansion, it has been suggested in [13] that, in the thermodynamic
limit $L \to \infty$, the value of the Binder cumulant at the critical point $\kappa = \kappa_c(\lambda)$ and,
equally, at a fixed ratio $Z_a/Z_p = 0.5425$ (the precise value is not important) of
partition functions with periodic and antiperiodic boundary conditions is a universal
constant $U^*$ independent on $\lambda$. We suppose that the latter statement is true, but
due not to the $\epsilon$-expansion. It is a consequence of some general argument of the RG theory: on the one hand, $U$ is invariant under the RG transformation and,
on the other hand, an unique fixed point (not necessarily the Wilson–Fisher fixed point) exists in the case of an infinite system, so that \( U \equiv U^* \) holds at \( L \to \infty \) and \( \kappa = \kappa_c(\lambda) \) where \( U^* \) is the fixed–point value of \( U \). The above conclusion remains true if we allow that the fixed point is defined not uniquely in the sense that it contains some irrelevant degree(s) of freedom (like \( c^* \) and \( \Lambda \) in the perturbative RG theory discussed in Sec. 2 of [3]) not changing \( U \). The numerical results in [16] confirm the idea that \( \lim_{L \to \infty} U(L) = U^* \) holds at criticality, where \( U^* \) is a universal constant independent on the specific microscopic structure of the Hamiltonian.

3 Estimation of the correction exponent \( \omega \)

Based on the idea that \( U^* \) is constant for a given universality class, here we estimate the correction–to–scaling exponent \( \omega \). According to [7], corrections to finite–size scaling for the magnetization of the actual 3D Ising and \( \lambda \varphi^4 \) models are represented by an expansion in terms of \( L^{-\omega} \) where \( \omega = 1/2 \). One expects that the magnetization (Binder) cumulant (2) has the same singular structure. Since \( \lim_{L \to \infty} U(L, \lambda) \equiv U^* \) holds at a fixed ratio \( Z_a/Z_p \), a suitable ansatz for estimation of \( \omega \) is [13]

\[
U(L, \lambda_1) - U(L, \lambda_2) \simeq \text{const} \cdot L^{-\omega} \quad \text{at} \quad Z_a/Z_p = 0.5425 ,
\]

which is valid for any two different nonzero values \( \lambda_1 \) and \( \lambda_2 \) of the coupling constant \( \lambda \). The data for \( \Delta U(L) = U(L, 0.8) - U(L, 1.5) \) can be read from Fig. 1 in [13] (after a proper magnification) without an essential loss of the numerical accuracy, i. e., within the shown error bars. Doing so, we have evaluated the effective exponent

\[
\omega_{\text{eff}}(L) = \ln \left[ \frac{\Delta U(L/2)}{\Delta U(L)} \right] / \ln 2 ,
\]

i. e., \( \omega_{\text{eff}}(12) \simeq 0.899 \), \( \omega_{\text{eff}}(16) \simeq 0.855 \), and \( \omega_{\text{eff}}(24) \simeq 0.775 \). These values are shown in Fig. 1 by crosses. Such an estimation, however, can be remarkably influenced by the random scattering of the simulated data points, particularly, at larger sizes where \( \Delta U(L) \) becomes small. This effect can be diminished if the values of \( \Delta U(L) \) are read from a suitable smoothed curve. A comparison to the original results (without the smoothening) provides some objective criterion of the accuracy of such estimations. We have found that \( \Delta U(L) \) within \( L \in [7; 24] \) can be well approximated by a second–order polinomial in \( L^{-1/2} \), as shown in Fig. 3. Without any claims about validity of such an approximation well outside of this interval, we can consider the least–squares fit in Fig. 2 as an appropriate smoothened curve from which we read \( \omega_{\text{eff}}(16) \simeq 0.8573 \) and \( \omega_{\text{eff}}(24) \simeq 0.7956 \). These values are depicted in Fig. 1 by empty circles. As we see, the results are similar to those obtained by a direct calculation from the original data points (crosses). However, the values obtained from the smoothened curve (circles) are more accurate and reliable. As regards the smallest size, we suppose that the original estimate \( \omega_{\text{eff}}(12) \simeq 0.899 \) is accurate enough even without any smoothening, since the values of \( \Delta U(6) \) and \( \Delta U(12) \) are large relative to the statistical errors.

In such a way, we see from Fig. 1 that the effective exponent \( \omega_{\text{eff}}(L) \) decreases remarkably with increasing of \( L \). According to GFD theory, \( \omega_{\text{eff}}(L) \) is a linear function of \( L^{-1/2} \) at \( L \to \infty \), as consistent with the expansion in terms of \( L^{-\omega} \) where \( \omega = 0.5 \). More data points, including larger sizes \( L \), are necessary for a
Figure 1: Effective correction–to–scaling exponent $\omega_{\text{eff}}(L)$ in the $O(n)$–symmetric $\lambda\varphi^4$ model with $n = 1$ (empty circles and crosses) and $n = 3$ (triangles), and $O(2)$–symmetric $dd – XY$ model (solid circles) depending on the system size $L$. The linear least–squares fits give row estimates of the asymptotic $\omega$ values $0.547$, $0.573$, and $0.625$ at $n = 1$, $2$, and $3$, respectively. The corresponding theoretical values of the GFD theory $1/2$, $5/9$, and $3/5$ (used in the $L^{-\omega}$ scale of the horizontal axis) are indicated by arrows. The dot–dot–dashed line shows the value $0.845(10)$ proposed in [13] for the 3D Ising universality class ($n = 1$).

Figure 2: The smoothened curve $\Delta U(L) = 0.003795 – 0.003232L^{-1/2} + 0.23433L^{-1}$ for an approximation of $\Delta U(L) = U(L, 0.8) – U(L, 1.5)$ within the interval $L \in [7; 24]$.
reliable estimation of the asymptotic exponent \( \omega = \lim_{L \to \infty} \omega_{\text{eff}}(L) \). Nevertheless, already a row linear extrapolation in the scale of \( L^{-1/2} \) with the existing data points yields the result \( \omega \approx 0.547 \) which is reasonably close to the exact value 0.5 (horizontal dashed line in Fig. 1) found within the GFD theory. The corresponding least–squares fit with circles (at \( L = 24, 16 \)) and cross (at \( L = 12 \)) is shown in Fig. 1 by a straight solid line. It is evident from Fig. 1 that the final result \( \omega = 0.845(10) \) (horizontal dot–dot–dashed line) reported in [13] represents some average effective exponent for the interval \( L \in [6; 24] \). It has been claimed in [13] that the estimates for \( \omega \) (cf. Tab. 2 in [13]) are rather stable with respect to \( L_{\text{min}} \), where \( L_{\text{min}} \) is the minimal lattice size used in the fit. Unfortunately, the analysis has been made in an obscure fashion, i. e., giving no original data, so that we cannot check the correctness of this claim. Besides, the estimates in Tab. 2 of [13] has been made by using an ansatz

\[
U(L, \lambda) = U^* + c_1(\lambda)L^{-\omega} \quad \text{at} \quad Z_a/Z_p = 0.5425 ,
\]

which is worse than (3). Namely, (4) and (5) are approximations of the same order, but (5) contains an additional parameter \( U^* \) which is not known precisely. The results of an analysis with the ansatz (3), reflected in Tab. 5 of [13], are not convincing, since only very small values of \( L_{\text{min}} \) (up to \( L_{\text{min}} = 6 \)) have been considered.

In any case, we prefer to rely on that information we can check, and it shows that the claim in [13] that \( \omega = 0.845(10) \) holds with \( \pm 0.01 \) accuracy cannot be correct, since \( \omega_{\text{eff}}(L) \) is varied in the first decimal place.

We have made a similar estimation of \( \omega \) for \( O(n) \)-symmetric spin models, namely, for the dynamically diluted \( XY \) (\( dd - XY \)) model simulated in [14] \( (n = 2) \) and for \( O(3) \)-symmetric \( \lambda \varphi^4 \) model simulated in [15]. In the case of the \( dd - XY \) model, parameter \( D \) (cf. Eq.(6) in [14]) plays the role of \( \lambda \) in (3). The data for the Binder cumulant in Fig. 1 of [14] look rather accurate, i. e., not scattered. This enables us to estimate \( \omega_{\text{eff}} \) just from the data at \( D = 1.03 \) and \( D = \infty \) (\( XY \) model). The resulting values of \( \omega_{\text{eff}} \) are depicted in Fig. 1 by solid circles. The scale of \( L^{-\omega} \) is used, where \( \omega = 5/9 \) is our theoretical value of the correction–to–scaling exponent at \( n = 2 \) consistent with the general hypothesis proposed in [1]. As we see, the solid circles can be well located on a smooth line which, however, is remarkably curved at smaller sizes. Due to the latter reason, we have used only the last three points (the largest sizes) for the linear fit (solid line) resulting in an estimate \( \omega \approx 0.573 \) which comes close to our theoretical value \( \omega = 5/9 = 0.555\ldots \)

The estimates of \( \omega_{\text{eff}} \) for the \( O(3) \)-symmetric \( \lambda \varphi^4 \) model are depicted in Fig. 1 (in the scale of \( L^{-\omega} \) with our \( \omega \) value 0.6) by triangles. The data have been extracted from Fig. 1 of [15] at \( \lambda_1 = 2 \) and \( \lambda_2 = \infty \). The obtained \( \omega_{\text{eff}}(L) \) values at \( L = 12, 16, \) and 24 well lie on a straight line (tiny–dashed line in Fig. 1) yielding an asymptotic estimate \( \omega \approx 0.625 \) which is reasonably close to our theoretical prediction \( \omega = 0.6 \). Hence, the \( \omega_{\text{eff}}(32) \) value deviates upwards unexpectedly. We suppose, this is due to an inaccurate simulation of the largest size \( L = 32 \), as explained below. We have depicted in Fig. 1 the ratio \( R(L) = (U(L, 2) - U^*)/(U^* - U(L, \infty)) \) evaluated from the data in Fig. 1 of [15] with \( U^* = 1.14022 \) (the average over three estimates at a fixed \( Z_a/Z_p \), given in Tab. 2 in [15]). According to [5], \( R(L) \) tends to a constant at \( L \to \infty \). The \( R(24) \) data point well lie on the smooth line (parabola) representing the least–squares fit to four smallest sizes \( L = 6, 8, 12, \) and 16, whereas the simulated \( R(32) \) value drops down unreasonably. So, it looks like a wrong simulation has been
Figure 3: The ratio $R(L) = (U(L,2) - U^*)/(U^* - U(L,\infty))$ for $O(3)$-symmetric $\lambda \phi^4$ model estimated from the MC data of [15]. The scale of $L^{-\omega}$ with $\omega = 0.6$ is used. The solid line (parabola) represents the least–squares fit including only four smallest sizes.

made at $L = 32$ to confirm the known RG estimate $\omega \approx 0.8$. Thus, our extrapolation in Fig. 1 (tiny–dashed line), omiting the point with $L = 32$, is justified.

In summary, the extrapolated $\omega$ values (Fig. 3) in all three cases $n = 1, 2, 3$ are reasonably close to our theoretical values $1/2$, $5/9$, and $3/5$ indicated by arrows. Only a small systematic deviation is observed. This, likely, is due to the error of linear extrapolation: the $\omega_{eff}(L)$ plots have a tendency to curve down slightly. The conventional (RG) estimate $\omega \approx 0.8$ more or less corresponds to effective exponents for currently simulated finite system sizes, but not to the asymptotic exponents.

The data for $n = 4$ also are available in [15]. Unfortunately, they are too much scattered for the actual analysis.

4 The critical coupling of 3D Ising and Heisenberg models

A conventional method to determine the critical exponent $\eta$ is a fit of the susceptibility data at criticality. For this, however, we need a very accurate value of the critical coupling (temperature). In this section we discuss the estimation of the critical coupling $\beta_c$ for 3D Ising and Heisenberg models.

The critical point of the standard 3D Ising model has been estimated in [16] with a 7–digit accuracy, i. e. $\beta_c = 0.2216545$. We have made our own fits with the MC data of [16] to check the accuracy of this estimation, and have obtained the same value within error bars of $10^{-7}$. We will use in our further analysis also a similar estimate $\beta_c = 0.383245$ [16] for the so called ”improved” 3D Ising model.

The critical coupling of the classical 3D Heisenberg model is known much less accurately than that of the 3D Ising model. Some of the known estimates are
Figure 4: The Binder cumulant $U$ vs system size $L$ in the 3D Heisenberg model at $\beta = 0.6929$ (bottom), $\beta = 0.692955$ (middle), and $\beta = 0.693$ (top). Symbols depict the MC data of \cite{20}, whereas lines represent the least–squares approximations of these data by a parabola. The solid line, coinciding with the universal critical value of the Binder cumulant $U^* = 0.61993(3)$, corresponds to the critical coupling $\beta_c \simeq 0.692955$.

$\beta_c = 0.6929(1)$ \cite{17}, $\beta_c = 0.693035(37)$ \cite{18}, and $\beta_c = 0.693001(10)$ \cite{19}.

In principle, the location of the critical point can be found with a high accuracy and reliability by simulations of the Binder cumulant $U(\beta, L)$ in close vicinity of the critical point, as it has been done in \cite{16} for the 3D Ising model. Taking into account the leading and the subleading corrections to scaling, we have

$$U(\beta_c, L) \simeq U^* + a_1 L^{-\omega} + a_2 L^{-2\omega}.$$  \hfill (6)

If the universal value of $U^*$ is known with a high precision, then the critical value of $\beta$ at which $U(\beta, L)$ coincides with (6) is well defined. Namely, at $\beta = \beta_c$ the quadratic (least–squares) extrapolation of $U(\beta, L)$ in the scale of $L^{-\omega}$ should yield $U^*$ at $L^{-\omega} \to 0$. In Fig. 4, we have shown the results of such an extrapolation with $\omega = 0.6$ (our theoretical value) at three different values of $\beta$, i. e., 0.6929 (lower dashed line), 0.692955 (solid line), and 0.693 (upper dashed line). The data for $U(\beta, L)$ have been extracted from Fig. 1 in \cite{20} via an approximation $U(\beta, L) \simeq U(\beta_0, L) + 0.06 L^{1.4}(\beta - \beta_0)$, where $\beta_0 = 1/1.4432$. Note that, in distinction to (2), now we use the conventional definition $U = 1 - (1/3)\langle m^4 \rangle / \langle m^2 \rangle^2$. A suitable estimate of $U^*$, taken from Tab. 2 in \cite{15}, is then $U^* = 0.61993(3)$. This value with the error bars is indicated in Fig. 4 by an arrow. As we see from Fig. 4, the estimate $\beta_c \simeq 0.692955$ is consistent with this value of $U^*$. Our estimation is rather stable, i. e., if the extrapolation is made in the scale of $L^{-0.8}$, we get practically the same result $\beta_c \simeq 0.692957$. Taking into account the curvature of the $U(\beta, L)$ plot at $\beta = 0.693$, it is unlikely that 0.693 could be the correct value of $\beta_c$ yielding $U^* = 0.61993(3)$ at $L \to \infty$. According to the strong variation of the extrapolated $U^*$ value with $\beta$, it is plausible that the error of our estimation $\beta_c \simeq 0.692955$ is about 0.00001 or even
Our result agree within the error bars with the value 0.6929(1) of [17], while the error bars of the estimates \( \beta_c = 0.693035(37) \) [18] and \( \beta_c = 0.693001(10) \) [19], in our opinion, are underestimated. As regards the value of [18], this is a result of a linear extrapolation (in the scale of \( L^{-1/0.7036} \)) of temperature values corresponding to extrema points for several physical quantities. However, the shift in \( \beta \) as large as 0.0001 is practically invisible in the scale of Fig. 3 in [18]. If one allows that the lines in this figure are curved very slightly, then even larger deviation in the extrapolated \( \beta_c \) value is possible. In other words, the proposed error bars ±0.000037, obviously, include only the statistical error and are underestimated since they ignore the possible systematic deviation due to the neglected corrections to scaling. A similar problem with the subleading correction persists in [19]. Namely, a linear extrapolation in Fig. 4 would give a larger \( \beta_c \) value, close to 0.693 (in agreement with that of [19]), but this value is shifted down to 0.692955 due to the subleading correction in the asymptotic expansion of \( U \). This correction has been neglected in the analysis of the Binder cumulant crossings in [19]. We have taken into account both the leading and the subleading corrections to scaling and, therefore, our value 0.692955 is more accurate than those proposed in [18] and [19], unless the data of [20] contain large systematical errors.

5 Fitting the susceptibility data at criticality

In this section we discuss some fits of MC data at criticality. According to the finite–size scaling theory, the susceptibility \( \chi \) near the critical point is represented by an expansion

\[
\chi = L^{2-\eta} \left( g_0(L/\xi) + \sum_{l \geq 1} L^{-\omega_l} g_l(L/\xi) \right),
\]

where \( g_l(L/\xi) \) are the scaling functions, \( \xi \) is the correlation length of an infinite system, \( \eta \) is the critical exponent related to the \( k^{-2+\eta} \) divergence of the correlation function in the wave vector space at criticality, and \( \omega_l \) are correction–to–scaling exponents, \( \omega_1 \equiv \omega \) being the leading correction exponent. The correlation length diverges like \( \xi \propto t^{-\nu} \) at \( t \to 0 \), where \( t = 1 - \beta / \beta_c \) is the reduced temperature. Thus, for large \( L \), in close vicinity of the critical point where \( tL^{1/\nu} \ll 1 \) holds Eq. (7) can be written as

\[
\chi = a L^{2-\eta} \left( 1 + \sum_{l \geq 1} b_l L^{-\omega_l} + \delta(t, L) \right),
\]

where \( a = g_0(0) \) and \( b_l = g_l(0) / g_0(0) \) are the amplitudes, and \( \delta(t, L) \) is a correction term which takes into account the deviation from criticality. In the first approximation it reads

\[
\delta(t, L) \simeq c \cdot tL^{1/\nu},
\]

where \( c \) is a constant.

We start our analysis with the standard 3D Ising model with the Hamiltonian

\[
H/T = -\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j .
\]
The fits of $\ln \left( \chi / L^2 \right)$ data at criticality (ansatz (8)) shifted by a constant $c$. Circles represent the MC data for 3D Ising model \[16\] at $\beta = 0.2216545$ ($c = 0$, empty symbols) and 3D Heisenberg model \[9\] at $\beta = 0.692955$ ($c = 0.55$, solid symbols). The corresponding fits with our (GFD) exponents ($\ln a = 1.065289, b_1 = -2.72056, b_2 = 8.18636, b_3 = -10.49614$ and $\ln a = 0.207324, b_1 = -1.22546, b_2 = 1.85823$) are shown by solid lines, whereas those with the exponents of \[13, 21\] ($\ln a = 0.430933, b_1 = 0.05850, b_2 = -7.74767, b_3 = 12.42890$ and $\ln a = -0.150242, b_1 = 0.03947, b_2 = -0.45033$) – by tiny–dashed lines. The empty boxes are MC data for 3–component 3D XY model \[22\], shifted by $c = 0.85$.

The critical point of this model with a 7–digit accuracy is $\beta_c \simeq 0.2216545$ (Sec. 4). From the maximal values of the derivative $\partial \ln \langle m^2 \rangle / \partial \beta \equiv \partial \ln \chi / \partial \beta$ evaluated in \[23\] we conclude that the shift of $\beta$ by $10^{-7}$ produces the variation of $\ln \chi$ at $L = 96$ near $\beta = \beta_c$, which does not exceed $4.7 \cdot 10^{-4}$ in magnitude. The latter means that, with a good enough accuracy, we may assume that $\beta_c$ is just 0.2216545 when fitting the susceptibility data at criticality within $L \in [4; 128]$. Here we mean the MC data given in Tab. 25 of \[16\]. We have made and compared several fits of these data to ansatz (8) with $\delta(t, L) = 0$ (more precisely, to the corresponding formula for $\ln \chi$) for two different sets of the critical exponents, i. e., our (GFD) and that proposed in \[13\]. The fits made with our exponents systematically improve relative to those made with the exponents of \[13\], as the system sizes grow and the approximation order increases. The necessity to include several correction terms is dictated by the fact that corrections to scaling are rather strong. According to the least–squares criterion, the fit with our exponents $\eta = 1/8$ and $\omega_l = l/2$ becomes better than that provided by the more conventional exponents $\eta = 0.0358(4), \omega_1 = 0.845(1), \omega_2 = 2\omega_1$, and $\omega_3 = 2$ \[13\] starting with $L_{\min} = 28$ (i. e., $L \in [L_{\min}; 128]$), if two correction terms ($l = 1, 2$) are included. In the case of three correction terms it occurs already at $L_{\min} = 11$. The four–parameter ($a, b_1, b_2, b_3$) fits to MC data (empty circles) within $L \in [14; 128]$ are shown in Fig. 5. The fit with our exponents (upper solid line) is relatively better at larger sizes. However, both fits (upper solid and dashed lines) look, in fact, quite similar, so that we cannot make unambiguous
conclusions herefrom.

We have shown in Fig. 5 also the three–parameter fits to the susceptibility data of the 3D Heisenberg model at $\beta = \beta_c \simeq 0.692955$ (Sec. 4) extracted from Fig. 6 in [9] by a suitable linear interpolation. The MC data within $L \in [12; 48]$ are shown by solid circles. The fit with our exponents ($\eta = 0.1$, $\omega_l = 0.6\ell$) is depicted by lower solid line, whereas that with the conventional RG exponents ($\eta = 0.0355$, $\omega = 0.782$ [21]) – by lower tiny–dashed line. Like in the case of 3D Ising model, the fit with our exponents looks slightly better, although the MC data are too inaccurate to make serious conclusions herefrom. Comparing the amplitudes given in the caption of Fig. 5, we see that corrections to scaling are remarkably weaker in the 3D Heisenberg model as compared to the 3D Ising model, so that the neglected third–order correction in the case of the Heisenberg model could be small enough even at sizes somewhat below $L = 12$. In this aspect, it is interesting to mention that the fit with our exponents $\eta = 0.1$ and $\omega_l = 0.6\ell$ (and not the other one) qualitatively correctly reproduces the shape of the actual $\ln(\chi/L^2)$ plot at $L < 12$ where it curves upwards to meet the condition $\chi(L = 1) = \langle \sigma^2 \rangle = 1$.

For comparison, we have shown in Fig. 5 also the MC data for 3D XY model [22] in which, however, only $x$ and $y$ components of the 3–component order parameter interact with each other. One believes [22] that this model belongs to the universality class of the standard XY model with the number of components $n = 2$. Unfortunately, we have not found in the recent literature more accurate explicit data for $n = 2$ case. As we see, the actual MC data (empty boxes) at $\beta_c$ evaluated approximately $\beta_c \simeq 0.6444$ [22] are rather scattered and, therefore, unsuitable for a refined analysis. Nevertheless, this is a typical situation where authors of such data make a very ”accurate” and ”convincing” estimation $\gamma/\nu = 1.9696(37)$ or $\eta = 0.0304(37)$ making a simple linear fit. However, the refined analysis given above has shown that even in the case of 3D Ising model, where the data are incompatibly more accurate, it is not so easy to distinguish between $\eta = 0.0358$ and $\eta = 1/8$. Moreover, a refined analysis prefer the second value which is much larger than those usually provided by linear fits at typical system syzes $L \leq 48$. This is particularly well seen in Fig. 6, where the effective critical exponent $\eta_{eff}(L)$ of the 3D Ising model, estimated via the linear fit within $[L; 2L]$, is depicted by solid circles. As we see, $\eta_{eff}(L)$ tends to increase well above the conventional value 0.0358 (horizontal dot–dot–dashed line). The shape of the $\eta_{eff}(L)$ plot is satisfactory well reproduced by a third–order polynomial in the actual scale of $L^{-1/2}$. Three such kind of least–squares approximations (at $L_{min} = 9, 10, 12$) are shown in Fig. 4. These fits do not provide very accurate and stable asymptotic values of $\eta$. Nevertheless, they are more or less in agreement with our theoretical prediction $\eta = 1/8$ (horizontal dashed line). Besides, the values of $\eta_{eff}$ are affected by the error in $\beta_c$ (about $10^{-7}$) only slightly, i. e., by an amount not exceeding 0.001.

6 A test for 3D Ising model with ”improved” action

Here we discuss some estimations of the critical exponents from the susceptibility data of 3D Ising model, reported in [16], with the so called ”improved” action (i. e., $H/T$). One of the problems with the standard 3D Ising model is that corrections to
Figure 6: The effective critical exponent $\eta_{\text{eff}}(L)$ (solid circles) obtained by fitting the susceptibility data of 3D Ising model at criticality ($\beta = 0.2216545$) within the interval $[L; 2L]$. The least-squares approximations obtained by fitting the $\eta_{\text{eff}}(L)$ data within $[L_{\text{min}}; 64]$ to a third-order polynomial in $L^{-1/2}$ are shown by dashed ($L_{\text{min}} = 9$), solid ($L_{\text{min}} = 10$), and tiny-dashed ($L_{\text{min}} = 12$) lines. The asymptotic value $\eta = 1/8$ of the GFD theory is indicated by a horizontal dashed line. The dot-dot-dashed line represents the $\eta$ value $0.0358$ proposed in [13].

scaling are strong. It has been proposed in [16] to solve this problem by considering a modified (spin–1) Ising model with the Hamiltonian

$$H/T = -\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j + D \sum_i \sigma_i^2,$$

(11)

where the spin $\sigma_i$ takes the values 0, ±1, with two coupling constants $\beta$ and $D$ adjusted in such a way that the leading correction to finite-size scaling vanishes for all relevant physical quantities (magnetization cumulant, energy per site, susceptibility, etc.) and their derivatives. Moreover, according to the claims in [16] (see the conclusions in [16]), the ratios of the leading and subleading corrections are universal, so that not only the leading but all (!) corrections should vanish simultaneously.

We have checked the correctness of these claims as described below. We have fitted the corresponding to (8) expression for $\ln \chi$ to the susceptibility data of the "improved" 3D Ising model [11] with $(\beta, D) = (0.383245, 0.624235)$ (this is an approximation of the critical point) given in [10] (Tab. 26). By fixing the exponents, the least-squares fit within $L \in [L_{\text{min}}; 56]$ (here $L = 56$ is the maximal size available in Tab. 26 of [10]), including the leading and the subleading correction to scaling, provides the effective amplitudes $a$, $b_1$, and $b_2$ depending on $L_{\text{min}}$. We have made a test with the critical exponents $\eta = 0.0358(4)$, $\omega = 0.845(10)$, and $\nu = 0.6296(3)$ proposed in [13]. These values are close to those of the usual RG expansions [21], but, as claimed in [13], they are more accurate. According to [13], the asymptotic expansion contains corrections like $L^{-n\omega}$ and $L^{-2n}$, where $n = 1, 2, 3, \ldots$ Thus we
Figure 7: The effective amplitudes $10b_1$ (circles) and $b_2$ (rhombs) in (8) estimated at fixed exponents $\eta = 0.0358$, $\omega_1 = 0.845$, $\omega_2 = 2\omega_1$, and $\nu = 0.6296$ by fitting the MC data within $L \in [L_{\min}; 56]$. Filled symbols correspond to $\delta(t, L) = 0$, empty symbols – to $\delta(t, L) = 10^{-6}L^{1/\nu}$. The effective amplitudes $b_1$ and $b_2$ estimated with the critical exponents of our GFD theory ($\eta = 1/8$, $\omega_l = l/2$) at $\delta(t, L) = 0$ are shown by "x" and "+", respectively. Lines represent the least-squares approximations by a fourth-order polynomial in $L$.

have $\omega_1 = \omega$ and $\omega_2 = 2\omega$. The resulting amplitudes $10b_1(L_{\min})$ and $b_2(L_{\min})$ are shown in Fig. 7 by circles and rhombs, respectively. We have depicted by filled symbols the results of the fitting with $\delta(t, L) = 0$, assuming that the critical coupling $\beta_c = 0.383245$ has been estimated in [13] with a high enough (6 digit) accuracy. The data points quite well fit smooth (tiny dashed) lines within $L_{\min} \in [4; 20]$, which means that the statistical errors are reasonably small. If the exponents used in the fit are correct and corrections to scaling are small indeed, then the convergence of the effective amplitudes to some small values is expected with increasing of $L_{\min}$. However, as we see from Fig. 7, the effective amplitudes tend to increase in magnitude acceleratedly as $L_{\min}$ exceeds 14. A small inaccuracy in $\beta_c$ value can be compensated by the term $\delta(t, L) \simeq e^*L^{1/\nu}$ in (8), where $e^* = ct$ (cf. Eq. (9)). The results of fitting with $e^* = 10^{-6}$ are shown in Fig. 7 by empty symbols. As we see, the expected inaccuracy in $\beta_c$ of order $10^{-6}$ does not change the qualitative picture. The increase of the effective amplitudes indicates that either the exponents are false, or the asymptotic amplitudes are not small (or both). This is our argument that the claims in [16] about very accurate critical exponents, extracted from the 3D Ising model with "improved" action, are incorrect.

For comparison, we have shown in Fig. 7 also the effective amplitudes $b_1(L_{\min})$ and $b_2(L_{\min})$ (by "x" and "+", respectively) estimated with the critical exponents of our GFD theory (8) ($\eta = 1/8$, $\omega_l = l/2$), assuming $\delta(t, L) = 0$. The effective amplitudes converge to some values with increasing of $L_{\min}$. These, however, are not the true asymptotic values, since the maximal size of the system has been eliminated to $L = 56$. 


7 A test for the standard 3D Ising model

A test with the effective amplitudes, as in Sec. 6, appears to be more sensitive tool as compared to the fits discussed in Sec. 5. Since more data points are available for the standard Ising model, we can make even better test than that in Sec. 6. We have fitted all data points in Tab. 25 of [16] within the interval \([L; 8L]\) to the theoretical expression for \(\ln \chi\) (consistent with (8)) to evaluate the effective amplitudes \(a\) and \(b_l\) with \(l = 1, 2, 3\) depending on \(L\). Exceptionally in the case if all the involved exponents are correct (exact) each effective amplitude can converge to a certain nonzero asymptotic value at \(L \to \infty\). In other words, if one tries to compensate the inconsistency in the exponent by choosing appropriate amplitude, then the amplitude tends either to zero or infinity at \(L \to \infty\).

We have shown in Fig. 8 the effective amplitudes \(\ln a(L)\) and \(b_l(L)\) in the case of our critical exponents \(\eta = 1/8\) and \(\omega_l = l/2\). As we expected, the effective amplitudes converge to some nonzero values with increasing of \(L\). This is a good numerical evidence that our critical exponents are true. The case with the exponents of \(\eta = 0.0358(4), \omega_1 = 0.845(10), \omega_2 = 2\omega_1,\) and \(\omega_3 = 2\) is illustrated in Fig. 4. As we expected, the effective amplitudes of our four–parameter fit (solid symbols) tend to diverge with increasing of \(L\), which shows that this set of critical exponents is false. One could object that, probably, the instability of the effective amplitudes is due to small errors in MC data. However, the amplitudes \(b_1(L)\) and \(b_2(L)\) of the more stable three–parameter fit \((l = 1, 2\) in \(\eta = 0.0358(4)\)) behave in a similar way (see empty symbols in Fig. 8). Moreover, the amplitude \(b_1(L)\) of the two–parameter fit, shown by crosses, increases almost linearly at large enough \(L\) instead of the expected (in a case of correct exponents) saturation like \(b_1(L) \simeq b_1 + \text{const} \cdot L^{-\omega}\). As regards
Figure 9: The effective amplitudes in Eq. (8) evaluated by fitting the susceptibility data of 3D Ising model at criticality within the interval of sizes $[L; 8L]$ with the critical exponents $\eta = 0.0358$, $\omega_1 = 0.845$, $\omega_2 = 2\omega_1$, and $\omega_3 = 2$ proposed in [13]. Solid symbols show the four-parameter fit: $50b_1(L)$ (circles), $b_2(L)$ (squares), and $b_3(L)$ (rhombus); empty symbols show the three-parameter fit: $100b_1(L)$ (circles) and $27b_2(L)$ (squares); crosses represent the amplitude of the two-parameter fit, i.e., quantity $190(b_1(L) + 0.34)$.

The convergence in Fig. 8 of the effective amplitudes at $L \to \infty$, it is possible only if both conditions are fulfilled, i.e., the exponents are correct and the MC data are accurate enough to ensure stable results. Thus, in any case, the analysis in Fig. 8 provides rather convincing evidence that our exponents are the true ones, which by itself rules out the possibility that those proposed in [13] could be correct. The results in Figs. 8 and 9 are affected insignificantly by a small inaccuracy of about $10^{-7}$ in the estimated $\beta_c$ value.

8 Some remarks about other numerical results

There exists a large number of numerical results in the published literature not discussed here and in our previous papers [3, 7]. A detailed review of these results is given in [24]. The cited there papers report results which disagree with the values of the critical exponents we have proposed. However, as regards the pure Monte Carlo study, we are quite confident that, just like in the actually discussed case of 3D Ising model, the increase of system sizes and/or use of higher-level approximations will lead to the conclusion that fits with our exponents are better than those with the conventional (RG) exponents. Particularly, a careful analysis of the effective exponents made in Sec. 3 and 4, as well as in Sec. 6 of [7] already has shown that the effective exponents deviate from the values predicted by the perturbative RG theory and converge more or less to those of the GFD theory at $L \to \infty$. Together with the analysis of the experiment with superfluid $^4$He [3], we have presented totally 6 independent evidences of such a behavior.
Formally, the finite–size effects on the obtained values of the critical exponents has been taken into account in many of cases considered in literature. However, the estimated effect strongly depends on that which kind of corrections to scaling is expected and included in the analysis. All the existing analysis (not counting our works), of course, are based on the assumption that the critical behavior of all physical quantities is characterised by the same correction exponent $\omega$ which is about 0.8 for $O(n)$–symmetric models with $n = 1, 2, 3, 4$. However, it is evident from the behavior of the partition function zeros of 3D Ising model [7] that $\omega$ cannot have so large value. Namely, the value of $(1/\nu) + \omega$ should be about 2 or even smaller, otherwise we arrive to a rather strong and obvious contradiction with the MC data for the real part of the partition function zeros [7]. The current analysis in Sec. 3 provides 3 independent evidences (for $n = 1, 2, 3$) that the correction exponent for the magnetization cumulant is remarkably smaller than 0.8. The numerical analysis often suggests that $\omega \approx 1$. This fact is perfectly explained by our theoretical concept: in some cases the amplitude of the leading correction term can be small as compared to that of the subleading term providing the effective correction exponent just about 1. The value of $\omega$ is crucial for an accurate correction–to–scaling analysis. If, e. g., we would assume that $\omega = 0.845$, then we could not arrive to a conclusion that $\eta = 1/8$ is a better choice for the 3D Ising model than $\eta = 0.0358(4)$, since all fits with $\eta = 1/8$ and $\omega = 0.845$ look relatively bad. This explains the fact that the usual estimations do not give $\eta \approx 1/8$, while this is just the correct value. We suppose that similar problems could arise also in other cases, particularly, if one uses some expression for the correlation length in finite system (like in [19]), as it has been discussed in [8].

We should not forget also about purely subjective factor that any signals about essential inconsistency between MC data and RG predictions usually are suppressed, i. e., they do not apper in the published literature. There are no doubts that such signals exist which can be mentioned even very easily, e. g., the behavior of the effective critical exponents $\omega_{eff}$ discussed in Sec. 3, or those evidences in [8] which appear as a result of unsophisticated analysis of MC data. As a result of an un–critical acceptance of anything which claims to confirm with a great accuracy the conventional (RG) values of the critical exponents and rejection of any contraarguments, the objective picture is distorted. This is the reason why almost all the published and reviewed papers usually claim to confirm with an almost unbelievable accuracy the predictions of the perturbative RG theory. It is impossible to check in detail all these papers, but our critical analysis in [8], [9], and here indicates that many of them are, at least, inobjective.

There exists some background for the conventional claims in the published literature that all the usual methods give consistent results which appear to be in a good agreement with the predictions of the perturbative RG theory. The perturbation expansions of the RG theory, as well as the techniques of high– and low–temperature series expansion are merely not rigorous extrapolation schemes which work not too close to criticality. As a result, these methods produce some pseudo or effective critical exponents which, however, often provide a good approximation just for the range of temperatures not too close to $T_c$ (critical temperature) where these methods make sense and, therefore, agree with each other. According to the finite–size scaling theory, $tL^{1/\nu}$ is a relevant scaling argument, so that not too small values of
the reduced temperature $t$ are related to not too large sizes $L \sim t^{-\nu}$. Therefore, one can understand that the MC results for finite systems often can be well matched to the conventional critical exponents proposed by high temperature (HT) and RG expansions. If, however, the level of MC analysis (i.e., the level of approximations used) is increased, then it turns out that the "conventional" critical exponents are not valid anymore, as it has been demonstrated in the current paper and in [8]. It is because the "conventional" exponents are not the asymptotic exponents. Correct values of the asymptotic exponents have been found in [8] considering suitable theoretical limits instead of formal expansions in terms of $\ln k$ (at criticality, where $k$ is the wave vector magnitude) or $\ln t$ (approaching criticality) which are meaningless at $k \to 0$ and $t \to 0$. These formal expansions lie in the basis of the RG expansions for the critical exponents. The founders and defenders of the perturbative RG theory, of course, will try to doubt our statement that the perturbative RG method is invalid at criticality. But it is impossible to doubt a mathematical proof. It has been proven in [8] that the assumption that the $\epsilon$-expansion works and provides correct results at $k \to 0$ leads to an obvious contradiction in mathematics (cf. Sec. 2 in [8]). This fact alone cannot be compensated even by an infinite number of numerical evidences supporting the "conventional" critical exponents coming from the RG expansions.

Our argument, based on the current numerical analysis, is the following. We have proposed here a very sensitive method (i.e., a study of effective amplitudes) which allows to test the consistency of a given set of critical exponents with the MC data including several (in our case up to 3) corrections to scaling. We have applied this method to one of the recent and most accurate numerical data for the susceptibility in 3D Ising model, and have got a confirmation that our critical exponents are true. It would be not correct to doubt our results based on less sensitive methods and lower-level approximations.

We prefer to rely just on the data of pure MC simulations because of the following reasons. The so called Monte Carlo RG (MCRG) method is not free of assumptions related to approximate renormalization. We would like only to mention that the MCRG study in [26] of 3D Ising systems of the largest (to our knowledge) available in literature sizes, i.e., up to $L = 256$, has not revealed an excellent agreement with the usual predictions of the perturbative RG. In particular, an estimate $\omega \approx 0.7$ has been obtained [26] which is smaller than the usual (perturbative) RG value $\omega \approx 0.8$, but still is larger than the exact value 0.5 predicted by the GFD theory. The high-temperature series cannot give more precise results than those extracted from the recent most accurate MC data, including the actual data of [16], since these series diverge approaching the critical point. One approximates the divergent series by a ratio of two divergent series (Pade approximation), but it is never proven that such a method converges to the exact result. It is interesting to compare the MC and HT estimates of the critical point for the standard 3D Ising model, i.e., $\beta_c \simeq 0.2216545$ (MC) [16] and $\beta_c = 0.221659 + 0.000002/ - 0.000005$ (HT) [25]. It is clear that the MC value is more accurate: if we look in [16], where the estimation procedure is well illustrated, we can see that $\beta_c$ is definitely smaller than 0.221659, and the error seems to be much smaller than the difference between both estimates 0.0000045. As we have mentioned already, our independent tests suggest that the error of the actual MC value is about $10^{-7}$. 
9 Conclusions

In summary of the present work, we conclude the following.

1. The leading correction–to–scaling exponent $\omega$ in $O(n)$–symmetric models on a three–dimensional lattice has been tested by analysing the recent Monte Carlo (MC) data. These tests have shown the incorrectness of some claims that $\omega$ has a very accurate value 0.845(10) at $n = 1$. A selfconsistent infinite volume extrapolation yields row estimates $\omega \approx 0.547$, $\omega \approx 0.573$, and $\omega \approx 0.625$ at $n = 1, 2$, and 3, respectively, in approximate agreement with the corresponding exact values $1/2$, $5/9$, and $3/5$ predicted by our recently developed GFD theory.

2. Considering the susceptibility data for 3D Ising model at criticality (Sec. 3), we conclude that the fits made with our (GFD) critical exponents systematically improve relative to those made with the exponents given in [13], as the system sizes grow and the approximation order increases.

3. The numerical analysis of the effective critical exponents in Sec. 3 and 5, as well as in Sec. 6 of [7] has shown that the effective critical exponents deviate from the values predicted by the perturbative RG theory and converge towards those of the GFD theory at $L \to \infty$. The same behavior has been observed in the experiment with superfluid $^4$He discussed in [3]. Totally, these are 6 independent evidences of such a behavior, suggesting that the above examples are not occasional or exceptional, but reflect a general rule.

4. Different sets of critical exponents (one provided by GFD theory, another proposed in [13]) predicted for the 3D Ising model have been tested by analysing the effective amplitudes (Sec. 3 and 5). While the usual fits of the susceptibility data do not allow to show convincingly which of the discussed here sets of the critical exponents is better, this method clearly demonstrates that the conventional critical exponents $\eta = 0.0358(4)$ and $\omega = 0.845(10)$ [13] are false, whereas our (GFD) values $\eta = 1/8$ and $\omega = 1/2$ are true.

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