Monte Carlo test of critical exponents in 3D Heisenberg and Ising models

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Abstract

We have tested the theoretical values of critical exponents, predicted for the three–dimensional Heisenberg model, based on the published Monte Carlo (MC) simulation data for the susceptibility. Two different sets of the critical exponents have been considered – one provided by the usual (perturbative) renormalization group (RG) theory, and another predicted by grouping of Feynman diagrams in $\phi^4$ model (our theory). The test consists of two steps. First we determine the critical coupling by fitting the MC data to the theoretical expression, including both confluent and analytical corrections to scaling, the values of critical exponents being taken from theory. Then we use the obtained value of critical coupling to test the agreement between theory and MC data at criticality. As a result, we have found that predictions of our theory ($\gamma = 19/14$, $\eta = 1/10$, $\omega = 3/5$) are consistent, whereas those of the perturbative RG theory ($\gamma \approx 1.3895$, $\eta \approx 0.0355$, $\omega \approx 0.782$) are inconsistent with the MC data. The seemable agreement between the RG prediction for $\eta$ and MC results at criticality, reported in literature, appears due to slightly overestimated value of the critical coupling. Estimation of critical exponents of 3D Ising model from complex zeroth of the partition function is discussed. A refined analysis yields the best estimate $1/\nu \approx 1.518$. We conclude that the recent MC data can be completely explained within our theory (providing $1/\nu = 1.5$ and $\omega = 0.5$) rather than within the conventional RG theory.

Keywords: Heisenberg model, Ising model, Monte Carlo data, critical exponents, partition function zeroth

1 Introduction

In our previous work [1], we have reported the possible values of exact critical exponents for the Ginzburg–Landau phase transition model predicted from a reorganized perturbation theory. These predictions are in exact agreement with the known exact and rigorous results in two dimensions [3], and are equally valid also in three dimensions. Our predictions have been compared to some original data of Monte
Carlo (MC) simulations and experiments [3, 4, 5], and a remarkable agreement has been found.

However, there is still rather paradoxical and unclear situation regarding the MC results. On the one hand, we have shown theoretically [1] the invalidity of the conventional RG expansions [6, 7, 8], but, on the other hand, the published papers on MC simulations usually claim to confirm the values of critical exponents coming from these expansions and being in contradiction to our results.

Contrary to the usual claims in the published papers that the values of critical exponents can be obtained from the Monte Carlo data with a striking accuracy, i.e. with an error much smaller than 0.01, our experience in analysis of several such data shows that in reality it is very difficult to extract accurate and reliable estimates therefrom. The problem is that a fitting of MC data to a simple theoretical ansatz (including no corrections to scaling) can provide a rather small statistical error, but the obtained result is not reliable since it contains an uncontrolled systematical error due to the neglected corrections to scaling. Moreover, confluent (i.e., those related to the universal properties of the critical point) and analytical corrections can be equally important at finite values of the reduced temperature at which the simulations have been done, since the amplitude of the leading analytical correction can be remarkably larger than that of the confluent correction. Our analysis of the susceptibility data for the three-dimensional Heisenberg model (Sec. 3) has shown that the estimated value of the critical exponent $\gamma$ decreases by several percents due to the confluent correction, and the result can be changed remarkably by the analytical correction too. Thus, both kind of corrections should be taken into account, but this is not possible in the usual applications related to the determination of critical exponents, since inclusion of both kind of corrections in a theoretical ansatz strongly increases the statistical errors.

As regards the fitting of MC data at criticality, only confluent corrections are present, but the usual estimations are rather sensitive to the precise value of the critical coupling. In this aspect, our estimation of the critical exponent $\eta$ [4] from the MC simulated fractal dimensionality of the three-dimensional Ising model at the critical point (i.e., from MC data of [3]) is preferable to a more conventional, but much more sensitive to the precise value of the critical coupling $\beta_c$, estimation of this exponent from the susceptibility data at criticality. According to the published results [4], the second method seems to give smaller values of $\eta$ in three dimensions (about 0.027 for Heisenberg model [4]) as compared to the first one (about 1/8 for Ising model [4]), but the reason for the discrepancy could be an inaccuracy in the estimated value of $\beta_c$. In the case of the Heisenberg model, this value has been overestimated, indeed, as discussed in Sec. 4. More recent MC results reported in [10] also provide rather small values of $\eta$ (about 0.04 for $O(n)$ models with $n = 2, 3, 4$). However, the infinite volume extrapolation in [10] is erroneous in view of our theory, and a selfconsistent treatment, based on our theoretical predictions, reveals no contradiction to the MC data (Sec. 3).

In the present work we have proposed a Monte Carlo test, based on a high quality susceptibility data [4], where the above discussed problems with corrections to scaling are solved on a higher level than it has been done in the currently published papers. Namely, our method enables us to test the agreement of MC data with given (fixed) theoretical values of critical exponents by taking into account both the leading
confluent and the leading analytical correction. Our test consists of a very accurate
determination of the critical coupling followed by a fitting of the susceptibility data
at criticality. It has shown (Sec. 5) that the actually discussed MC data are in
agreement with our theoretical values of critical exponents, but not with those of
the RG expansions.

2 Critical exponents from our theory

Our theory provides possible values of exact critical exponents \( \gamma \) and \( \nu \) for the \( \phi^4 \)
model with \( O(n) \) symmetry (\( n \)-component vector model) with the Hamiltonian

\[
H/T = \int \left[r_0 \phi^2(x) + c(\nabla \phi(x))^2 + u \phi^4(x)\right] dx ,
\]

where \( r_0 \) is the only parameter depending on temperature \( T \), and the dependence is
linear. At the spatial dimensionality \( d = 2, 3 \) and \( n = 1, 2, 3, \ldots \) these values are [1]

\[
\gamma = \frac{d + 2j + 4m}{d(1 + m + j) - 2j} , \\
\nu = \frac{2(1 + m) + j}{d(1 + m + j) - 2j} ,
\]

where \( m \geq 1 \) and \( j \geq -m \) are integers. At \( n = 1 \) we have \( m = 3 \) and \( j = 0 \) to fit the
known exact results for the two-dimensional Ising model. As proposed in Ref. [1],
in the case of \( n = 2 \) we have \( m = 3 \) and \( j = 1 \), which yields in three dimensions
\( \nu = 9/13 \) and \( \gamma = 17/13 \).

In the present analysis the correction–to–scaling exponent \( \theta \) for the susceptibility
also is relevant. The susceptibility is related to the correlation function in the Fourier
representation \( G(k) \), i. e., \( \chi \propto G(0) \). In the thermodynamic limit, this relation
makes sense at \( T > T_c \), where \( T_c \) is the critical temperature. According to our
theory, \( G(0) \) can be expanded in a Taylor series of \( t^{2\nu-\gamma} \) at \( t \to 0 \). In this case the
reduced temperature \( t \) is defined as \( t = r_0(T) - r_0(T_c) \propto T - T_c \). Formally, \( t^{2\gamma-2\nu} \)
appears as second expansion parameter in the derivations in Ref. [1], but, according
to the final result represented by Eqs. (2) and (3), \((2\gamma-2\nu)/(2\nu-\gamma)\) is a natural
number. Some of the expansion coefficients can be zero, so that in general we have

\[
\theta = \ell \left(2\nu - \gamma\right) ,
\]

where \( \ell \) may have integer values 1, 2, 3, etc. One can expect that \( \ell = 4 \) holds at
\( n = 1 \) (which yields \( \theta = 1 \) at \( d = 2 \) and \( \theta = 1/3 \) at \( d = 3 \)) and the only nonvanishing corrections are those of the order \( t^\theta, t^{2\theta}, t^{3\theta} \), since the known corrections
to scaling for physical quantities, such as magnetization or correlation length, are
analytical in the case of the two–dimensional Ising model. Here we suppose that
the confluent corrections become analytical, i. e. \( \theta \) takes the value 1, at \( d = 2 \).
Besides, similar corrections to scaling are expected for susceptibility \( \chi \) and mag-
netization \( M \) since both these quantities are related to \( G(0) \), i. e., \( \chi \propto G(0) \) and
\( M^2 = \lim_{x \to \infty} \langle \phi(0)\phi(x) \rangle = \lim_{V \to \infty} G(0)/V \) hold where \( V = L^d \) is the volume and
\( L \) is the linear size of the system. The above limit is meaningful at \( L \to \infty \), but
\( G(0)/V \) may be considered as a definition of \( M^2 \) for finite systems too. The latter
means that corrections to finite–size scaling for $\chi$ and $M$ are similar at $T = T_c$. According to the scaling hypothesis and finite–size scaling theory (Sec. 3), the same is true for the discussed here corrections at $t \to 0$. Thus, the expected expansion of the susceptibility $\chi$ looks like $\chi = t^{-\gamma} \left(a_0 + a_1 t^{\theta} + a_2 t^{2\theta} + \cdots \right)$.

Our general hypothesis is that $j = j(n)$ and $\ell = \ell(n)$ monotonically increase with $n$ to fit the known exponents for the spherical model at $n \to \infty$. In particular, we expect that $j(n) = n - 1$, $\ell(n) = n + 3$, and $m = 3$ hold at $n = 1, 2, 3$ and, probably, also in general. This hypothesis is well confirmed by MC results discussed here and in Ref. [9].

We allow that different $\ell$ values correspond to the leading correction–to–scaling exponent for different quantities related to $G(k)$. The expansion of $G(k)$ by itself contains a nonvanishing term of order $t^{2\nu - \gamma} \equiv t^{\nu'}$ (in the form $G(k) \approx t^{-\gamma} [g(k t^{-\nu}) + t^{\nu'} g_1(k t^{-\nu})]$ with $g_1(0) = 0$, since $\ell \geq 1$ holds in the case of susceptibility) to compensate the corresponding correction term (produced by $c(\nabla \phi)^2$) in the equation for $1/G(k)$ (cf. [1]). The latter means, e. g., that the correlation length $\xi$ estimated from an approximate ansatz like $G(k) \propto 1/\left[k^2 + (1/\xi)^2\right]$ used in [3, 10] also contains a correction proportional to $t^{\nu'}$. Since $\eta \nu$ has a rather small value, the presence of such a correction (and, presumably, also the higher order corrections $t^{2\nu'}, t^{3\nu'}, \ldots$) makes the above ansatz unsuitable for an accurate numerical correction–to–scaling analysis. Due to this reason the susceptibility data, but not the correlation length data of Ref. [3], are used in our further analysis.

The correction $t^{\nu'}$ is related to the correction $L^{-\eta}$ in the finite–size scaling expressions at criticality. The existence of such a correction in the asymptotic expansion of the critical real–space Green’s (correlation) function, i. e. $\tilde{G}(rL) \propto L^{2-\eta-\delta} \left(1 + O(L^{-\eta})\right)$ where $r$ is a constant, is well confirmed by our recent (preliminary) results for the 2D Ising model. These results for $L = 2, 4, 6, \ldots, 16$ have been obtained by an exact numerical transfer–matrix algorithm. In such a way, the infinite volume extrapolation in [10] appears to be incorrect, therefore the obtained there results do not represent a serious argument against our theory. Moreover, if the extrapolation in [10] is done including the correction $L^{-\eta}$, then the results for $O(n)$ models with $n = 2, 3$ appear to be in a satisfactory agreement (within the extrapolation errors) with our values $\eta = 1/9$ and $\eta = 1/10$, respectively.

Our consideration can be generalized easily to the case where the Hamiltonian parameter $r_0$ is a nonlinear analytical function of $T$. Nothing is changed in the above expansions if the reduced temperature $t$, as before, is defined by $t = r_0(T) - r_0(T_c)$. However, analytical corrections to scaling appear (and also corrections like $(T - T_c)^{m+n\delta}$ with integer $m$ and $n$) if $t$ is reexpanded in terms of $T - T_c$ at $T > T_c$. The solution at the critical point remains unchanged, since the phase transition occurs at the same (critical) value of $r_0$.

### 3 Estimation of the critical exponent $\gamma$ from MC data

In this section we discuss the estimation of the susceptibility exponent $\gamma$ for the classical three–dimensional Heisenberg model. Our analysis is based on the fitting of the susceptibility (MC) data to a theoretical ansatz. According to the finite–size scaling theory, the susceptibility $\chi$ depending on the reduced temperature
\[ t = 1 - \beta/\beta_c \] (where \( t > 0 \)) and the linear size of the system \( L \) reads

\[ \chi = L^{\gamma/\nu} g \left( L/\xi \right) , \tag{5} \]

where \( g(L/\xi) \) is the scaling function and \( \xi \sim t^{-\nu} \) is the correlation length of an infinite system. Eq. (5) holds precisely at \( L \to \infty \) and \( t \to 0 \) for any given value of \( L/\xi \). At finite values of \( t \) and \( L \) corrections to (5) exist. Eq. (5) can be rewritten as

\[ \chi = t^{-\gamma} f \left( tL^{1/\nu} \right) , \tag{6} \]

where \( g(y) = y^{-\gamma/\nu} f \left( y^{1/\nu} \right) \). In the thermodynamic limit \( L \to \infty \) Eq. (6) reduces to \( \chi = b_0 t^{-\gamma} \), where \( b_0 = \lim_{x \to \infty} f(x) \) is the amplitude. A natural extension of Eq. (6), including corrections to scaling, is

\[ \chi = t^{-\gamma} \sum_{l \geq 0} t^\gamma_l f_l \left( tL^{1/\nu} \right) , \tag{7} \]

where \( \gamma_0 = 0 \), \( f_0(x) = f(x) \), and the terms with \( l > 0 \) represent all the corrections in the asymptotic expansion of \( \chi \) at \( t \to 0 \) for any given value of \( x = tL^{1/\nu} \). In the thermodynamic limit we have \( \lim_{x \to \infty} f_l(x) = b_l \), where \( b_l \) are the amplitudes. The most important correction terms in the sum over \( l \) are the leading confluent correction \( b_1 t^{\gamma_1} \) with the exponent \( \gamma_1 = \theta \) and the leading analytical correction \( b_2 t^{\gamma_2} \) with \( \gamma_2 = 1 \). Although \( \theta < 1 \) holds, the analytical correction also should be included at finite values of \( t \) used in practical simulations: because of absence of a direct correlation between the amplitudes of confluent and analytical corrections, the ratio \( r = b_2/b_1 \) can be arbitrarily large. One can expect that the higher order confluent corrections (i. e., those proportional to \( t^{2\theta} \), \( t^{3\theta} \), etc.) are small as compared to the leading confluent correction, and the same is true for analytical corrections. We consider the case of small \( t \) and large \( x \), i. e., small \( f_l(x) - b_l \). In this case Eq. (7) can be written as

\[ \chi \simeq t^{-\gamma} \left[ 1 + b \left( t^\theta + rt \right) \right] f \left( tL^{1/\nu} \right) , \tag{8} \]

where \( b = b_1/b_0 \) is a constant.

We have used the susceptibility data simulated by an improved (cluster) MC algorithm reported in Ref. [9] (\( \tilde{\chi}^{imp} \) vs \( \beta \), tab. IV in [9]) to estimate the critical exponent \( \gamma \) by fitting the data to (8). Such an estimation has been done in [9], neglecting either the analytical or the confluent correction and setting \( f \left( tL^{1/\nu} \right) = b_0 \). Since in the actual simulations the scaling argument \( x = tL^{1/\nu} \) has large enough values, about 6 or 7, which are varied only slightly, the latter approximation is reasonable. We have used even better approximation where \( \ln f(x) \) has been linearized within the narrow range of \( x \) variation, and the simulated data points for \( \ln \chi \) have been fitted to the resulting theoretical expression

\[ \ln \chi(t, L) = a - \gamma \ln t + \ln \left[ 1 + b \left( t^\theta + rt \right) \right] + p tL^{1/\nu} , \tag{9} \]

where \( a \) and \( p \) are constants. The minimum of the sum of the squared deviations for \( N \) data points \( S(N) \) corresponds to the least–squares fit. Besides, it is reasonable to use the least–squares method just for \( \ln \chi \), but not for \( \chi \), since the errors for \( \ln \chi \)
Figure 1: Estimation of the critical exponent $\gamma$ in 3D Heisenberg model. Solid line shows the standard deviation $\sigma$ of the simulated data points from the analytical curve (9) as a function of $\gamma$ with parameters $a$, $b$, $p$, and $\beta_c$ obtained from the least-squares fit at $\nu = 5/7$, $\theta = 3/7$ (our theoretical values), and $r = 0$. The dotted curve corresponds to fixed $p = 0$. The minimum of the solid curve gives the least-squares estimate $\gamma = 1.345$. All fits (for different data sets) lie in the marked area which is shifted only slightly, as indicated by thin vertical dashed lines, if the RG values of $\nu$ and $\theta$ are used instead of ours. Our theoretical value $\gamma = 19/14$ (thick vertical dashed line) is inside of the marked region, whereas that of the RG theory (vertical dot-dot-dashed line at $\gamma = 1.3895$) is outside.

Data points are comparable, i.e., the relative but not the absolute errors are more or less equal. At large $N$, the inaccuracy in the fitted curve due to the statistical errors can be characterised by the standard deviation $\sigma = (S(N)/[N(N-1)])^{1/2}$. Obviously, the minimum of $\sigma$ corresponds to the least-squares fit at any given $N$.

We have illustrated in Fig. 1 the estimation of $\gamma$ by minimizing $\sigma$ with respect to the parameters $a$, $b$, $p$, and $\beta_c$ (where $\beta_c$ is incorporated in (9) via $t = 1 - \beta/\beta_c$) at fixed exponents $\theta = 3/7$ and $\nu = 5/7$, taken from our theory (Sec. 2). The analytical correction to scaling has been neglected by setting $r = 0$. The solid line shows the accuracy of the fit, i.e., the value of $\sigma$, depending on the choice of the exponent $\gamma$. The minimum of $\sigma$, indicated by a vertical dotted line, is located at $\gamma \simeq 1.345$, which corresponds to the least-squares fit. The dotted curve corresponds to the case of fixed $p = 0$. From this we can see that inclusion of the term $ptL^{1/\nu}$ in (9), responsible for the variation of the scaling function $f(x)$, affects the result only slightly.

In spite of the very high accuracy of the fit (about 0.02% error in $\chi$), the minimum in $\sigma$ is too broad for a reliable estimation of $\gamma$ with, e.g., $\pm 0.01$ accuracy. This is a problem which usually appears if we use a high-level approximation including many fitting parameters. If the analytical correction also is included, then the situation becomes even worse, i.e., the $\sigma$ vs $\gamma$ plot is an almost horizontal line. Neglection of both (confluent and analytical) corrections, as it has been done finally in (9), is not
a solution of the problem since the result is affected significantly by the confluent correction. Namely, the obtained value of $\gamma$ is shifted from 1.389 to 1.345. According to our estimation, the statistical error for the latter result is remarkably smaller than the difference between these two values, so that the second value is better. Another problem is that the estimated value of $\gamma$ depends on $\theta$ and $\nu$. This effect, however, is relatively small. By the conventional RG values $\theta = 0.55$ and $\nu = 0.7073$ we obtain $\gamma \simeq 1.354$.

Like in Ref. [11], we have estimated the possible statistical error of our result $\gamma \simeq 1.345$ by comparing the values of $\gamma$ for a large number of different data sets generated from the original one (with 18 data points) by omitting some (1 to 6) data points. The data points have been omitted more or less randomly, but not the neighbouring points and not the first and the last point simultaneously, to ensure a sufficiently uniform distribution of the used $t$ values and to avoid a significant narrowing of the total interval covered by these values. The largest deviations from the central $\gamma$ value 1.345 have been observed omitting the data points No. 1, 6, 10, 14, and 17 (tab. IV in [9]), which yielded $\gamma \simeq 1.322$, and the data points No. 2, 5, 8, 11, and 14, which yielded $\gamma \simeq 1.366$. Thus, all the fits gave $1.322 \leq \gamma \leq 1.366$ at $r = 0$, $\theta = 3/7$ and $\nu = 5/7$. This interval is marked in Fig. 1 by thin solid lines. At $\theta = 0.55$ and $\nu = 0.7073$ the borders of this region are shifted slightly, as indicated by thin vertical dashed lines. These manipulations enable us to estimate the possible statistical error in both cases, i. e., $\gamma = 1.345 \pm 0.023$ at $\theta = 3/7$ and $\gamma = 1.354 \pm 0.020$ at $\theta = 0.55$. These, in fact, are maximal errors, i. e., since we never have observed larger deviations, the probability that the value extracted from exact data would be outside of the error bars is vanishingly small.

It is a remarkable fact that our theoretical value $\gamma = 19/14 \simeq 1.35714$ (thick vertical dashed line) lies inside the region of maximal statistical errors, whereas that of the RG theory, i. e. $\gamma \simeq 1.3895$ indicated by a do–dot–dashed line, is clearly outside of this region. This result can be changed by the analytical correction. However, if the ratio of amplitudes $r$ in Eq. (9) is positive, then the least–squares fit with respect to the parameters $a$, $b$, $p$, and $\beta_c$ always yields the central value of $\gamma$ (with all 18 data points included) in the range from 1.345 to 1.369 at $\theta = 3/7$ and $\nu = 5/7$. Here $\gamma = 1.369 \pm 0.013$ corresponds to the case of purely analytical correction to scaling obtained by formally setting $\theta = 1$. In such a way, selfconsistent estimations at $r > 0$ yield $\gamma$ values which are reasonably close to our prediction $\gamma = 19/14$. Precise agreement is reached at $r \simeq 1.17$.

Unfortunately, we have no proof that $r$ is positive. If we allow that $r < 0$, then a large uncertainty appears. In this case $\gamma$ can take the values as small as, e. g., 1.1 (at $\theta = 3/7$, $\nu = 5/7$, and $r \approx -1.35$) and as large as 1.4 (at $\theta = 0.55$, $\nu = 0.7073$, and $r \approx -1.8$). The actual MC data do not allow to find the true value of $r$ (unless we assume that our exponents are true and, therefore, $r \approx 1.17$), since the standard deviation of the least–squares fit is almost independent on $r$.

4 Estimation of the critical coupling

Based on the method developed in Sec. 3, here we determine the critical coupling $\beta_c$ for the three–dimensional Heisenberg model assuming that critical exponents $\gamma$,
Figure 2: Estimation of the critical coupling $\beta_c$ by fitting the MC data to ansatz (9) with fixed exponents taken from our (thick solid line) and RG (thin solid line) theory. The minimums of $\sigma$ vs $\beta_c$, used as a fitting parameter, give the least–squares estimates for the true $\beta_c$ value, as indicated by vertical dotted lines and arrows. The vertical dashed line indicates a value of $\beta_c$ proposed in [9, 10].

$\theta$, and $\nu$ are known from theory. The latter ensures a very small statistical error. The coefficients in (9) are found by the least–squares method. The resulting value of the standard deviation $\sigma$ vs $\beta_c$, used as a fitting parameter, is shown in Fig. 2. The thick solid line corresponds to our critical exponents $\gamma = 19/14$, $\nu = 5/7$, and $\theta = 3/7$, whereas the thin solid line – to the conventional (RG) exponents $\gamma = 1.3895$, $\nu = 0.7073$, and $\theta = 0.55$. The minimums of these curves, indicated by vertical dotted lines, are located at $\beta_c \approx 0.692795$ and $\beta_c \approx 0.692855$, respectively, corresponding to the least–squares estimates for the true values of the critical coupling. The estimation of maximal statistical errors, as in Sec. 3, leads to the following conclusions:

1. If our values of the critical exponents $\gamma = 19/14$, $\nu = 5/7$, and $\theta = 3/7$ are true, then

$$\beta_c = 0.692795^{+0.000030}_{-0.000043}.$$  \hfill (10)

2. If the true values of the critical exponents are close to those predicted by the RG theory, i.e., $\gamma = 1.3895$, $\nu = 0.7073$, and $\theta = 0.55$, then

$$\beta_c = 0.692855^{+0.000029}_{-0.000043}.$$  \hfill (11)

The estimation in [9, 10] gave $\beta_c \approx 0.6930$. This value is indicated in Fig. 2 by a vertical dashed line. As we see, it clearly does not correspond to the best fit. To clear up the reason for the discrepancy, let us discuss the Binder’s cumulant crossing technique used in [9] and [10] for the estimation of $\beta_c$. In this approach, the
Figure 3: Estimation of the critical coupling by the Binder’s cumulant crossing technique. The straight line represents the least-squares fit of (12) to the MC data for crossing points $T_{\text{cross}}$. The zero intercept gives $\beta_c = 1/T_c \simeq 0.69286$. For comparison, the approximation $T_{\text{cross}} - T_c \propto 1/\ln b$ (where $b$ is Binder parameter) is shown by thin solid line.

magnetization cumulants for different lattice sizes $L$ and $L'$ are plotted as a function of $\beta$ to find the intersection point $\beta = \beta_{\text{cross}}$. According to the theory [12],

$$
\beta_{\text{cross}}(L, b) - \beta_c \propto L^{-(1/\nu) - \omega} \frac{1 - b^{-\omega}}{b^{1/\nu} - 1}
$$

holds at large $L$, where $L$ is the size of the smaller lattice, $b = L'/L$ is the Binder parameter, and $\omega = \theta/\nu$. The estimation in [11] has been done by approximating the term $\rho = (1 - b^{-\omega})/(b^{1/\nu} - 1)$ in Eq. (12) with $\text{const}/\ln b$. We have made and have illustrated in Fig. 3 our own estimation of $\beta_c$ from Eq. (12), using the data for $T_{\text{cross}} = 1/\beta_{\text{cross}}$ extracted from Fig. 3 in Ref. [11]. According to (12), $\beta_{\text{cross}}$ is a linear function of $\rho$ at a fixed $L$. The same is true for $T_{\text{cross}}$ in vicinity of $T_c$. The straight line in Fig. 3 corresponds to the linear least-squares fit for $T_{\text{cross}}$ vs $\rho$ at $L = 16$ (with our exponents $\omega = 3/5$ and $\nu = 5/7$) which yields (at $\rho = 0$) $\beta_c \simeq 0.69286$. This value agree with (10) and (11) within the error bars $\pm 0.0001$ proposed in [9]. In fact, the data points are too much scattered to consider such an estimation reliable. Due to this reason, we have not tried to estimate $\beta_c$ from the data of $L = 12$ which are even more scattered. We have depicted in Fig. 3 by thin solid line the fit, corresponding to the approximation $T_{\text{cross}} - T_c \propto 1/\ln b$, made in [9] at $L = 16$. As we see, in the scale where the original ansatz (12) yields a straight line this approximation is represented by a curve providing an underestimated value of $T_{\text{cross}}$ at $\rho = 0$, i.e., an overestimated $\beta_c \simeq 0.6930$ instead of $\beta_c \simeq 0.69286$. Obviously, this approximation is the reason for the discrepancy. Note that other kind of estimations in [9] provided a bit smaller $\beta_c$ values, closer to ours.
Figure 4: Our fit to the susceptibility ($\chi$) data of [9] for 3D Heisenberg model at and near criticality. Only two coefficients $a$ and $b$ have been used as fitting parameters in (14) for the thick solid curve and solid circles representing $\ln(\chi/L^2)$ vs $\ln L$ at criticality according to our critical exponents ($\eta = 0.1$, $\gamma = 19/14$, $\omega = 0.6$) and $\beta_c \approx 0.692795$ estimated independently in Sec. 4. The same fit at RG exponents with the corresponding $\beta_c$ value 0.692855 is represented by the dot–dot–dashed line and empty circles. Thin solid lines show our three–parameter fit at $\beta = 0.6925$ (empty squares), $\beta = 0.6930$ (crosses), and $\beta = 0.6933$ (empty rhombs). The linear fit of [9] is shown by tiny dashed line.

5 The test of consistency at $T = T_c$

Consequently following the conclusions (10) and (11) made in Sec. 4, here we test the agreement between theory and MC data at criticality.

According to the finite–size scaling theory, the susceptibility at the critical point is given by

$$\chi \propto L^{\gamma/\nu} \left(1 + bL^{-\omega} + \ldots\right),$$

where $b$ and $\omega = \theta/\nu$ are the amplitude and the exponent of the leading correction to scaling. The dots stand for further corrections. Eq. (13) can be rewritten as

$$\ln \left(\chi/L^2\right) \simeq a - \eta \ln L + \ln \left(1 + bL^{-\omega}\right),$$

where $a$ is a constant and $\eta = 2 - \gamma/\nu$ is the critical exponent describing the asymptotic long–wave behavior of the correlation function (i. e. $G(k) \sim k^{-2+\eta}$) at $T = T_c$. We have read from Fig. 6 in Ref. [9] the values of $\chi$ near $\beta_c$ and have made the linear interpolation between $\beta = 0.6927$ and $\beta = 0.6929$ to estimate $\chi$ at the values of the critical coupling given by (10) and (11). So obtained $\chi$ values are depicted in Fig. 4 by solid and empty circles, respectively. The corresponding two parameter ($a$ and $b$ in Eq. (14)) least–squares fits with fixed exponents are shown by thick solid line (our case) and dot–dot–dashed line (RG case). If $\eta$ is considered as a fitting parameter, then in our case the least–squares fit yields $\eta \simeq 0.105$ in close
agreement with the theoretical value 0.1, whereas in the RG case it yields $\eta \simeq 0.076$ in a remarkable disagreement with the theoretical value 0.0355. It can be seen also from Fig. 6 of Ref. 3 that the dot–dot–dashed line with $a = -0.17034$ and $b = 0.1178$, obtained at fixed $\eta = 0.0355$, does not provide a satisfactory fit to the data, i.e., this line is curved in a wrong direction.

Our values of critical exponents provide an excellent fit to the MC data not only at $\beta = \beta_c$, but also at small deviations $t = 1 - \beta / \beta_c$ from the critical point considered in Fig. 6 of Ref. 3. Our fit $\chi = 1.1266 L^{1.9} (1 - 0.4944 L^{-0.6} - 0.58 t L^{1.4})$ is shown in Fig. 4 by solid lines. This approximation is consistent with the finite–size scaling theory at large $L$ and small $t L^{1/\nu}$. The data points in Fig. 4 correspond to $12 \leq L \leq 48$. At smaller $L$ values the second–order corrections to scaling, neglected in our ansatz, could be relevant. The solid curve at $\beta = 0.6930$ is the most linear one within $12 \leq L \leq 48$, as it is evident from Fig. 4 where the straight–line fit of $\chi$ is shown by a tiny dashed line. It is evident also that the good linearity of $\ln (\chi / L^2)$ vs $\ln L$ in this region does not mean that $\beta_c \simeq 0.6930$ and $\eta \simeq 0.027$.

One of the arguments in 3, supporting the idea that $\eta$ has a very small value ($\eta < 0.05$), is based on the simulated data for $\chi$ vs the correlation length $\xi$ for finite systems. However, the variation of $\eta_{\text{eff}}$ with $\xi$ in Fig. 12 of Ref. 3 can be well explained by presence of corrections of the kind $\xi^{-m \eta}$, where $m = 1, 2, \ldots$ and $\eta = 1/10$, consistent with the correction–to–scaling analysis in Sec. 2 (see remarks regarding the actual approximation for $\xi$). In this case $\eta_{\text{eff}}$ can behave nonmonotonously, as well. As regards other arguments in 3 in support of the conventional RG values of critical exponents, they are weaker than our contraarguments discussed here, since all the final estimates in 3 are obtained neglecting corrections to scaling. Note also that such kind of simple estimations not always give very small values of $\eta$. In particular, the values of about 0.15 follow from MC study of Heisenberg fluid 13. In view of our theory and presented here analysis of the MC method, the discrepancy between the so called ”lattice” and ”off–lattice” critical exponents discussed in 13 can be well understood as an error of about ±0.07 (in $\eta$) of the above discussed simple estimations.

It is noteworthy that a large variety of experimental measurements in Ni discussed in 14, confirm our values of critical exponents $\gamma = 19/14 = 1.357\ldots$, $\beta = (d-2+\eta) \nu/2 = 11/28 = 0.3928\ldots$, and $\delta = (d+2-\eta)/(d-2+\eta) = 49/11 = 4.4545\ldots$ rather than those of the RG theory ($\gamma \simeq 1.3895$, $\delta \simeq 4.794$, and $\beta \simeq 0.3662$ 11).

6 Comparison to 3D Ising model

In this section we discuss the recent MC results 15 for the complex zeroth of the partition function of the three–dimensional Ising model. Namely, if the coupling $\beta$ is a complex number, then the statistical sum has zeroth at certain complex values of $\beta$ or $u = e^{-\beta}$. The nearest to the real positive axis values $\beta^0$ and $u^0$ are of special interest. Neglecting the second–order corrections, $u^0$ behaves like

$$u^0 = u_c + A L^{-1/\nu} + B L^{-(1/\nu) - \omega}$$

(15)

at large $L$, where $u_c = e^{-\beta_c}$ is the critical value of $u$, $A$ and $B$ are complex constants, and $\omega$ is the correction–to–scaling exponent. According to the known results (see,
e. g., the solution given in [13]), the partition function zeroth correspond to complex values of \(\sinh(2\beta)\) located on a unit circle in the case of 2D Ising model, so that \(A\) is purely imaginary. The latter means that the critical behavior of real and imaginary parts of \(u_0^0 - u_c\) essentially differ from each other, i. e., \(\text{Re} \ (u_0^0 - u_c) \propto L^{-(1/\nu) - \omega}\) and \(\text{Im} \ (u_0^0) \propto L^{-1/\nu}\) (where, in this case of \(d = 2\), \(\nu = \omega = 1\)) at \(L \to \infty\). The MC data of [15], in fact, provide a good evidence that the same is true in three dimensions.

Unfortunately, the authors of Ref. [15] have not tried to find the objective truth regarding the behavior of the complex zeroth, but only have searched the way how to confirm the already known estimates for \(\nu\). Their treatment, however, is rather doubtful. First, let us mention that, in contradiction to the definition in the paper, \(\nu\) regarding the behavior of the complex zeroth, but only have searched the way how to coincide with the known exact result at \(d = 2\), \(\nu = 2/3\) and \(\omega = 1/2\), i. e., \((1/\nu) + \omega = 2\).

To obtain a more complete picture, we have considered separately the real part and the imaginary part of \(u_0^0 - u_c\). We have calculated \(u_0^0\) from \(\beta_0^0\) data listed in Tab. I of [13] and have estimated the effective critical exponents \(y_{eff}(L)\) and \(y_{eff}''(L)\), separately for \(\text{Re} \ (u_0^0 - u_c)\) and \(\text{Im} \ (u_0^0)\), by fitting these quantities to an ansatz \(\text{const} \cdot L^{-y_{eff}}\) and \(\text{const} \cdot L^{-y_{eff}''}\), respectively, at sizes \(L\) and \(L/2\). The value of \(u_c\) consistent with high– and low– temperature series [17] as well as MC [18] estimations of the critical coupling, \(\beta_c \simeq 0.221659\), have been used. The results are shown in Fig. 3. As we see, \(y_{eff}'\) (empty circles) claims to increase above \(y_{eff}''\) (solid circles) when \(L\) increases. This is a good numerical evidence that, like in the two–dimensional case, the asymptotic values are \(y' = \lim_{L \to \infty} y_{eff}'(L) = (1/\nu) + \omega\) and \(y'' = \lim_{L \to \infty} y_{eff}''(L) = 1/\nu\). According to our theory, the actual plots in the \(L^{-1/2}\) scale are linear at \(L \to \infty\), as consistent with the expansion in terms of \(L^{-\omega}\). The linear least–squares fits are shown by solid lines. The zero intercepts 1.552 and 1.913 are in approximate agreement with our theoretical values 1.5 and 2 indicated by horizontal dashed lines. The relative discrepancy of about 4%, presumably, is due to the extrapolation errors and inaccuracy in the simulated data.

The behavior of \(y_{eff}'\) is rather inconsistent with the RG predictions. On the one hand, \(y_{eff}\) claims to increase above \(y_{eff}''\) and also well above the RG value of \(1/\nu\) (the lower dod–dot–dashed line at 1.5863), and, on the other hand, the extrapolation yields \(y'\) value (1.913) which is remarkably smaller than \((1/\nu) + \omega \simeq 2.3853\) (the upper dot–dot–dashed line) predicted by the RG theory. For selfconsistency, we should use the linear extrapolation in the scale of \(L^{-\omega}\) with \(\omega = 0.790\) (the RG value). However, this extrapolation (tiny dashed line in Fig. 3), yielding \(y' \simeq 1.757\), does not solve the problem in favour of the RG theory.

The data points of \(y_{eff}'\) look (and are expected to be) less accurate than those of \(y_{eff}''\), since \(\text{Re} \ (u_0^0 - u_c)\) has a very small value. The \(y_{eff}''\) data do not look scattered, therefore they allow a refined analysis with account for nonlinear corrections. To
Figure 5: Effective critical exponents for the real (empty circles) and the imaginary (solid circles) part of complex partition–function–zeroth of 3D Ising model depending on $L^{-1/2}$, where $L$ is the linear size of the system. Solid lines show the linear least–squares fits. The asymptotic values from our theory are indicated by horizontal dashed lines, whereas those of the RG theory – by dot–dot–dashed lines. A selfconsistent extrapolation within the RG theory corresponds to the tiny dashed line.

obtain stable results, we have included the data for smaller lattice sizes $L = 3$ and $L = 4$ given in [19]. In principle, we can use rather arbitrary analytical function $\phi(\beta)$ to evaluate the effective critical exponent

$$y''_{\text{eff}}(L) = \ln \left[ \text{ln} \phi \left( \beta_0^I(L/2) \right) / \text{ln} \phi \left( \beta_0^I(L) \right) \right] / \text{ln} 2$$

and estimate its asymptotic value $y''$. For an optimal choice, however, $y''_{\text{eff}}(L)$ vs $L^{-\omega}$ plot should be as far as possible linear to minimize the extrapolation error. In this aspect, our choice $\phi = \exp(-\beta)$ is preferable to $\phi = \exp(-4\beta)$ used in [19]. We have tested also another possibility, i. e. $\phi = \sinh(2\beta)$, providing almost optimal results in the case of 2D Ising model. In Fig. 6, we have shown the slope of $y''_{\text{eff}}$ vs $L^{-1/2}$ curve, calculated from the MC data of [15, 19], for $\phi = \exp(-\beta)$ (empty circles) and $\phi = \sinh(2\beta)$ (solid circles). It is evident that in both cases the slope cannot be reasonably approximated by a linear function of $L^{-1/2}$, but can be quite well described by a parabola. The latter means that $y''_{\text{eff}}(L)$ can be satisfactorily well approximated by a third–order (but not by a second–order) polynomial in $L^{-1/2}$. The corresponding four parameter least–squares fits are shown in Fig. 6. They yield $y'' \simeq 1.473$ in the case of $\phi = \exp(-\beta)$ (long–dashed line) and $y'' \simeq 1.518$ at $\phi = \sinh(2\beta)$ (solid line). It is evident from Fig. 6 that in the latter case we have slightly better linearity of the fit, therefore $1/\nu \simeq 1.518$ is our best estimate of the critical exponent $1/\nu$ from the actual MC data. Thus, while the row estimation provided the value $y'' = 1/\nu \simeq 1.552$ which is closer to the RG prediction $1/\nu \simeq 1.5863$ (horizontal dot–dot–dashed line), the refined analysis reveals remarkably better agreement with
Figure 6: Slope of the $y''_{\text{eff}}$ vs $L^{-1/2}$ plot in Fig. 5 (including also smaller sizes $L$). The empty circles correspond to $\phi = \exp(-\beta)$, whereas the solid circles to $\phi = \sinh(2\beta)$. The corresponding least–squares fits $1.1840 - 8.507 L^{-1/2} + 19.09 L^{-1} + 0.6669 - 3.645 L^{-1/2} + 9.275 L^{-1}$ are shown by long–dashed line and solid line, respectively.

Figure 7: Effective critical exponent $y''_{\text{eff}}(L)$ for the imaginary part of the complex partition–function–zeroth as a function of $L^{-1/2}$, where $L$ is the linear size of the system. The empty circles correspond to $\phi = \exp(-\beta)$, whereas the solid circles to $\phi = \sinh(2\beta)$. The corresponding least–squares fits $y''_{\text{eff}}(L) = 1.4731 + 1.3345 L^{-1/2} - 4.7657 L^{-1} + 6.8962 L^{-3/2}$ and $y''_{\text{eff}}(L) = 1.5180 + 0.7301 L^{-1/2} - 2.0397 L^{-1} + 3.318 L^{-3/2}$ are shown by long–dashed line and solid line, respectively. Our asymptotic value $y'' = 1/\nu = 1.5$ is indicated by horizontal dashed line, whereas that of the RG theory (1.5863) – by dot–dot–dashed line.
our (exact) value \(1/\nu = 1.5\) (horizontal dashed line).

7 Conclusions

In summary, we conclude the following.

1. Corrections to scaling for different physical quantities near and at criticality have been discussed in framework of our recently developed theory [1] (Sec. 2).

2. The critical exponent \(\gamma\) for 3D Heisenberg model has been estimated by fitting the original susceptibility (MC) data of [3] to an ansatz of finite–size–scaling theory which includes the leading confluent correction–to–scaling term (Sec. 3). The obtained estimates (\(\gamma = 1.345 \pm 0.023\) and \(\gamma = 1.354 \pm 0.020\)) agree within error bars with our theoretical value \(\gamma = 19/14 \simeq 1.35714\) and disagree with the conventional RG value \(\gamma \simeq 1.3895\). Taking into account also the leading analytical correction, a selfconsistent estimation always yields the central value of \(\gamma\) in the range of \(1.345 \leq \gamma \leq 1.369\), i.e., reasonably close to our (exact) value 19/14, if the ratio of amplitudes \(r\) for analytical and confluent corrections is varied from 0 to \(\infty\).

3. Based on MC data for susceptibility in 3D Heisenberg model, a very accurate estimation of the critical coupling has been made at given values of critical exponents (Sec. 4), taking into account both confluent and analytical corrections to scaling. These estimates, combined with fits in vicinity of the critical point (Sec. 3), allowed us to test the consistency between theoretical values of critical exponents and actual MC data. As a result, we have found that our values (\(\eta = 1/10, \gamma = 19/14, \omega = 3/5\)) are consistent, whereas those of the RG theory (\(\eta \simeq 0.0355, \gamma \simeq 1.3895, \omega \simeq 0.782\)) are rather inconsistent with the MC data.

4. Recent Monte Carlo data for complex zeroth of the partition function in 3D Ising model have been discussed (Sec. 3). The actual MC data suggest that, like in 2D Ising model, the critical behavior of the real part differs from that of the imaginary part. It can be explained reasonably by our exponents \(\nu = 2/3\) and \(\omega = 1/2\), but not by those (\(\nu \simeq 0.6304\) and \(\omega \simeq 0.799\)) of the conventional RG theory. Our best estimate of the critical exponent \(\nu\) from the MC data, i.e. \(1/\nu \simeq 1.518\) or \(\nu \simeq 0.659\), is in a good agreement with the theoretical (exact) value 2/3.

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