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# A new approach to critical exponents in phase-transitions of spin-systems

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**Abstract**

We investigate a method to obtain critical exponents using standard numerical simulation techniques for spin systems. We show that by analyzing the inverse of the logarithmic derivative of the susceptibility $\chi$ with respect to temperature the accuracy in determining $\gamma$ can be increased significantly. The method is tested on the two- and three-dimensional Ising models but this alternative approach is thought to be most useful for spin systems on non-periodic structures like quasi-crystals and fractal lattices where the finite size scaling method is difficult to apply. 

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*Keywords:* Monte Carlo simulations; Critical exponents determination

## 1. Introduction and method

For Monte Carlo simulation commonly used for studying phase transitions and critical exponents [1,2] there exist two possibilities to extract the necessary information to obtain critical exponents. In the region close to the critical temperature one uses "finite size scaling" [3] which allows to determine very precisely the exponents. It is based on the assumption of a smooth and predictive dependence of the critical properties on system size. In non-translation invariant systems, for instance fractal lattices and Penrose lattices, or edges and corners [4] this assumption may not be valid. Therefore, it is necessary to investigate alternatives. In the second region further away from the

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critical temperature where the correlation length $\xi$ is smaller than the system size $L$, one can also determine the critical exponents by fitting directly the critical behavior, provided it has already set in. As an example for both methods, FSS and a direct fit see Ref. [5].

Thus, even though finite size scaling is expected to produce better results whenever applicable, the objective of this article is to improve the second method for cases where an alternative is necessary.

In the vicinity of the critical temperature $T_c$ a thermodynamic quantity like the susceptibility $\chi$ can be approximated by

$$\chi = |T - T_c|^{-\gamma}(a_0^{\pm} + a_1^{\pm}(T - T_c)^{\omega_1} + a_2^{\pm}(T - T_c)^{\omega_2} + \cdots) \tag{1}$$

with the critical exponent $\gamma$ and the "amplitudes" $a_0^+$ or $a_0^-$ referring to the high-temperature phase (HTP) with $T > T_c$ or to the low temperature phase (LTP) $T < T_c$, respectively. The importance of the correction to scaling with the amplitudes $a_i^{\pm}$ and the exponents $\omega_i > 0$, due to irrelevant fields in the language of the renormalization group, is difficult to assess for a "direct fit" to (1). Neglecting them in the determination of $\gamma$ at least three additional parameters $T_c$, $a_0^+$ and $a_0^-$ have to be determined. To decrease this number we calculate $\chi/\chi'$ instead, that is

$$\frac{\chi}{(\partial/\partial T)\chi} = -\frac{(T - T_c)}{\gamma}(1 + b_1^{\pm}(T - T_c)^{\kappa_1} + b_2^{\pm}(T - T_c)^{\kappa_2} + \cdots) \tag{2}$$

with $b_i^{\pm}$ and $\kappa_i$ related to the parameters of the corrections to scaling $a_i^{\pm}$ and $\omega_i$ of (1). The derivative $\chi'$ is calculated by means of higher moments as discussed in the next section. Using (2) as the starting point, besides $\gamma$ the only free parameter to determine is $T_c$. Neglecting the correction to scaling it is a linear fit. The only price one has to pay is the stronger statistical fluctuation of the derivative of $\chi$.

In general, the region where (1) or (2) can be used as good approximation is unknown. The importance of higher order corrections grows with the distance from $T_c$ noticeable as a deviation from the straight line behavior of (2). Thus, it is necessary to simulate the system as close as possible to $T_c$. However, when $\xi$ becomes very large we are confronted with the problem of too large a simulation time, since we require $L \gg \xi$. Neglecting critical slowing down the CPU time needed to simulate a given number of independent samples of a $d$-dimensional system of size $L$ is proportional to $L^d$. So the limited CPU-time suppresses highly accurate numerical results for large system sizes near $T_c$ and thus the results for the high- and low-temperature phase will be separated by a more or less wide gap, where no reliable result exists. On the HTP side of the gap, $a_i^+$ is to be used in (1), while $a_i^-$ must be used on the LTP side. The same applies to (2) for $b_i^{\pm}$. To use all data in the same fit and to keep the number of free parameters as small as possible, a theta-function is used,

$$a^{\pm} = a^+\theta(T - T_c) + a^-(1 - \theta(T - T_c)) \tag{3}$$

where $\theta(x)=1$ for $x\geqslant 0$ and $\theta(x)=0$ otherwise. As we will see below, this "bridging of the gap" makes the fitting to the modification (2) very sensitive for its first order, $1/\gamma$, and it strongly profits from the gap.

A few points, in principle only two, that is one in the LTP and the other in the HTP region, are sufficient to determine $\gamma$. In fact, a fit to (2) allows an estimate for $\gamma$ in a very short time (up to a factor 50 less CPU-time with two points compared to a fit to (1) using all points). However, to control the accuracy one certainly needs more information.

In the following the methods using Eqs. (1) and (2) are applied to the two-dimensional Ising model concentrating on the comparison of the two methods and especially on the statistical errors, while the exact results serve as control [6–12].

## 2. Application to 2D-Ising

We considered systems of size $L$ in the range 100–350 periodic boundary conditions imposed. In the LTP, Wolff's algorithm [13,14] was used and in the HTP the Swendsen–Wang algorithm [15] was used to reduce critical slowing down. The simulations were carried out at temperatures between 2.10 and 2.55, where $T_c=2/\ln(\sqrt{2}+1)\approx 2.27$. It has been checked with the help of Fourier transform of the correlation function that $L\geqslant 10\xi$ [16].

In each simulation, three million measurements were made after each cluster update and 500.000 steps were done for equilibration. Since we want to compare the direct fit to (1) and the modification using (2), special care has been taken to estimate the errors using the Jackknife method [17].

For each temperature $T$ we calculated the following quantities:

$$E=-J\sum_{\langle i,j\rangle}s_i s_j\,, \tag{4}$$

$$\chi_1=\langle m\rangle=\frac{\langle M\rangle}{N}\,, \tag{5}$$

$$\chi_2=\chi=\frac{\langle M^2\rangle-\langle M\rangle^2}{Nk_BT}\,, \tag{6}$$

$$\chi_3=\frac{\langle M^3\rangle-3\langle M\rangle\langle M^2\rangle+2\langle M\rangle^3}{Nk_B^2T^2}\,, \tag{7}$$

$$\chi_4=\frac{\langle M^4\rangle-4\langle M\rangle\langle M^3\rangle+12\langle M^2\rangle\langle M\rangle^2-3\langle M^2\rangle^2-6\langle M\rangle^4}{Nk_B^3T^3}\,, \tag{8}$$

where for the energy $E$ the sum is over all nearest neighbors and for the magnetization $M$ over all $N=L^2$ spins. The thermodynamic averages are given by $\langle\cdots\rangle$ and the susceptibilities, $\chi_n$, are the $n$th derivative of the free energy with respect to the magnetic

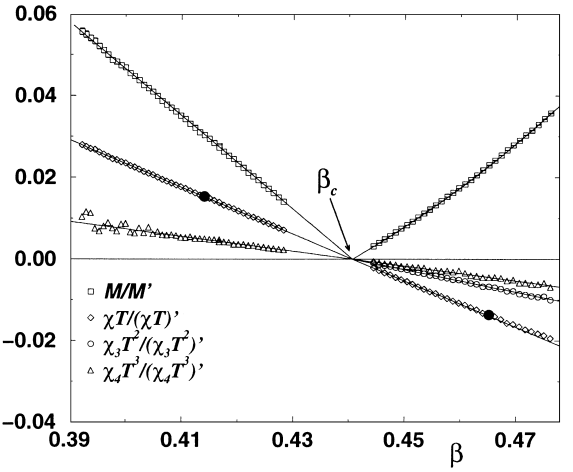


Fig. 1. $(\chi T)/(\chi T)'$ and other ratios as a function of the inverse temperature $\beta = 1/T$. $\langle M\rangle/\langle M'\rangle$ is scaled by a factor of 10 in the LTP $\beta > \beta_c$. Its slope gives the inverse of $\beta$ and of $\gamma/2$ in the HTP ($\beta < \beta_c$). The slope of $(\chi T)/(\chi T)'$ gives $\gamma^{-1}$, $(\chi_3 T^2)/(\chi_3 T^2)'$ gives $\gamma_3^{-1}$ and $(\chi_4 T^3)/(\chi_4 T^3)'$ gives $\gamma_4^{-1}$. All curves intersect at $\beta_c = 0.440686\ldots$. The error bars for $\langle m\rangle/\langle m'\rangle$ and $\chi/\chi'$ are smaller than the symbols. The solid lines are exact for $\langle m\rangle/\langle m'\rangle$, approximations otherwise (for $\chi/\chi'$ see Ref. [8]). The two filled circles serve as an example for the two-point-fitting method.

field. In addition, we calculated $\chi_n T^{n-1}$ as well as $\chi_n/\chi_n'$ and $\chi_n T^{n-1}/(\chi_n T^{n-1})'$. As higher order corrections are usually smaller if a function contains a factor $T^{n-1}$ we used these to calculate the exponents of $\chi_n$. For the same reason we take the derivative with respect to $\beta = 1/T$ rather than to $T$. We obtain

$$\frac{\partial}{\partial\beta}\langle A\rangle = (\langle A\rangle\langle E\rangle - \langle AE\rangle)\,. \tag{9}$$

Because $\langle M\rangle$ is calculated as $\langle|M|\rangle$ [2], Eqs. (5)–(8) are numerically valid only in the LTP, while in the HTP we set $\langle M^{2n+1}\rangle = 0$.

In Fig. 1 the ratios $\langle f\rangle/\langle f'\rangle$ for Eqs. (5)–(8) are plotted as a function of the inverse temperature $\beta = 1/T$. The complete results can be found at `http://www.physik.fu-berlin.de/~pruess/ising2d.data.200001`. As expected all the graphs intersect in zero at $\beta_c = 1/T_c$.

We fitted the numerical results to

$$\langle f\rangle = |\beta - \beta_c|^{-\mu(f)}(a_0^{\pm} + a_1^{\pm}(\beta - \beta_c) + a_2^{\pm}(\beta - \beta_c)^2 + \cdots)\,, \tag{10}$$

$$\langle f\rangle/\langle f\rangle' = \frac{(\beta - \beta_c)}{-\mu(f)}(1 + b_1^{\pm}(\beta - \beta_c) + b_2^{\pm}(\beta - \beta_c)^2 + \cdots)\,, \tag{11}$$

whereas for $a_i^{\pm}$ and $b_i^{\pm}$ (3) is used. In the case of 2D-Ising it is reasonable to put $\omega_i = i$ from (1) and $\kappa_i = i$ (2), respectively. The critical exponents $\mu()$ are known exactly: $\mu()$ of $\langle m\rangle$ is $-\beta = -\frac{1}{8}$, of $\chi$ is $\gamma = \frac{7}{4}$, of $\chi_3$ is $\gamma_3 = \frac{29}{8}$, of $\chi_4$ is $\gamma_4 = \frac{11}{2}$ and of $\xi$ is $\nu = 1$.

To show the field of application and the benefits of modification 2, we restricted the following analysis to a set of data between $T = 2.150$ and 2.230 and between $T = 2.335$

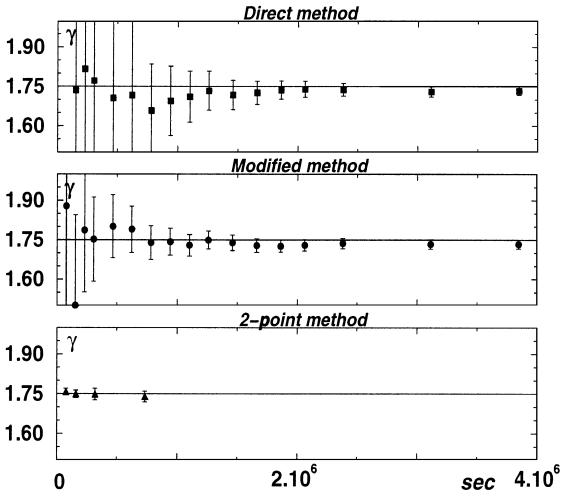


Fig. 2. Results for $\gamma$ as a function of simulation time normalized to a common PC using different methods explained in the text. The exact value $\frac{7}{4}$ is indicated by the straight line.

and 2.415, where 17 points are in LTP and the same number in HTP. We are indeed not interested in obtaining very precise estimates for the exponents, which are well known for the 2D-Ising-model, but to show the differences of the two approaches. For both methods we used one correction term, which means four parameters for the modification (2) and six for the direct method (1). For an unknown system eventually more data points in the vicinity of the critical temperature and more parameters are required, especially the correction to scaling $\kappa_i$ and $\omega_i$.

Using all available points in the interval, the results for $\gamma$ by the direct method is $\gamma_{\chi T}^{\text{direct}} = 1.733(16)$ and $\gamma_{\chi T/(\chi T)'}^{\text{mod.}} = 1.733(17)$ by the modification (2). In Fig. 2 we have plotted the estimated value and error of $\gamma$ as a function of CPU-time. The various values of $\gamma$ in the plot were generated by excluding more and more data from the fit and thus enlarging the gap step by step symmetrically around $T_c$, in order to simulate the quality of the results if less CPU-time is available. The figure shows, that the method 2 strongly profits from the gap: If the full CPU-time is available, i.e., without skipping any data points, both methods give very similar results. For less CPU-time, i.e., if the gap is enlarged, the error bar for the estimate of $\gamma$ by our modification grows only slowly. Skipping 14 data points the error doubles, while the error of the direct method increases nearly fivefold.

In the last row of Fig. 1 quick and rough estimates for $\gamma$ are plotted, which are produced by two-point fits of pairs of data symmetrically around $\beta_c$. On the one hand, they are less reliable; on the other, they need up to a factor 50 less CPU-time. For example, the estimate for $\gamma$ using the pair with the smallest amount of CPU-time within the range of data we used (see the two filled circles in Fig. 1) is $\gamma_{\chi T/(\chi T)'}^{2\text{ points}} = 1.761(13)$. One might argue that the quality of the two-point fits depends on the fact that the ratio of the amplitudes of the correction in (1), $a_i/a_0$ are the same as in LTP and

HTP. However, we show below that even in the case of 3D-Ising, where $b_i^+ \neq b_i^-$ is expected, this method still works.

One could add a correction to (1) and (2) of the form $c^{\pm}|T - T_c|^{\omega}$ [18] with $c$ and $\omega$ as additional free parameters, which usually appear in more complicated systems. This is just another degree of freedom for both methods and in our special case this leads to slightly better results for the modification (2), while the direct fit does not converge any more, since the number of free parameters is too large.

We have to determine a second exponent, to get the remaining ones from the scaling laws. In our special case of 2D-Ising the specific heat, $c_H$, is inaccessible due to its logarithmic divergence. But typically the moments of the energy have large fluctuations, which cause bad estimates for $\alpha$ in general. Moreover $c_H$ possesses usually a non-singular part and therefore needs a special treatment.

However, the more complex magnetic quantity, for example $\chi_4$, has also large errors due to the large number of terms and large moments, which must be included in the calculation. In Fig. 1 one can see the fluctuation of $\chi_4$ and $\chi_3$. In our simulation we found $\gamma^{\mathrm{mod}}_{\chi_4 T^3/(\chi_4 T^3)'} = 5.51(98)$, very close to the exact result (5.5), but with a too large error.

As mentioned above, we expect method (2) to profit from the fact that data points exist on both sides. However, $\langle M \rangle$ and in general every quantity, which consists of odd powers of $\langle M \rangle$, vanishes in the HTP region. Surprisingly, the fit of $\langle m \rangle / \langle m' \rangle$ gives $\beta^{\mathrm{mod.}}_{M/M'} = 0.1261(18)$, very close to the exact value of 0.125. The direct fit of $\langle m \rangle$ did not converge, due to the too small number of data points.

## 3. Application to 3D-Ising

An additional test is to calculate $\gamma$ for the three-dimensional Ising model. We make use of the simple two-point method taking the inverse temperatures $1/T_< = 0.2270$ and $1/T_> = 0.2163$ between the critical value $1/T_c = 0.2216544(3)$ known with high precision from simulations (see Ref. [21]). Using for the system sizes $L = 64$ for the temperature in the LTP and $L=40$ for the HTP, we are certain that $\xi \ll L$ from previous investigations [19]. With $5 \times 10^5$ MCS-steps for equilibration and $3 \times 10^6$ for statistics we obtain $1/T_c = 0.2219(2)$ and $\gamma = 1.284(42)$. Of course, one does not obtain the precision of the renormalization group calculations with $\gamma = 1.2397(13)$ [20], but the result obtained from only two points and thus calculated in a very short time agrees sufficiently well. Since the two-point method is quite sensitive to the correction terms in (2), that is $b_i^+ \neq b_i^-$ for the three-dimensional Ising model, one cannot expect high accuracy.

## 4. Conclusion

We have shown how to improve the method of directly fitting and extracting critical exponents. This improved method uses the results further away form the critical region,

where the correlation length has to be smaller than the system size. Although simulations of large systems are required a substantial gap around the critical temperature can be left without significantly increasing the inaccuracy contrary to the method using a direct fit. In addition, our modification is capable of giving a very quick estimate for critical exponents from only a few data points.

The modification can be applied directly in all dimensions, for Potts or vector spins and on all systems where finite size scaling has difficulties like Penrose and fractal lattices and edges and corners [4].

Again we want to stress that we want to propose the method (2) as an alternative to the direct fit (1), not to the finite sizes scaling method, which is expected to give at least comparable estimates for critical exponents in similar or shorter time-whenever applicable.

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