Monte Carlo method for spin models with long-range interactions

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Abstract

We introduce a Monte Carlo method for the simulation of spin models with ferromagnetic long-range interactions in which the amount of time per spin-flip operation is independent of the system size, in spite of the fact that the interactions between each spin and *all* other spins are taken into account. We work out two algorithms for the q-state Potts model and discuss the generalization to systems with other interactions and to O(n) models. We illustrate the method with a simulation of the mean-field Ising model, for which we have also analytically calculated the leading finite-size correction to the dimensionless amplitude ratio $\langle m^2 \rangle^2 / \langle m^4 \rangle$ at the critical temperature.

1 Introduction

The study of systems with long-range interactions is notoriously difficult, due to the large number of interactions that has to be taken into account. This has discouraged the application of Monte Carlo methods, whereas only very few exact solutions are available for these models. Furthermore, other numerical analyses of these systems suffer from serious difficulties. They often truncate the interaction beyond a certain distance, thus introducing errors in the calculation, or are restricted to small system sizes, which limits the accuracy that can be obtained in a finite-size analysis [1]. Here, we present a Monte Carlo method for the simulation of spin models with long-range interactions which is capable of simulating large systems within a reasonable amount of computing time. The algorithm, which is based on the well-known Wolff cluster method [2], does not make any approximation except for the inherent statistical errors. In the process of cluster formation the amount of time per spin visit is independent of the system size, despite the fact that each spin interacts with *all* other spins in the system. This fact, together with the reduction of critical slowing down in cluster algorithms, makes this algorithm very suitable for the study of critical phenomena in models with long-range interactions. Therefore it will allow an accurate numerical analysis of ferromagnetic long-range models.

The outline of this paper is as follows. In section 2 we start with a brief review of the Wolff cluster algorithm. In section 3 we discuss two efficient cluster-building algorithms. We illustrate the Monte Carlo method in section 4 with some simulations of the mean-field Ising model, for which we have also calculated the leading finite-size correction to the dimensionless amplitude ratio $\langle m^2 \rangle^2 / \langle m^4 \rangle$ at the critical temperature. Section 5 contains generalizations of the algorithm to other systems as well as our conclusions.

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2 Cluster methods

Cluster algorithms for spin models are based on the Kasteleyn–Fortuin mapping of the Potts model on a bond percolation model [3, 4]. The Potts Hamiltonian $\mathcal{H}_{\mathrm{P}}$ is given by

$$\beta\mathcal{H}_{\mathrm{P}} = -K \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} \quad (\sigma = 1, \ldots, q) \,, \tag{1}$$

where $\sum_{\langle ij \rangle}$ denotes a summation over all nearest-neighbor pairs and q is the possible number of states for each spin. The partition function is thus given by

$$Z_{\mathrm{Potts}} = \sum_{\{\sigma_i\}} \exp(-\beta\mathcal{H}_{\mathrm{P}}) \,. \tag{2}$$

It can be shown that this is equivalent to the Whitney polynomial [5], which gives the partition function of the random-cluster model,

$$Z_{\mathrm{RC}} = \sum_{G} q^C v^l \,, \tag{3}$$

where $\sum_G$ denotes a sum over all graphs on the lattice, l denotes the number of bonds in the graph, $v = e^K - 1$ and C is the number of connected components in the graph. A connected component is a cluster of spins connected directly or indirectly by bonds (a single, isolated spin is regarded as a cluster as well).

The fact that all spins belonging to one connected component are in the same state and uncorrelated with all other spins in the system forms the basis of the cluster method. Let us briefly review the Wolff cluster method for the Ising model. First, a random site is chosen, which contains the first spin of the cluster. Then bonds are activated between this spin and its neighbors, with probability

$$p(\sigma_i, \sigma_j) = \delta_{\sigma_i \sigma_j} \frac{v}{1+v} = \delta_{\sigma_i \sigma_j} (1 - e^{-K}) \,, \tag{4}$$

where K is the Potts coupling between neighboring spins. This process is repeated iteratively by activating bonds between each newly added spin and its neighbors, thus creating a *cluster* of spins connected by active bonds. Then all the spins in this cluster are reversed and a new cluster is formed. The great advantage of the Wolff cluster algorithm for this system compared to the Metropolis algorithm is the drastic change in critical slowing down. E.g., for the two-dimensional Ising model the dynamical critical exponent z is reduced from $z \approx 2.1$ to $z \approx 0.35$ [6] and for the mean-field Ising model it is even suggested that z is reduced from $z \approx 2$ to $z \approx 0$ [7]. So, roughly speaking, for a system consisting of L^d spins, the amount of time to reach equilibrium is decreased by a factor $\mathcal{O}(L^2)$.

The Kasteleyn–Fortuin mapping can also be applied to systems with different interaction strengths by associating a certain type of bond with each type of interaction. The corresponding generalization of eq. (3) is then [5]

$$Z = \sum_{G} q^C v_1^{l_1} v_2^{l_2} v_3^{l_3} \ldots \,, \tag{5}$$

where now l_i denotes the number of bonds of class i in the graph and $v_i = e^{K_i} - 1$ (K_i is the coupling constant or interaction energy between a spin pair connected by a bond of class i).

This allows the application of the Wolff cluster method to spin models with an arbitrary number of different interactions, in particular long-range interactions. With each value of the interaction strength, i.e. with each spin distance, we associate a different bond class. Then, we activate bonds between each spin in the cluster and *all* other spins in the system with a probability p of a bond that depends on the interaction strength between the two spins. Once a complete cluster has been formed, its spins are reversed and the formation of a new cluster is started. In this article, we present a method

in which the number of operations required to activate a bond is independent of the number of spins in the system. The efficiency of this method can be illustrated by the following simple example. If p were equal for each spin pair, one out of p^{-1} spins would be added to the cluster, and it would take $\mathcal{O}(p^{-1}) \sim \mathcal{O}(L^0)$ operations per spin to update a configuration, compared to $\mathcal{O}(L^d)$ operations *per spin* for a Metropolis algorithm. Taking into account the decrease in critical slowing down, we see that the efficiency of this method is typically a factor $\mathcal{O}(L^{d+2})$ larger than the conventional Monte Carlo algorithm.

3 Building clusters in systems with long-range interactions

3.1 Long-range Hamiltonian

In systems with long-range interactions, the Hamiltonian (1) is generalized to

$$\beta\mathcal{H}_{\mathrm{LR}} = -\sum_{\langle ij \rangle} K_{ij}\delta_{\sigma_i\sigma_j} \ , \tag{6}$$

where the sum runs over all spin pairs. As an example, we will take $K_{ij} = f/r_{ij}^{d+\sigma}$ $(f > 0)$, which is one of the most commonly studied long-range interactions [8]. Here r_{ij} denotes the distance between spins σ_i and σ_j, d is the dimensionality of the system and $\sigma > 0$ is a parameter which determines the power-law decay of the interaction. We have written the exponent as the sum of d and σ to emphasize the fact that the integrated interaction does not converge for $\sigma \leq 0$.

We now have to devise an algorithm to build a cluster of spins, activating bonds between each pair of spins with a probability given by eq. (4) with K replaced by K_{ij}. For simplicity we discuss here a one-dimensional system. We start with a spin on a randomly chosen site and activate bonds between this spin and all other spins in the system with a probability $\delta_{\sigma_i\sigma_j}p_m$, where p_m denotes the probability of activating a bond between two identical spins at distance m (in units of lattice spacing). Generalizing eq. (4), we find $p_m(\sigma_i, \sigma_j) = 1 - \exp(-fm^{-(d+\sigma)}) \equiv 1 - \exp(-K_m)$. Each time we activate a bond, the corresponding spin is added to the cluster. Furthermore, the spin address is placed on the *stack*. This is a list of spin addresses from which an address is removed once it has been read. When all neighbors of the first spin have been considered, we read a new spin from the stack and repeat the process. This cycle ends when the stack is empty, i.e. if all neighbors of all spins in the cluster have been considered. The spin from which we are currently activating bonds will be called the *current spin*. To avoid considering each single bond, we introduce the concept of the *cumulative bond probability*. This is a quantity from which we can derive the distance of the first spin (with respect to the current spin) which has to be added to the cluster, assuming that this spin is identical to the other spins in the cluster. The probability that the first bond is activated at a distance j from the current spin is given by

$$P(j) = (1 - p_1)(1 - p_2)\ldots(1 - p_{j-1})p_j \ . \tag{7}$$

The cumulative bond probability is defined as

$$C(j) \equiv \sum_{n=1}^{j} P(n) \ . \tag{8}$$

Now, if a random number $(\in [0, 1\rangle)$ between $C(j-1)$ and $C(j)$ is drawn, the first bond has to be activated between the current spin and the spin at a distance j, provided that they are parallel. Since the next bond must be activated between the current spin and a spin at a distance $k > j$, we have to shift P as follows:

$$P_j(k) = (1 - p_{j+1})(1 - p_{j+2})\ldots(1 - p_{k-1})p_k \ , \tag{9}$$

and eq. (7) is simply a special case of eq. (9). The generalized version of eq. (8) is given by

$$C_j(k) = \sum_{n=j+1}^{k} P_j(n) \; . \tag{10}$$

Substituting for p_m, which is the bond probability (4) without the Kronecker delta (which is applied *after* the selection of the spin), we find:

$$C_j(k) = 1 - \exp\left(- \sum_{n=j+1}^{k} K_n \right) \; . \tag{11}$$

In the following subsections we consider two possibilities of calculating the bond distance k from a given $C_j(k)$. Let us here mention one detail that we have omitted in the above discussion. In eqs. (7) and (9), p_m denotes the probability of activating a bond to a spin at distance m. This means that this is the probability of a bond to the right *or* to the left. This can be taken into account by doubling the interaction strength K_m. Once a bond distance m has been obtained, its direction can be determined by an additional random number. Some care has to be exercised to ensure that a bond at the same distance but in the opposite direction is still allowed.

3.2 Look-up table

The first possibility is the construction of a look-up table. This means that we carry out the sum in (11) explicitly for a large number of distances k, up to a certain cutoff and store the results in a table.[1] Then, after drawing a random number, we can derive the corresponding bond distance from this table. This method is very fast, since we have to calculate all cumulative probabilities only once, but it has two major drawbacks. First, all bonds beyond the cutoff are neglected, which introduces an unacceptable error in the case that the interaction decays very slowly, i.e. when σ is small. We address this problem in the next subsection. Secondly, this method is not feasible in more than one dimension, as the number of distances for which the cumulative bond probability has to be calculated increases quickly with the dimensionality of the system (for a fixed cutoff).

3.3 Continuous bond probability

We may also approach the summation problem as follows. The sum in eq. (11) can be approximated by an integral:

$$\sum_{n=j}^{k} K_n = \sum_{n=j}^{k} \frac{f}{n^{d+\sigma}} \approx f \int_{j-\frac{1}{2}}^{k+\frac{1}{2}} \mathrm{d}x \; x^{-(d+\sigma)} \; . \tag{12}$$

By replacing the sum by this integral we still have an exact Monte Carlo scheme, but the interaction has been altered from $K_{ij} = f/|i-j|^{d+\sigma}$ (discrete) to the continuous function

$$K(|i-j|) = f \int_{|i-j|-\frac{1}{2}}^{|i-j|+\frac{1}{2}} \mathrm{d}x \; x^{-(d+\sigma)} \; . \tag{13}$$

Since both interactions exhibit the same long-range behavior, we expect the same universal properties, e.g. the same critical exponents. However, their short-range behavior differs, so all non-universal quantities, such as the critical temperature, will have different values. The cumulative probability of activating a bond to a spin at a distance between j and k is now given by

$$C(j,k) = 1 - \exp\left(-f \int_{j-\frac{1}{2}}^{k+\frac{1}{2}} \mathrm{d}x \; x^{-(d+\sigma)} \right) \; . \tag{14}$$

[1] Only the cumulative probabilities for the case $j = 0$ have to be calculated, as one can obtain $C_j(k)$ for general j from $C_0(k)$ by a simple rescaling.

The important feature of eq. (14) is that the integral can be carried out explicitly, allowing us to equate $C(j,r)$ to a random number and solve this equation for r (j is a constant determined by the previously activated bond). We can estimate the difference between the discrete and the continuous interaction by expanding the integrand in eq. (13) in a Taylor series,

$$K(m) = \int_{m-\frac{1}{2}}^{m+\frac{1}{2}} \mathrm{d}x \, \frac{f}{x^{d+\sigma}} = K_m + K_m^{(2)} \int_{m-\frac{1}{2}}^{m+\frac{1}{2}} \mathrm{d}x \, \frac{1}{2}(x-m)^2 + \mathcal{O}(K_m^{(4)}) \approx K_m + \frac{1}{24} K_m^{(2)} \; . \tag{15}$$

So up to leading order in $1/m$ the relative difference between K_m and $K(m)$ is given by

$$\frac{1}{24} \frac{K_m^{(2)}}{K_m} = \frac{(d+\sigma)(d+\sigma+1)}{24m^2} \; . \tag{16}$$

The continuous bond probability provides an excellent solution to the first problem posed in section 3.2. We do not have to neglect the bonds beyond the cutoff, but can simply calculate the bond distance from eq. (14), where j is larger than the cutoff. Since the difference between the discrete and the continuous bond probability decays quickly with increasing distance, we can make the error in this approximation arbitrarily small by increasing the cutoff. Furthermore we can apply the method of the continuous bond probability for any number of dimensions.

4 Mean-field model

As an illustration of the method described in this article, we have carried out a Monte Carlo simulation of the mean-field model, described by the Hamiltonian

$$\beta \mathcal{H}_{\mathrm{MF}} = -\frac{K}{2N} \sum_i \sum_{j \neq i} \sigma_i \sigma_j \quad (\sigma = \pm 1) \; , \tag{17}$$

in which N is the number of spins in the system. This model can be regarded as an extremely long-range system, since each spin interacts equally with every other spin. It is equivalent to the system described by eq. (6) with $K_{ij} = f/r_{ij}^{d+\sigma}$ in the limit $\sigma \downarrow 0$, where periodic boundary conditions are employed and K_{ij} must be suitably normalized. It has been solved exactly and exhibits a phase transition at $K = 1$ (see e.g. ref. [9, Chapter 3]; note the difference in the coupling constant in eq. (3.1.3) of this reference compared to eq. (17) above). Furthermore, it has classical values for the critical exponents α, β, γ and δ. It should be noted that for this particular model a relatively efficient Monte Carlo simulation can be carried out even with the Metropolis algorithm, since the total interaction energy between one spin σ_i and all the other spins is simply given by

$$-\frac{K}{2N} \sum_{j \neq i} \sigma_j = -\frac{K}{2N} (M - \sigma_i) \; . \tag{18}$$

Here $M = Nm = \sum_j \sigma_j$ is the total magnetization. Of course, this is only possible because the coupling between all spin pairs is equal in this model. In our simulations, which serve purely as a test for the algorithm described above, we have *not* used the total magnetization. We have carried out Monte Carlo simulations for systems with sizes in the range $4 - 64000$, constructing 10^6 Wolff clusters per simulation. This took less than 30 hours of CPU-time on a modest workstation, of which approximately 20 hours were spent on the two largest system sizes, consisting of 32000 and 64000 spins, respectively. We have sampled the dimensionless amplitude ratio

$$Q \equiv \frac{\langle m^2 \rangle^2}{\langle m^4 \rangle} \; , \tag{19}$$

which is related to the fourth-order cumulant introduced by Binder [10]. In the thermodynamic limit, at $T = T_{\mathrm{c}}$, this ratio is equal to $4\Gamma(\frac{3}{4})^2/\Gamma(\frac{1}{4})^2 \approx 0.456947$. In the appendix, we derive an expression

for $Q(T_c)$ for finite systems to order $1/N$ by expansion of the partition function. The form of this expansion (33) agrees with the expression for Q_N obtained from finite-size scaling [11],

$$Q_N = Q_\infty + a_1 N^{y_i} + a_2 N^{2y_i} + a_3 N^{3y_i} + a_4 t N^{y_t} + a_5 (t N^{y_t})^2 + \dots \ . \tag{20}$$

Here y_i is the leading irrelevant exponent (which is derived in the appendix as well), y_t is the temperature exponent and t represents the temperature field, in which we have also included an irrelevant term,

$$t = (K - K_c)[1 + a_6 N^{y_i}] \ , \tag{21}$$

where K_c denotes the critical coupling. Note that we have expressed the scaling function in terms of N. If one prefers to identify the mean-field model with an Ising model at its upper critical dimension $d = 4$, one should replace N by L^4.

The Monte Carlo data for $Q(T_c)$ as function of the system size are shown together with the exactly calculated values in figure 1. In figure 2, Q is plotted against the coupling for a range of system sizes. Fitting our data to expression (20), we have obtained the following results.

	Theory	MC
Q_∞	0.456947	0.4565(5)
K_c	1.0	0.99998(3)
y_t	0.5	0.498(4)
y_i	-0.5	$-0.52(4)$
a_1	0.214002	0.219(6)

Here the theoretical values of the critical coupling, the temperature exponent and the irrelevant exponent are understood to be exact values. The numbers in parentheses represent the error in the last decimal. In order to obtain maximum accuracy we have only varied one parameter at a time in our fitting procedure, fixing the remaining parameters at their theoretical values. Varying several parameters simultaneously yields comparable results, but with larger errorbars. Given the amount of computer time invested, the accuracy of the Monte Carlo data is very good and the agreement between the theoretical values and the results of the Monte Carlo simulations is quite satisfactory.

5 Generalizations and conclusions

The algorithm described in section 3 can be generalized in several ways. First, the form of the interaction may be modified. As long as the interaction is an integrable function of the distance, this generalization is completely straightforward. If the interaction is not integrable, one can use a look-up table in the one-dimensional case, whereas an approximation scheme may be devised for a system of higher dimensionality. Secondly, the algorithm may also be applied to long-range XY and Heisenberg models. The generalization to these systems is as follows. First, for each new cluster a spin-flip direction i is chosen at random. Then each spin which may be added to the cluster is selected just as in the case of the Potts model, i.e. with a probability $1 - \exp(-K)$, where K is the Potts coupling of the model. However, the condition in the Potts model that only bonds between identical spins are activated, which is expressed by the Kronecker delta in eq. (6), must be replaced by the condition that the bond between $\vec{\sigma}_1$ and $\vec{\sigma}_2$ is activated with probability

$$\frac{1 - \exp(\min[0, K\sigma_{1,i}\sigma_{2,i}])}{1 - \exp(-K)} \ . \tag{22}$$

The numerator in this expression is equal to that derived by Wolff [2, eq. (5)], where $\sigma_{k,i}$ refers to the projection in direction i of spin $\vec{\sigma}_k$. It should be noted that the spin from which we are currently activating bonds, $\vec{\sigma}_1$, has already been flipped, which explains the absence of a minus sign in front of K. The denominator comes from the fact that we have selected spin $\vec{\sigma}_2$ with a probability $1-\exp(-K)$.

So once a spin has been selected, its component in direction i is reversed with a probability given by eq. (22). Thus the algorithm described above can be extended to general O(n) models, just as the original Wolff algorithm.

In conclusion we can summarize this paper as follows. We have introduced a Monte Carlo cluster method for the efficient simulation of spin models with long-range interactions. We have worked out the algorithm for algebraically decaying interactions, which is the most commonly studied case. Extensive simulations for this case will be presented elsewhere. Here we have illustrated the feasibility of our method by carrying out simulations for the exactly solved mean-field Ising model. Finally we have indicated how the method can be applied to models with other interactions and to general spin models.

A Calculation of the dimensionless critical-point amplitude ratio $\langle m^2 \rangle^2 / \langle m^4 \rangle$ in the mean-field model

Denoting the number of spins in the system by N and the number of down spins by r, the partition function of the mean-field model is

$$Z = \sum_{r=0}^{r=N} c(r) \; , \tag{23}$$

with

$$c(r) = \frac{N!}{r!(N-r)!} \exp\left(\frac{1}{2} K \frac{(N-2r)^2 - N}{N} \right) \; . \tag{24}$$

The average magnetization per spin is given by $m \equiv (N-2r)/N$. Replacing the sum in eq. (23) by an integral (which introduces an error of order $1/N$) and changing the integration variable from r to m we find

$$Z = \frac{N}{2} \int_{-1}^{+1} \mathrm{d}m \; \tilde{c}(m)[1 + \mathcal{O}(1/N)] \; , \tag{25}$$

with

$$\tilde{c}(m) = \frac{N!}{[\frac{1}{2}N(1-m)]![\frac{1}{2}N(1+m)]!} \exp\left(\frac{1}{2} K (Nm^2 - 1) \right) \; . \tag{26}$$

The factor $N/2$ in eq. (25) comes from the Jacobian which appears due to the change of variables. Likewise, we can write expressions for the average square magnetization and the average of the fourth power of the magnetization,

$$\langle m^2 \rangle = \frac{N}{2Z} \int_{-1}^{+1} \mathrm{d}m \; m^2 \tilde{c}(m)[1 + \mathcal{O}(1/N)] \; , \tag{27}$$

$$\langle m^4 \rangle = \frac{N}{2Z} \int_{-1}^{+1} \mathrm{d}m \; m^4 \tilde{c}(m)[1 + \mathcal{O}(1/N)] \; . \tag{28}$$

To find the behavior of these quantities for large N, we can expand $\ln(\tilde{c}(m))$ using Stirling's formula, which yields

$$\ln(\tilde{c}(m)) = -\frac{1}{2}[N(1-m)+1] \ln[\frac{1}{2}N(1-m)] - \frac{1}{2}[N(1+m)+1] \ln[\frac{1}{2}N(1+m)] + \frac{1}{2}Nm^2 + f + \mathcal{O}(1/N) \; , \tag{29}$$

where f contains all terms not depending on m and we have set $K = 1$, because we want to evaluate all quantities at T_c. Expanding in m we find ($\hat{f}$ is a new constant equal to f plus additional terms not depending on m)

$$\ln(\tilde{c}(m)) = -\frac{1}{12}Nm^4 - \frac{1}{30}Nm^6 - \frac{1}{56}Nm^8 + \frac{1}{2}m^2 + \frac{1}{4}m^4 + \frac{1}{6}m^6 + \hat{f} + \dots \,. \tag{30}$$

Substituting this for $\tilde{c}(m)$ in eq. (25) and expanding the exponentials yields

$$Z = \frac{N}{2}e^{\hat{f}} \int_{-\infty}^{+\infty} \mathrm{d}m \; e^{-\frac{1}{12}Nm^4} \left(1 - \frac{1}{30}Nm^6 + \frac{1}{2}m^2\right) \left[1 + \mathcal{O}(1/N)\right], \tag{31}$$

where we have also extended the integral boundaries to $\pm\infty$, which introduces an error which decays exponentially with N. For the evaluation of eq. (31) we use

$$I_k = \int_{-\infty}^{+\infty} \mathrm{d}m \; m^k \exp\left(-\frac{1}{12}Nm^4\right) = \left(\frac{12}{N}\right)^{\frac{k+1}{4}} \frac{1}{2}\Gamma\left(\frac{k+1}{4}\right) \,. \tag{32}$$

Thus, each factor m in the integrand yields an extra factor $N^{-1/4}$ in the result and terms of the form Nm^{k+4} are of the same order as terms of the form m^k. Therefore we retain only the terms up to order m^2 and Nm^6 in eq. (30). After some elementary calculations we find for the dimensionless ratio (19)

$$Q = 4\left(\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}\right)^2 + \frac{16}{5}\sqrt{3}\left(\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}\right)^3 \frac{1}{\sqrt{N}} + \mathcal{O}\left(\frac{1}{N}\right) \approx 0.456947 + 0.214002\frac{1}{\sqrt{N}} + \mathcal{O}\left(\frac{1}{N}\right) \,. \tag{33}$$

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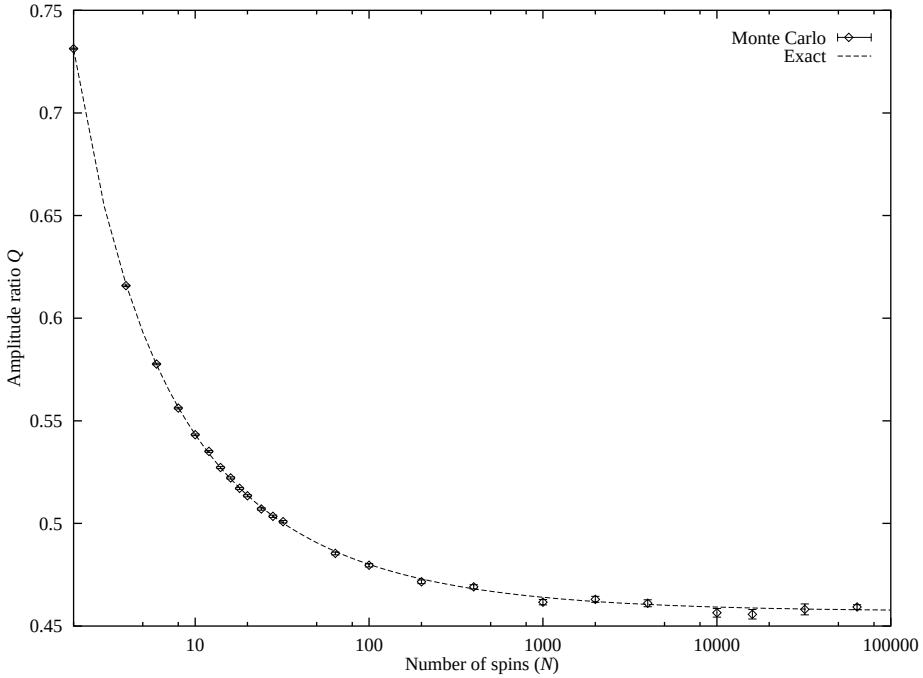

Figure 1: Comparison between exact (dashed line) and Monte Carlo data for the dimensionless amplitude ratio Q at the critical temperature for system sizes in the range 2–64000. For most systems, the size of the errorbars does not exceed the symbol size. The exact data for system sizes smaller than 10000 were obtained by explicit summation over all values of the magnetization, whereas the data for larger systems were calculated from eq. (33).

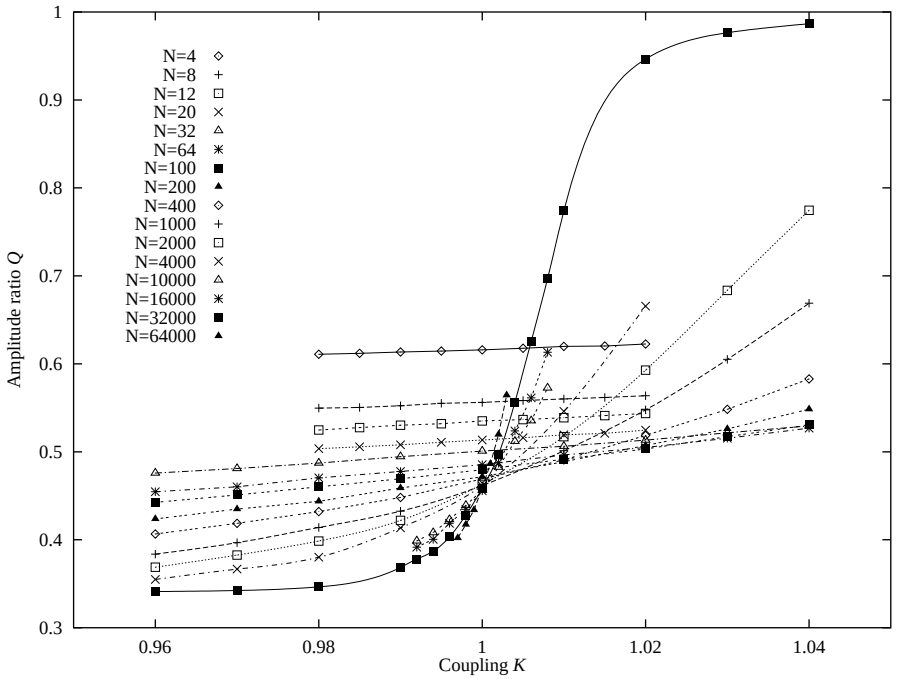

Figure 2: The dimensionless amplitude ratio Q as function of temperature for several system sizes. For clarity the following system sizes that were used in the finite-size analysis have been omitted from the figure: $N = 6, 10, 14, 16, 18, 24, 28$. The size of the errorbars does not exceed the symbol size. Note the large corrections to scaling for small systems.