

Broad Histogram Method

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Monte Carlo simulations of thermodynamic models are usually performed according to Boltzmann's canonical distribution, with a fixed temperature T . This can be very time consuming on the computer since one needs to do a new computer run for each value of T . Salzburg *et al* invented and Ferrenberg and Swendsen perfected the histogram method to circumvent this, by measuring the Boltzmann probability distribution as a function of the energy E , for a fixed T . Instead of repeating the simulations for another value T' , the measured probability distribution is simply reweighted through analytic manipulations of the Boltzmann formula. The simulated Boltzmann probability distribution has, however, exponentially decaying tails. Therefore the statistics are poor away from the peak which is centered around the average energy. Since the peak of the new T' is centered somewhere on these tails, the histogram method only works well for very small system sizes. We present a quite different approach, defining a non-biased random walk along the E axis with long range power-law decaying tails, and measuring directly the degeneracy $g(E)$, without thermodynamic constraints. Our arguments are general (model independent), and the method is shown to be exact for the 1D Ising ferromagnet. Also for the 2D Ising ferromagnet, our numerical results for different thermodynamic quantities agree quite well with exact expressions.

I. Introduction

The Monte Carlo approach is a fundamental tool to study the thermodynamic properties of model systems^[1]. Instead of taking into account all possible states of the system, thermal averages are performed among a finite set of states. These states form a random Markovian sequence generated according to a dynamic rule which has as attractor fixed point the canonical Boltzmann probability distribution

$$P_T(E) = \frac{1}{Z_T} g(E) \exp(-E/T) \quad (1)$$

for each possible energy value E , where T is the fixed temperature, $g(E)$ is the degeneracy of energy level E , and

$$Z_T = \sum_E g(E) \exp(-E/T) \quad (2)$$

is the partition function. Note that E corresponds to the total energy, and we have taken the Boltzmann constant $k_B = 1$. There are many different dynamic rules obeying this probability distribution - the first one being introduced in Ref.^[2]. According to this rule one tries to make some random movement in phase space, for instance through a one-spin flip, starting from the current state of the system. If this movement leads to a decrease of the energy, it is performed. If, however, an energy increment ΔE would result from this movement, it is only performed with probability $\exp(-\Delta E/T)$. By repeating this rule many times, one forms the quoted Markovian sequence of states, the

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thermal average $\langle Q \rangle_T$ of some quantity Q (magnetization, susceptibility, specific heat, etc.) is then simply the arithmetic mean of this quantity over the visited states. Of course, one must take care of statistical correlations and fluctuations, in order to get accurate values. There are many standard procedures^[1] to do this.

Normally one needs to calculate $\langle Q \rangle_T$ as a function of T . So, one is forced to repeat the entire procedure described in the last paragraph for each different value of T . In order to save computer time, an appealing strategy^[3] consists in extracting out the T dependence from equations (1) and (2). Note that T only appears in the Boltzmann weight exponents, making this task easy. First, the distribution $P_T(E)$ itself is measured by accumulating in a histogram the number of visits to each value of E , during the Markovian sequence of simulated states. Then, one can infer another distribution $P_{T'}(E)$ corresponding to a different value T' **without** performing any further computer run, simply by reweighting equations (1) and (2). This approach is known as the histogram method, and has been popularized by Ref. [4]. In order to obtain the average $\langle Q \rangle_T$, one needs to accumulate also in another histogram the measured values of Q corresponding to each energy E . The thermal average at temperature T is then

$$\langle Q \rangle_T = \sum_E \langle Q(E) \rangle P_T(E) \quad , \quad (3)$$

where $\langle Q(E) \rangle$ means the average value of Q obtained at fixed energy E , i.e. the microcanonical average. Once one has the reweighted distribution $P_{T'}(E)$, equation (3) can be applied to obtain $\langle Q \rangle_{T'}$ for other (not simulated) temperatures T' .

The probability distribution $P_T(E)$ presents a sharp peak at $\langle E \rangle_T$ and decays exponentially on both sides. The larger the system size, the narrower this peak. Thus, the computer measured $P_T(E)$ is only reliable around the peak, the statistics being poor in the exponential tails. The reweighting procedure corresponds to replacing the Boltzmann factors appearing in equations (1) and (2) by other Boltzmann factors corresponding to the new value T' , transforming the whole function $P_T(E)$ into $P_{T'}(E)$. In particular, the probability values are reduced near the former peak, and en-

hanced near the new peak position $\langle E \rangle_{T'}$. However, since the statistics is poor near this new peak position, the inferred $P_{T'}(E)$ is not accurate. That is why the histogram method, in spite of its elegant reasoning, has difficulties in practice^[5].

In the present work, we introduce a new method conceived to avoid the exponential tails responsible for the drawback of the histogram method. It is presented in the next section. Section III is devoted to show that our technique is exact for the simple case of the Ising ferromagnet in one dimension, and to compare our numerical results with the exactly known values for the same model in two dimensions. Technical details concerning the computer implementation of the method for the Ising ferromagnet are presented in section IV (which the reader can skip). Concluding remarks are made in section V.

II. The Method

In this section, we will not restrict ourselves to any particular model. Suppose one only knows how to compute the energy E of some given state of the system in the thermodynamic limit (in practice, the system may be a large but finite one). Our reasoning is based on two steps. First, we define a non-biased random walk along the E axis. For that purpose, one needs first to define a set of dynamic movements. For instance, in the case of N Ising spins one can adopt one-spin flips giving raise to N possible movements starting from each state. Other dynamics (cluster flips, continuous spin dynamics, etc.) can also be adopted, depending on the problem being treated. Within this predefined dynamics, starting from the current state with energy E , consider all possible movements changing this state. These movements can be classified into two classes^[6]:

$$\text{class 1: } E \longrightarrow E - \Delta E$$

$$\text{class 2: } E \longrightarrow E + \Delta E \quad ,$$

where $\Delta E > 0$. Suppose for the moment that all possible movements have the same $|\Delta E|$. This hypothesis is not important, and will be disregarded at the end. In the physical region of positive temperatures, $g(E)$ is a monotonically fast increasing function of the energy, and thus the number of possible movements of class 2 is larger than the corresponding possibilities for

class 1. In this way, if one naively defines the dynamics by performing any randomly tossed movement, the energy will increase monotonically up to the maximum entropy region corresponding to infinite temperature. This naive dynamic rule corresponds to a biased random walk along the energy axis. In order to construct a **non biased** random walk, we propose the following dynamics: if the currently chosen movement belongs to class 1, it is accepted and performed; if, however, it belongs to class 2, it is accepted and performed only with probability $N_{\text{dn}}/N_{\text{up}}$, where N_{dn} and N_{up} are the total numbers of possible movements of classes 1 and 2, respectively, counted at the current state. This acceptance probability removes the bias, forcing the probabilities of increasing or decreasing the energy to be equal. Note that N_{dn} and N_{up} correspond to the **potential** possible movements from which only one would be actually performed at each step. Within this dynamic rule the region already visited along the energy axis increases its width proportionally to $\Delta E\sqrt{t}$, like a random walk, where t is the number of performed movements, i.e. the length of the Markovian sequence of states. This makes our method completely distinct from any other based on the Boltzmann distributions, for which the visited energies are confined to narrow windows due to the quoted exponential tails. Fig. 1 shows the number of visits as a function of the energy for the Ising ferromagnet in two dimensions obtained by both methods.

The second step of our reasoning concerns the direct measurement of $g(E)$. Following the non biased random walk dynamics defined above, the probability for the energy to jump from E to $E + \Delta E$ is the same as that of jumping back from $E + \Delta E$ to E . This can be mathematically stated as

$$\langle N_{\text{up}}(E) \rangle g(E) = \langle N_{\text{dn}}(E + \Delta E) \rangle g(E + \Delta E) \quad (4)$$

where the averages are again microcanonical. Equation (4) can be rewritten as

$$\ln g(E + \Delta E) - \ln g(E) = \ln \frac{\langle N_{\text{up}}(E) \rangle}{\langle N_{\text{dn}}(E + \Delta E) \rangle} \quad (5)$$

or

$$\beta(E) \equiv \frac{d \ln g(E)}{dE} = \frac{1}{\Delta E} \ln \frac{\langle N_{\text{up}}(E) \rangle}{\langle N_{\text{dn}}(E + \Delta E) \rangle} \quad (5)$$

allowing one to measure $g(E)$ and thus the entropy change, from the averages $\langle N_{\text{up}}(E) \rangle$ and $\langle N_{\text{dn}}(E) \rangle$ accumulated during the random walk.

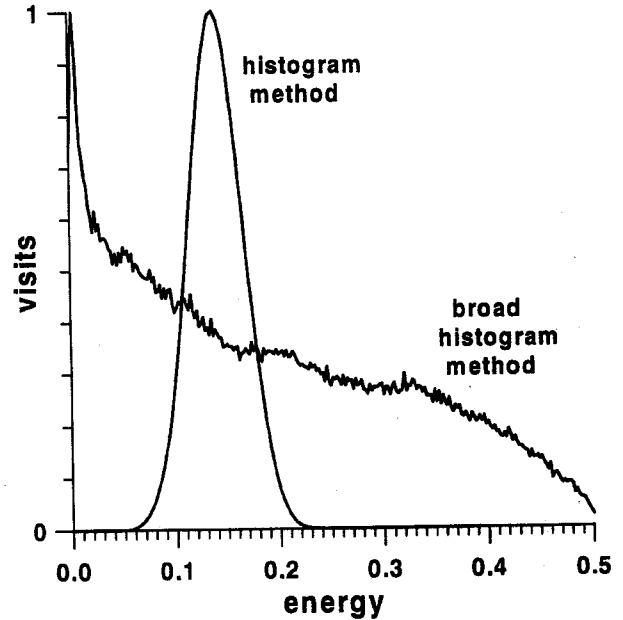


Figure 1. Number of visits as a function of energy obtained from the histogram method^[3,4] (fixing the temperature at the critical value), and from the present method, for the Ising ferromagnet on a 32×32 square lattice. The energy values are displayed by the density of broken bonds. On that scale the whole physical positive-temperature range is between 0 (ground state) and 0.5 (infinite temperature), while the critical point corresponds to 0.146. Within the present method, the whole physical energy range is explored for any system size. In contrast, the histogram method explores only a narrow window, the larger the system size the narrower is this window: namely, for $L = 32$ (shown in the figure), 64, 128 and 256, we found widths 0.061, 0.031, 0.015 and 0.007, respectively.

Our method consists, then, in performing the random walk dynamics defined above, and accumulating values in four histograms along the E axis: the number of visits; the quantity Q one is interested in; the average number N_{up} of movements of class 1; and N_{dn} corresponding to class 2. At the end, $g(E)$ is determined by eq. (5), and the thermal average $\langle Q \rangle_T$ by equations (1), (2) and (3).

As a last remark, let us stress that no thermodynamic concepts are present in our method. Equations like (1), (2) and (3) involve **two completely different ingredients**: 1) how the system exchanges energy with the environment, in the particular present case through

the Boltzmann equilibrium distribution represented by the exponential term $\exp(-E/T)$; and 2) the system itself, i.e., how its internal energy levels are distributed along the energy axis, represented here by its spectrum $g(E)$. Our method concerns only the latter, i.e., the **signature** of the system, independent of its environment or thermal exchanges. The thermal average sums whose results are exemplified in Figs. 3 and 4 are performed only **after** the Markovian process was finished, and the spectrum $g(E)$ of the system had already been determined by the method. In this sense, conceptually, our method is completely distinct from all other based on thermodynamic grounds. It is just this independence from thermodynamic constraints which frees us from the narrow window distributions characteristic of statistical physics, allowing to obtain rather cheaply the overview through the whole space of states. Ironically, is just in the study of statistical physics where our method could become a powerful tool. Another important feature of this thermodynamic-constraint freedom characteristic of our method is the complete absence of critical slowing down, distinguishing it from others once more.

III. Ising Ferromagnet Test

Consider a ring with N Ising spins pointing up or down. Each pair of neighboring spins may either be parallel or anti-parallel, the contribution of this pair to the total energy being zero or one, respectively. In other words, the total energy $E = 0, 2, 4 \dots$ is the number of broken bonds (neighboring spins pointing in opposite directions). In this case, the exact degeneracy can be easily obtained as

$$g_{1D}(E) = 2 \frac{N!}{E!(N-E)!}, \quad (6)$$

or

$$\beta(E) = \frac{1}{2} \ln \frac{(N-E)^2}{E^2}, \quad (7)$$

where we have taken the thermodynamic limit $N/2 > E \gg 1$.

Let's consider one-spin flips and implement our method in this case. A movement will belong to class 1 if the spin to be flipped is currently surrounded by two broken bonds. On the other hand, class 2 corresponds

to spins parallel to both neighbors. In both cases, the energy jump is $\Delta E = \pm 2$. Neglecting ΔE compared to E , one obtains the averages

$$\langle N_{dn}(E) \rangle = \frac{E^2}{N} \quad (8)$$

corresponding to the probability $(E/N)^2$ of finding two neighboring broken bonds, and analogously

$$\langle N_{up}(E) \rangle = \frac{(N-E)^2}{N}. \quad (9)$$

Comparing eqs. (8) and (9) with eqs. (5) and (7) we see that our method gives the exact result (6) for the 1D Ising ferromagnet.

The exact degeneracy $g_{2D}(E)$ of the Ising ferromagnet in two dimensions was also recently derived for finite systems^[7], by using the algebraic software MATHEMATICA, from closed forms already known^[8] for finite square lattices. We use it for another non trivial test of our method. Fig. 2 shows the plot of $\ln g(E)$ obtained by our simulation, for a 32×32 square lattice and the exact curve^[7]. They are indistinguishable on the scale of the plot.

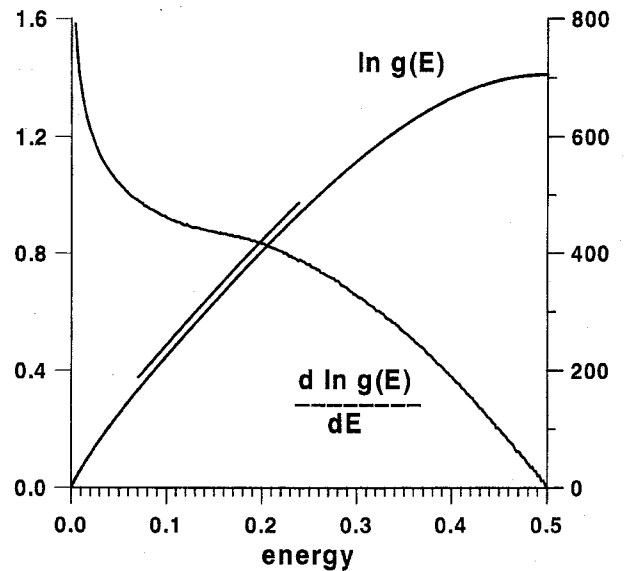


Figure 2. Degeneracy $g(E)$ for the Ising ferromagnet on a 32×32 square lattice (the exact result^[8] could be explicitly obtained up to this size, through an algebraic MATHEMATICA program^[7]). The energy values are displayed by the density of broken bonds. The plot contains both the exact curve and the results of our simulations and they are indistinguishable at this scale. The shorter line displayed slightly above corresponds to the histogram method^[3,4] for which the results remain restricted inside the narrow windows mentioned on the caption of Fig. 1. Also shown is the derivative which is the quantity we directly measured.

Now, we no longer have the same absolute value ΔE for all possible one-spin flips. Spins surrounded by zero or four parallel neighbors correspond to $\Delta E = 4$ and belong to classes 1 or 2, respectively. Analogously, spins surrounded by one or three parallel neighbors correspond to $\Delta E = 2$ and also belong to classes 1 or 2, respectively. One can adopt two distinct strategies to deal with this feature. First, one can divide classes 1 and 2 into sub-classes 4 and 2, storing four histograms: $N_{\text{dn}}^{(4)}(E)$, $N_{\text{dn}}^{(2)}(E)$, $N_{\text{up}}^{(2)}(E)$ and $N_{\text{up}}^{(4)}(E)$ counting spins surrounded by zero, one, three or four parallel neighbors, respectively. At the end one can measure the degeneracy $g_{2D}(E)$ by two independent approaches, either using eq. (5) with $\langle N_{\text{up}}^{(4)}(E) \rangle$, $\langle N_{\text{dn}}^{(4)}(E) \rangle$ and $\Delta E = 4$, or, alternatively, with $\langle N_{\text{up}}^{(2)}(E) \rangle$, $\langle N_{\text{dn}}^{(2)}(E) \rangle$ and $\Delta E = 2$. The second strategy corresponds to store only two histograms for $N_{\text{up}}^{1/\Delta E}(E)$ and $N_{\text{dn}}^{1/\Delta E}(E)$, replacing eq. (5) by the equivalent form

$$\beta(E) \equiv \frac{d \ln g(E)}{dE} = \ln \frac{\langle N_{\text{up}}(E)^{1/\Delta E} \rangle}{\langle N_{\text{dn}}(E + \Delta E)^{1/\Delta E} \rangle} \quad (10)$$

Adopting the first strategy, we confirmed that within the statistical accuracy, both determinations of $g_{2D}(E)$ give the same result. They also agree with the values obtained through the second strategy which is particularly adapted to models where various possible values of ΔE occur.

Fig. 3 shows the averaged energy and specific heat, obtained by the present method, also indistinguishable from the exact curves^[9]. The inset shows the exact specific heat blowed up near the peak as a continuous line, within the error bars of our results represented by the crosses. For a larger lattice, Fig. 4 shows also the magnetization and susceptibility which can be compared with canonical Monte Carlo simulations^[10], since they are not yet known exactly for finite lattices. In order to break the global spin flip symmetry, the magnetization here is considered as the average of the absolute difference between the population fractions of spins up and down. In both Figs. 3 and 4 we considered the energy as twice the number of broken bonds in order to fit the usual form $-J \sum S_i S_j$ of the Ising Hamiltonian.

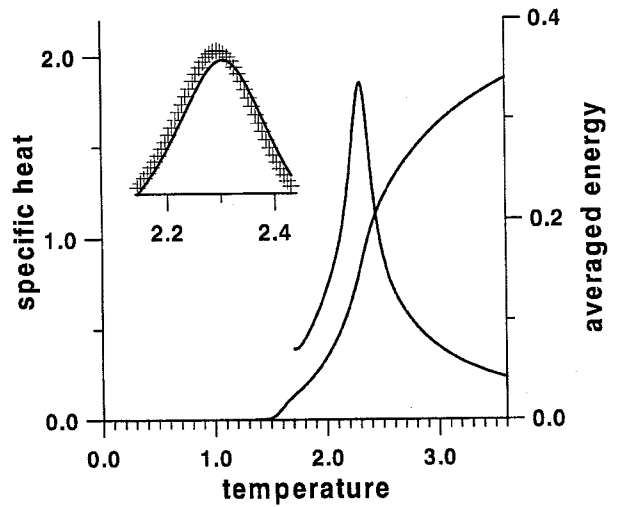


Figure 3: Averaged energy and specific heat obtained from the present method for the Ising ferromagnet on a 32×32 square lattice. The inset compares the exactly known curve^[9] with our results (symbols of the same size of the error bars), near the specific heat peak: these curves are indistinguishable at the larger scale. Concerning CPU time, we took less than 40 minutes on a PENTIUM PC running at 66Mhz, 50% more than the histogram method at the same conditions.

IV. Technical Details

We have written a C program using some multispin coding tricks^[11] in order to accelerate the code. In particular, we have adopted the multilattice approach^[12] storing the states of 32 lattices in a $L \times L$ square array of 32-bit integers, where L is the linear size of the lattice. All 32 samples are processed in parallel by using as often as possible bitwise logical operations instead of algebraic ones^[11]. The sites to be flipped are tossed at random. We adopted the pseudo random number generator which consists in the multiplication of the current random 32-bit odd unsigned integer R with 65539, i.e.

$$R = 65539 \times R, \quad (11)$$

where only the first (less significant) 32 bits of the result are kept. This truncation is automatically done by most compilers. Different random numbers are tossed for the 32 lattices. We have also adopted periodic boundary conditions. The starting state is random and then thermalized by 10 entire lattice sweeps at the critical temperature (Metropolis dynamics). The physical positive-temperature range of energies corresponds to $0 \leq e \leq 0.5$, where e is the energy per bond. Since

the Onsager critical energy corresponds to $e \approx 0.146$, we decided to restrict our random walk energy range to $0 < e < 0.4$, tossing a new initial state every time the current energy goes out of this range. All our numerical results correspond to the kind of calculations described in this paragraph (except for data shown in Figs. 1 and 2, for which we have extended the range up to $e = 0.5$).

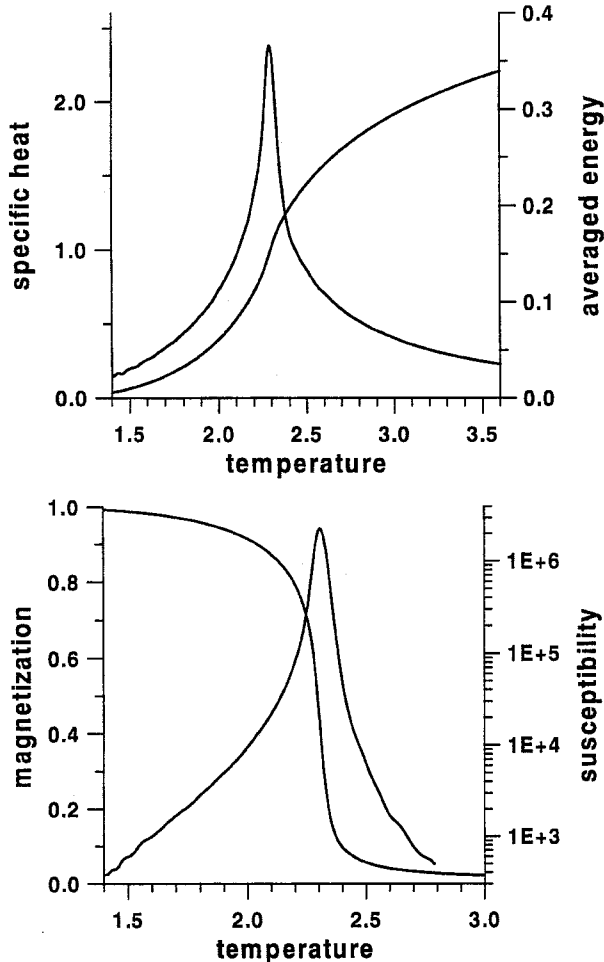


Figure 4: Curves obtained from the present method for the Ising ferromagnet on a 128×128 square lattice. Only 10^4 whole lattice sweeps are used, the same amount adopted for the smaller lattices in previous figures.

Implementing our method as described above, the correlations between successive states decay slowly: around 10 lattice sweeps must be taken between successive data picked for latter averages, in order to obtain good, correlation-free results. Another characteristic feature of Ising one-spin flip dynamics is the frequent blocking of the system in certain pathological low energy states^[13]. If for instance, the square lattice presents a vertical strip of up spins in adjacent columns, all other spins pointing down, the Markovian sequence

will be blocked in this state. This does not change the results, because we only store values to perform the averages if the current state differs from the previous one, but computer time is wasted by these blockings.

In order to accelerate the code, we decided to overcome both problems quoted in the previous paragraph. To do this, we introduced 5 (non-averaging) lattice sweeps of the Metropolis dynamics after each lattice sweep using our random walk dynamics. The fixed temperature adopted for these 5 extra thermalization sweeps corresponds to that of the current energy as measured by equation (10) (note that eq. (10) is formally equal to the statistical definition of the inverse temperature), extracting the averages from the values already accumulated in the histograms $N_{\text{up}}^{1/\Delta E}$ and $N_{\text{dn}}^{1/\Delta E}$. In order to improve efficiency even more one can use the ratio between the corresponding values already accumulated in the histograms instead of the current instantaneous ratio between the numbers of class 1 and class 2 spins.

As a result of all these acceleration tricks the total computer time is less than 40 minutes on a PENTIUM PC running at 66MHz frequency, for $(1 + 5) \times 10^4$ lattice sweeps for 32 samples of size 32×32 . The 64×64 lattice simulation is 4 times slower, and so on. These times are only 50% larger than we measured for the histogram method under the same conditions.

Conclusions

We have presented a new histogram Monte Carlo method which as compared to the traditional one based on temperature^[3,4] is based on histograms measured from a random walk along the energy axis. These histograms have the advantage of having much broader tails allowing to extrapolate to a much larger range of temperatures with a rather small number of samples. We have tested our method on the two-dimensional Ising model and succeeded in reproducing thermodynamic quantities with high accuracy over the entire physical temperature scale with very little effort.

Our method is very general and could be useful for instance for simulations of spin glasses or spin models in three dimensions. Work in this direction is in progress.

Acknowledgments

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