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AN APPLICATION OF A CLUSTER MONTE CARLO METHOD TO THE HEISENBERG MODEL

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A Monte Carlo method with boundary conditions of a self-consistent maximum entropy type has been applied to the classical Heisenberg model.

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1. Introduction

The investigation of phase transitions using computer simulations is extremely time consuming even for simple lattice models.[1] Apart from the system size a very important aspect is the choice of boundary conditions (i.e., which environment should be used to surround the sample) in order to minimize the surface effects on the system and mimick bulk behavior.

Two standard choices are to use periodic boundary conditions (PBC) or to leave free space around the box. The first method is ubiquitously used in simulations and amounts to having exact replicas of the system, filling the space as required by the range of the pair interaction assumed to exist between the particles. Although greatly superior to a free space boundary, using periodic boundary conditions leads to relatively large smearing and broadening of the dependence of the heat capacity and of the order parameter on the temperature. This in turn means that relatively large samples, with many thousands of particles, have to be used to locate the transition even to a moderate precision.

Another possibility, introduced by Binder for the Heisenberg model,[2] is the Self-consistent Monte Carlo (SMC) in which the interactions with the spins outside the

sample box are replaced by interactions with an external magnetic field that couples to the surface particles, and whose strength is adjusted self-consistently.

Yet another type of boundary condition is proposed in the Cluster Monte Carlo (CMC) method,[3] employed here, originally developed to perform simulations of nematic liquid crystal (LC) models. This method is based on replacing the missing interactions at the sample surface by interactions with ghost particles whose orientations are sampled from a distribution generated in accordance with the internal ordering of the lattice using the Maximum Entropy principle.

The method has been applied to a number of LC models: the second rank Lebwohl-Lasher Hamiltonian for nematics,[3] a pure P_4 model,[4] and a ferroelectric system with first and second rank interactions.[5] The results of all these simulations are very satisfactory in the sense that they can be compared with larger lattice simulations in which periodic boundary conditions have been employed.

Here we present an application of the Cluster Monte Carlo method to the classical Heisenberg model that we shall recall in the next section, in Sec. 3 we briefly describe the CMC method whilst in Sec. 4 we present the main results of the simulations performed. A comparison with other recent simulations[6] is also provided.

2. The Heisenberg Model

This classical model, extensively studied using various approximate theories and computer simulations,[2,6,7] is defined on a simple cubic lattice by the pair Hamiltonian:

$$\begin{aligned} U_{ij} &= -\epsilon_{ij}\mathbf{S}_i \cdot \mathbf{S}_j \\ &= -\epsilon_{ij}\cos(\beta_{ij}) \end{aligned} \tag{1}$$

where $\mathbf{S}_i$'s are three-dimensional unit vectors ('spins') located at the lattice sites, ϵ_{ij} is (for the standard isotropic ferromagnetic case) a positive constant, ϵ, for nearest neighbours spins i and j and zero otherwise. The model shows a second-order phase transition from the ordered ferromagnetic phase to the disordered paramagnetic phase at a reduced temperature $T^* \equiv kT/\epsilon \approx 1.45$.[6]

3. The Cluster Monte Carlo

3.1. *Generalities*

As mentioned before the peculiarity of the CMC method is the use of a particular type of boundary conditions where the space surrounding the simulation sample is filled with a set of spins which have, on average, the same magnetization and ordering properties of the spins inside the sample. To do this in a system with nearest neighbour interactions, we add a layer of ghost particles that represent the relevant part of the external world W, to the sample box B (see Fig. 1). Notice that the shape of the box can be chosen quite freely and that it does not have to fill space as with periodic boundary conditions. For instance, a spherical shape can be chosen by suitably carving a sphere from a cubic lattice,[8] as we have actually

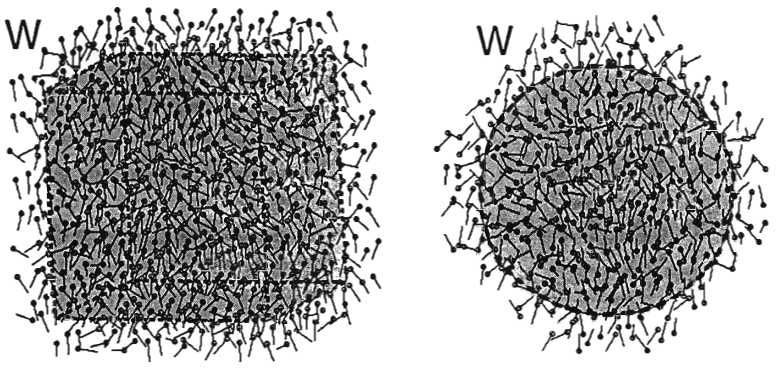

Fig. 1. Visualization of lattices with CMC boundary conditions. The sample box (grey area) is surrounded by a layer of ghost particles of the external 'world' W.

done here. This is schematically shown in Fig. 1.

The desired global average of a quantity A is written as an average over all the external 'world' configurations of Monte Carlo averages calculated with this outside configuration fixed, i.e.,

$$\begin{aligned} \langle A\rangle_G &= \langle\langle A\rangle_{[W]}\rangle_W \\ &\approx (1/M_W)\sum_{[W]}\langle A\rangle_{[W]}\,. \end{aligned} \tag{2}$$

The Cluster Monte Carlo algorithm can then be schematically summarized as follows:

— Calculate a set of relevant observables (order parameters, magnetization) inside the sample box. In particular calculate the first L' orientational order parameters $\langle P_L\rangle$, average of the Legendre polynomials $P_L(\cos\beta_i)$, where β_i is the angle between the spin S_i and the preferred orientation of the system (the magnetization axis or director).

— Obtain an approximate orientational distribution consistent with these observables using the maximum entropy principle.[9] The best Information Theory inference for the singlet orientational distribution of the particles outside the sample based on the order parameters $\{\langle P_L\rangle\}$, $L = 0, \ldots, L'$, and thus implicitly assuming spherical or uniaxial symmetry is :

$$P(\cos\beta) = \exp\left[\sum_{L=0}^{L'} a_L P_L(\cos\beta)\right]\,. \tag{3}$$

In practice in the present case we keep the first two relevant order parameters, $\langle P_1\rangle \equiv \langle M\rangle$ (magnetization) and $\langle P_2\rangle$, so that the most likely distribution will be of the form

$$P(\cos\beta) = \frac{\exp[a_1 P_1(\cos\beta) + a_2 P_2(\cos\beta)]}{\int_0^\pi d\beta \sin\beta \exp[a_1 P_1(\cos\beta) + a_2 P_2(\cos\beta)]}, \tag{4}$$

where the coefficients a_1, a_2 are determined from the constraint that the available $\langle P_L\rangle$ can be reobtained by averaging $P_L(x)$ over the distribution, i.e., by solving the non-linear system

$$\langle P_1\rangle_L = \frac{\int_0^\pi d\beta \sin\beta P_1(\cos\beta) \exp[a_1 P_1(\cos\beta) + a_2 P_2(\cos\beta)]}{\int_0^\pi d\beta \sin\beta \exp[a_1 P_1(\cos\beta) + a_2 P_2(\cos\beta)]} \tag{5}$$

$$\langle P_2\rangle_L = \frac{\int_0^\pi d\beta \sin\beta P_2(\cos\beta) \exp[a_1 P_1(\cos\beta) + a_2 P_2(\cos\beta)]}{\int_0^\pi d\beta \sin\beta \exp[a_1 P_1(\cos\beta) + a_2 P_2(\cos\beta)]}. \tag{6}$$

We use $\langle\ldots\rangle_L$ to indicate that the averages are taken with respect to the laboratory magnetization direction. Notice that the coefficients $a_1(\langle P_1\rangle, \langle P_2\rangle)$ and $a_2(\langle P_1\rangle, \langle P_2\rangle)$ are defined in a domain delimited by the inequalities

$$\frac{2}{3}\langle P_2\rangle^2 + \frac{1}{3} \leq \langle P_1\rangle \leq \left[\frac{2}{3}\langle P_2\rangle + \frac{1}{3}\right]^{\frac{1}{2}}. \tag{7}$$

and these restrictions follow in turn from Schwarz's inequality applied to the specific trigonometric form of the first and second rank Legendre polynomials.[5]

— Generate the set of outside ghosts needed to define the boundary layer by sampling from this distribution.

— Perform Metropolis Monte Carlo updates of the lattice,[10] and monitor the observables.

— When the observables change from the ones competing to the outside environment in a statistically significant way,[3] repeat the generation of the outside environment.

— Calculate a grand average of the previous results to get $\langle A\rangle_G$.

4. Simulation and Results

We have investigated the Heisenberg model using this Cluster Monte Carlo method on a $8 \times 8 \times 8$ lattice, and on jagged spherical droplets carved from lattices of linear dimension $L = 10$, 16, 24, and containing 304, 1568, and 5832 spins, respectively.

The simulations were meant to be independent from each other, and were run in cascade starting from a completely ordered ferromagnetic configuration or from an equilibrated configuration at the nearest lower temperature. A controlled evolution with a rejection ratio not too far from 0.5 has been maintained.[11]

We have calculated several thermodynamic observables: energy, heat capacity, magnetization, the order parameters up to the fourth rank one, and the pair orientational correlation functions.

4.1. *The heat capacity*

The dimensionless heat capacity C_V^* plays an important role in this kind of investigation, if only because the phase transition is located by the temperature at which its peak occurs. It is obtained by differentiating the average energy with respect to temperature as previously described. In brief, here the energy values are interpolated and smoothed using a five point orthogonal formula, before performing the numerical differentiation with an inversion method on the energy written as an integral of the heat capacity with respect to temperature.[12] The overall results for the heat capacity as obtained from the CMC of spherical samples are reported in Fig. 2. The maximum of C_V^* occurs at $T^* \equiv kT/\epsilon \approx 1.45$ for all of the three cases shown. The peak height does not change significantly but becomes sharper when increasing the number of spins, as expected for a continuous transition.

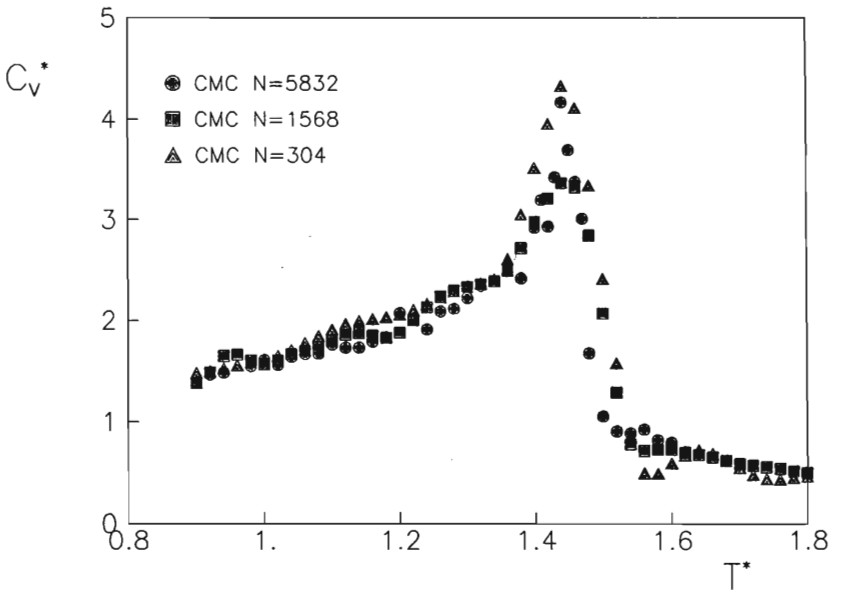

Fig. 2. Temperature dependence of the heat capacity for the three spherical samples studied using the CMC method.

4.2. *The magnetization*

We have calculated the magnetization with respect to the instantaneous ordering direction, $\langle M \rangle \equiv \langle P_1 \rangle_\lambda$, and with respect to the Z laboratory axis $\langle M \rangle_L \equiv \langle P_1 \rangle_L$.

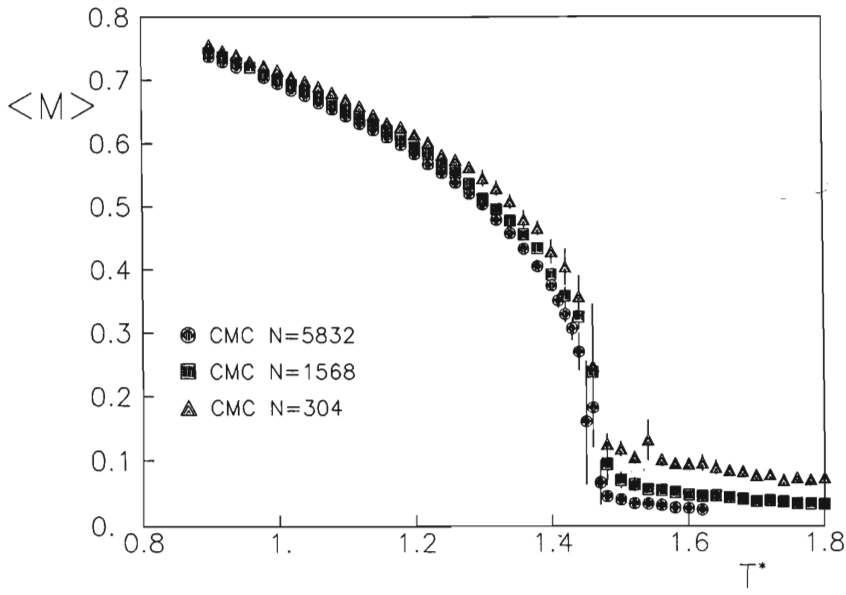

Fig. 3. The magnetization $\langle M \rangle$ calculated with CMC and a spherical sample with $N = 304, 1568$, and 5832 spins.

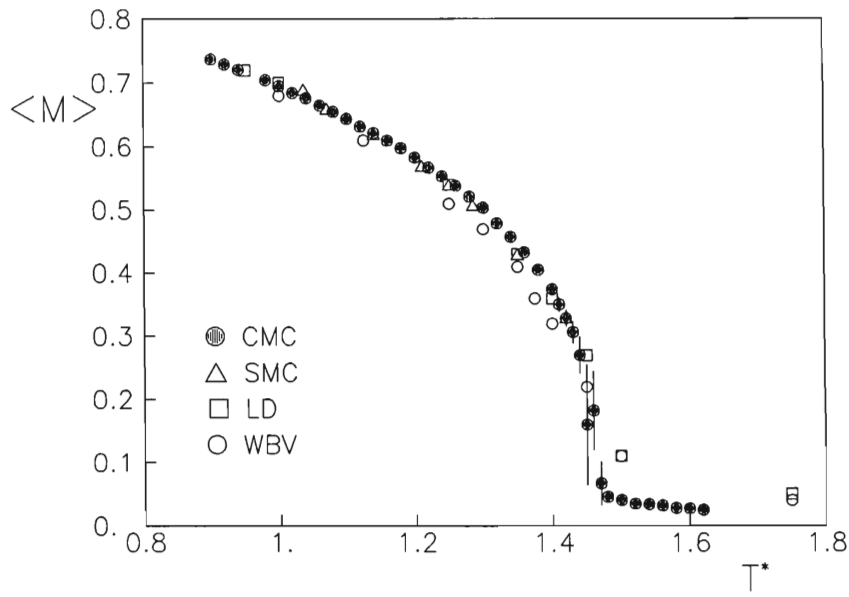

Fig. 4. The magnetization $\langle M \rangle$ obtained from a CMC simulation of a sphere with N=5832. Data from PBC simulations of 8192 spins (WBV)[7] and of 4096 spins (LD)[6] and SMC simulation of 4096 spins[2] are also reported.

$\langle M \rangle_\lambda$ has been calculated from the unit vector $\mathbf{u}_i$, specifying the spin orientation, and the director $\mathbf{d}^J$ (i.e., the mean direction of the spins of all the system in the Jth configuration) obtained from the eigenvector corresponding to the largest eigenvalue of the ordering matrix.[5] The average over K configurations then gives:

$$\langle M \rangle_\lambda = \frac{1}{KN} \sum_J^K \left| \sum_i^N \mathbf{u}_i \cdot \mathbf{d}^J \right| . \tag{8}$$

In Fig. 3, we show our results for the different system sizes. The results are in good agreement with those of previous simulations performed using periodic boundary conditions on $16 \times 16 \times 16$ [6] and $16 \times 16 \times 32$ [7] lattices, and the Self-consistent Monte Carlo with 4096 spins[2] as can be seen in Fig. 4.

4.3. *The orientational correlation functions*

The spin-spin correlation function of rank one, defined as:

$$G_1(r) = \langle P_1(\cos \beta_{ij}) \rangle_r \tag{9}$$

gives the correlation between the orientations of two spins separated by a distance r. It is calculated choosing a spin i as the origin, and summing the contribution in Eq. 8 for all the spins j falling at a distance r, repeating the calculation for a set of origins. $G_1(r)$ then starts from 1 at distance $r = 0$, and decays to a plateau with a value equal to the square of the magnetization if there is long range order.

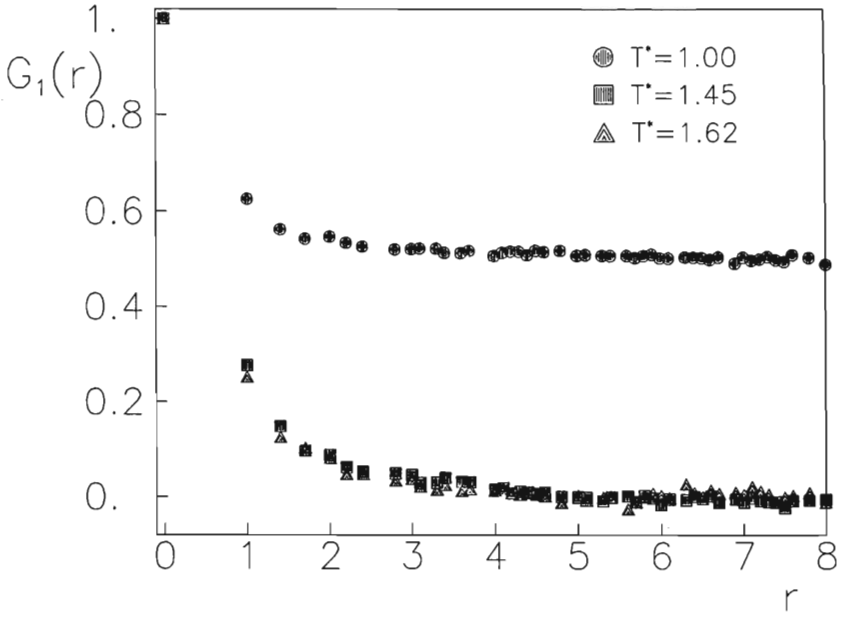

Fig. 5. The spin-spin correlation function plotted against separation r in lattice units as obtained from the CMC simulation of a $N = 8 \times 8 \times 8$ system, at three selected temperatures.

Using PBC, the results of $G_1(r)$ are correct only up to $r = L/2$ because spurious correlation effects appear when the distances approach L, since the spins are replicated with their exact orientations at the position $r = L + 1$. In the CMC method this does not happen and $G_1(r)$ has a correct asymptotic behavior (up to the box length) as shown in Fig. 5 for a $8 \times 8 \times 8$ lattice at three selected temperatures.

5. Conclusions

We have applied the Cluster Monte Carlo method to the classical Heisenberg model, and we have shown that the method presents various advantages in comparison with PBC simulations. We can conclude that:

— The CMC method gives results in accordance with the results[2,6,7] of previous simulations and reproduces correctly the characteristics of the second-order phase transition for the Heisenberg model, and the transition temperature.

— In this method, the orientational pair correlation function has the correct aymptotic behavior and does not grow up unphysically for spins whose distances approach the box length as in PBC simulations.

— The CMC method permits simulations of samples of different shape (we have used cubical and spherical samples), and gives results independent of the sample shape.[13]

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