Monte Carlo studies of antiferromagnetic spin models in three dimensions

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We study several antiferromagnetic formulations of the O(3) spin model in three dimensions by means of Monte Carlo simulations. We discuss about the vacua properties and analyze the phase transitions. Using Finite Size Scaling analysis we conclude that all phase transitions found are of first order.

1. Introduction

The study of antiferromagnetic models (AFM) may give us some insights on the formulation of non trivial relativistic quantum field theories, as they present a very rich phase space and, presumably, new universality classes [1]. They are also interesting as related with models describing high temperature superconductors [2]; the two dimensional quantum Heisenberg antiferromagnet in the low temperature region can be described by a non linear $\sigma$ model in three dimensions [2].

We study in this contribution several formulations of three dimensional antiferromagnetic sigma models as a first step in these directions.

It is clear that we must go beyond the naive formulation of an O(3) $\sigma$ model in a cubic lattice with only nearest neighbors coupling

$$-S = \beta \sum_{\text{nn}} \sigma_i \cdot \sigma_j,$$  \hspace{1cm} (1)

where $\sigma_i$ is a three components normalized real vector, as it can be easily seen that the antiferromagnetic system ($\beta < 0$) is trivially related with the ferromagnetic one obtained by the staggered transformation

$$\sigma_{x,y,z;\beta} \rightarrow \sigma_{x,y,z}(-1)^{x+y+z} ; -\beta$$  \hspace{1cm} (2)

We will consider three models that break the symmetry (2) making the vacuum frustrated:

1. A two parameter model with nearest (nn) and next to nearest (nnn) neighbor couplings

$$-S = \beta_1 \sum_{\text{nn}} \sigma_i \cdot \sigma_j + \frac{1}{2} \beta_2 \sum_{\text{nnn}} \sigma_i \cdot \sigma_j$$  \hspace{1cm} (3)

Under the transformation (2) the second sum in (3) does not change so it is not possible to map the negative $\beta_2$ values onto positive ones.

2. A face centered cubic lattice (FCC) whose geometry explicitely breaks the symmetry (2). Other cubic lattices like the BCC (interior centered cubic) and the tetrahedrical (diamond) fail to do so. Notice also that by setting $\beta_1 = 0$ in (3) two FCC sublattices are decoupled.

3. A Fully Frustrated model constructed by defining the following set of couplings

$$\beta_{x,y,z;0} = \beta(-1)^{x+y},$$
$$\beta_{x,y,z;1} = \beta(-1)^z,$$
$$\beta_{x,y,z;2} = \beta,$$  \hspace{1cm} (4)

where $\beta_{x,y,z;\mu}$ is the coupling of the link pointing in the $\mu$ direction from the $x,y,z$ lattice site, the values $\mu = 0, 1, 2$ correspond to the $x,y,z$ directions respectively. This model presents a $Z_2$ local gauge symmetry: it is invariant under a change of the sign of a particular spin and a simultaneous change of the sign of the couplings at the links starting from the same site.
2. The simulation

We have used mainly the Metropolis algorithm for the updating with several overrelaxation steps. For the largest lattice size \( L = 64 \) the number of Monte Carlo sweeps performed after thermalization, has been of the order of \( 10^6 \), while for the smaller lattices that number has been even greater. We have checked in all cases that the autocorrelation time was much smaller than the total Monte Carlo time used for measures.

We have found the Wolff’s single cluster algorithm \[4\] to be very inefficient near to the antiferromagnetic transition, because the size of the biggest cluster usually represents a very large fraction of the total lattice volume. For this reason, we have used it only to study the ferromagnetic transition.

As observables we have measured the energies
\[
E_1 = \frac{1}{3V} \sum_{nn} \sigma_i \cdot \sigma_j, \quad (5)
\]
\[
E_2 = \frac{1}{6V} \sum_{nnn} \sigma_i \cdot \sigma_j, \quad (6)
\]
with \( V \) being the lattice volume. In the case of the FCC lattice we only measure \( E_2 \), while in the Fully Frustrated model (see \[3\] for details) the sign of the coupling has to be properly taken into account.

For antiferromagnetic phases the standard definition of the magnetization as \( M = \frac{1}{V} \sum_i \sigma_i \) is not an order parameter. For the first two models we have instead considered a staggered magnetization defined as
\[
M'_a = \frac{1}{V} \sum_i (-1)^a \sigma_i, \quad (7)
\]
where \( a = x, y, z \). For the third model we have constructed the following set of vectors
\[
M'_p^{(i,j,k)} = \frac{8}{V} \sum_{x,y,z \text{ (even)}} \sigma_{x+i,y+j,z+k}, \quad (8)
\]
with \( i, j, k = 0, 1 \). It can be checked that the mean values of the previous quantities are independent of \( i, j, k \). We shall refer to it as the period two magnetization.

In practice we measure the magnetizations squared from which we compute the Binder cumulant and the susceptibility defined respectively as
\[
U_L = 1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2}, \quad \chi = V \left( \langle M^2 \rangle - \langle |M| \rangle^2 \right). \quad (9)
\]

Another interesting quantity is the correlation length. To avoid problems with fluctuations and asymmetric lattices we use the second momentum definition considered in ref. \[5\], valid only for the disordered phase
\[
\xi = \left( \frac{g_0/g_1 - 1}{4 \sin^2(\pi/L)} \right)^{1/2}. \quad (10)
\]
where \( g_0 \) and \( g_1 \) are the Fourier transforms of the propagator \( G(r_i - r_j) = \langle \sigma_i \cdot \sigma_j \rangle \) at zero and minimal nonzero momentum respectively.

The derivatives of the energies and magnetizations with respect to the couplings can be computed as connected correlations. For instance, the specific heat matrix can be expressed as
\[
C_{i,j} = \frac{\partial E_i}{\partial \beta_j} = 3V \left( \langle E_i E_j \rangle - \langle E_i \rangle \langle E_j \rangle \right). \quad (11)
\]

We have used a Finite Size Scaling Analysis to compute the critical point and the critical exponents associated with the phase transitions. Measuring for instance the maxima of the specific heat and the susceptibility, using the spectral density method, we obtain
\[
C \sim L^{\alpha/\nu}, \quad \chi \sim L^{\gamma/\nu}. \quad (12)
\]
The critical temperature can be obtained from the scaling behavior of the crossing point \( \beta_{L_1, L_2} \)
\[
\frac{1}{\beta_c} - \frac{1}{\beta_{L_1, L_2}} \sim \frac{1}{\log(L_1/L_2)}. \quad (13)
\]
The critical exponent \( \beta \) may be computed from the magnetization
\[
\langle |M| \rangle_{\beta_c} \sim L^{-\beta/\nu}. \quad (14)
\]
For first order phase transitions however the scaling behavior presents fictitious critical exponents
\[
\nu = \frac{1}{d}, \quad \alpha = 1, \quad \gamma = 1. \quad (15)
\]
3. Results

We have analyzed the phase diagram of the two parameter model (see figure 1). We have found three phases: ferromagnetic and antiferromagnetic separated by a disordered (paramagnetic) phase. The order parameter for the paramagnetic-ferromagnetic (P-F) transition line is the magnetization, while for the paramagnetic-antiferromagnetic (P-A) we use the staggered magnetization. Along the P-F line we find, for

\[ \beta_2 = 0 \]

the standard \( \sigma \) model critical point, for \( \beta_1 = 0 \) the original lattice is decoupled into two sublattices and it is equivalent to the ferromagnetic FCC model with \( \beta = 0.619(5) \). We have measured the critical exponents on those points along the P-F line, checking that they agree well with known values of the standard \( \sigma \) model. The exponent \( \nu \) has been obtained with a 2\% of accuracy.

Along the P-A line we have measured along fixed directions the specific heat, susceptibility, staggered magnetization and correlation length at the following points in the \((\beta_1, \beta_2)\) plane

\[ \mathbf{A} = (\beta_1 = 2, \beta_2 = -1.2511(13)) \]
\[ \mathbf{B} = (\beta_1 = 0.85763(8), \beta_2 = -2\beta_1) \] \hspace{1cm} (16)
\[ \mathbf{C} = (\beta_1 = 0.5, \beta_2 = -2.3899(12)) \]

We have found very difficult to reach the asymptotic behavior even for large lattice sizes. We should emphasize that it is even harder to attain at the point \( \mathbf{B} \). Assuming the results of the \( L = 64 \) as asymptotic we found that the growth of the specific heat is compatible with an \( \alpha/\nu = 3 \) while lower exponents can be readily discarded.

From an analysis of the magnetic susceptibility we exclude a second order transition. The energy histograms (see figure 2) confirm this assumption, for large enough \( L \) they present a clear two peak structure with an stable inter-peak distance. We point out that even for the smaller lattice sizes where the two peaks cannot be resolved the specific heat and the susceptibility give strong indications of the transition first order character.

\[ \beta_1 \]

\[ \beta_2 \]

Figure 1. Phase diagram for the two parameter model. The solid line corresponds to the P-F transition and the dashed line to the P-A transition. The point where \( \beta_2 = 0 \) is the standard \( \sigma \) model critical point. The points where \( \beta_1 = 0 \) correspond to the critical ferromagnetic and antiferromagnetic critical points of the FCC model.

\[ \mathbf{A} \]
\[ \mathbf{B} \]
\[ \mathbf{C} \]

Figure 2. Energy histogram for \( L = 32 \) (solid), \( L = 48 \) (dashes) and \( L = 64 \) (dot-dashes) at \( \mathbf{B} \).

To estimate the correlation length according to (10), we have to simulate in the disordered phase and then extrapolate the results in order to obtain the values at the critical point. We have found the following values for the correlation lengths defined in (10)

\[ \xi^A \sim 7 \quad \xi^B \sim 12 \quad \xi^C \sim 7 \] \hspace{1cm} (17)
with statistical errors of the order of 10%. These values explain \textit{a posteriori} the difficulties found in reaching, especially for point B, the asymptotic region.

The second model considered is the FCC lattice with antiferromagnetic coupling. Classically the ground state presents a $O(3)^L$ degeneracy group. However, when thermal fluctuations are taken into account a collinear ground state is selected (see [3] for details). This is an example on Villain’s \textit{order from disorder} [6]. In the absence of another interaction that fixes the global direction, there remains a $Z_2^L$ degeneracy.

We have performed a numerical simulation in the $L = 24$ lattice in the low temperature phase ($\beta = -5 < \beta_c$) that confirms the collinear ground state structure. Each of the $2^L$ ground states is very stable under Monte Carlo evolution with a local update algorithm. Extrapolating to infinite volume the transition point, in the assumption of a first order behavior, we obtain

$$\beta_{c}^{\text{FCC}} = -4.491(2).$$  \hspace{1cm} (18)

The energy histogram of the $L = 32$ lattice presents a clear double peak that establishes the first order nature of the transition, although for that lattice size the asymptotic behavior has not been reached.

Finally let us present our results for the Fully Frustrated model. As the hamiltonian of this model is invariant under the transformation (2) we will consider only the $\beta \geq 0$ case. We obtain a phase transition, between a disordered phase for small $\beta$ and an ordered one with a complicated structure, at

$$\beta_{c}^{\text{FF}} = 2.26331(13)$$  \hspace{1cm} (19)

The ground state in the ordered phase is highly degenerate. We have checked for $L = 2$, by means of numerical and analytical methods, that the equilibrium configurations, in the $\{e_1, e_2, e_3\}$ space where $e_i \equiv \mathbf{\sigma}(r_0) \cdot \mathbf{\sigma}(r_i)$, lay inside the hexagon perpendicular to the (1,1,1) vector with vertices at $(1, \frac{2\sqrt{3}}{3}, \frac{\sqrt{3}}{3})$ and permutations. For $L > 2$ the equilibrium configurations concentrate around the six corners of the hexagon in a region whose size decreases with increasing lattice size.

The finite size scaling analysis of the specific heat shows that this is a weak first order phase transition with a hard to reach thermodynamic limit. From the $L = 8$ to $L = 24$ values we find good agreement with $\alpha/\nu = 1$ while from the $L = 24$ to $L = 64$ we find an increasing value that tends to $\alpha/\nu = 3$ as expected for a weak first order phase transition. We only observe an incipient two peak structure in the energy histogram for $L = 64$. For the susceptibility we find a behavior compatible with a first order character. From the bigger lattices we quote $\gamma/\nu \sim 3$.

We therefore conclude that the order parameter for the transition, i.e. the period two magnetization becomes a discontinuous function of $\beta$ in the thermodynamic limit.

4. Conclusions

We have explored three models with internal $O(3)$ symmetry that are antiferromagnetic or develop frustration. We conclude that all the antiferromagnetic transitions found are of first order.

We have checked that the ferromagnetic line belongs to what seems to be the only universality class for $O(3)$ models in three dimensions.

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