STUDY OF A PLANAR LATTICE MODEL
WITH $P_4$ INTERACTION

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Abstract

A planar square lattice model with 3-d spins interacting with nearest neighbours through a potential $-\epsilon P_4(\cos\theta_{ij})$ is studied by Monte Carlo technique. Lattice sizes from 10\times10 to 30\times30 are considered for calculating various thermodynamic averages. A 80\times80 lattice has been used to obtain the pair correlation function. To accurately ascertain the order of the phase transition the Ferrenberg-Swendsen technique has been used on a 120\times120 lattice. Our study predicts that the system exhibits a first order phase transition which is confirmed by the twin-peaked nature of the distribution function. The pair correlation function shows an algebraic decay at low temperatures and an exponential decay at high temperatures. Mean field and Two-site Cluster calculations have also been performed and the latter is found to predict the thermodynamic averages fairly accurately.

PACS number(s) : 61.30., 61.30. Gd., 64.70. M.
Key Words : Lattice Models, Monte Carlo

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The phenomenon of fluctuation destruction of long range order in two dimensional systems with a continuous symmetry is well known in literature and is referred to as the Mermin-Wagner-Berezinski theorem. Thus there can be no true long range order in such systems. Systems with power law decay of order parameter correlation function are said to have quasi-long-range order (QLRO). The much studied XY-model has a Hamiltonian $H = -\epsilon \sum_{x,\mu}(\sigma(x), \sigma(x + \mu))$ where $\sigma(x)$ is a two component unit vector at the site $x$ of a square lattice, $\mu$ denotes the two directions of the lattice and $\langle \sigma(x), \sigma(y) \rangle$ denotes the scalar product of the spin vectors $\sigma(x)$ and $\sigma(y)$. There are topological point defects in the two dimensional XY model and vortex unbinding leads to a QLRO-disorder transition which is second order [1].

The question that naturally arises is whether systems with $d=2, n\geq 2$ (where $d$ is the system dimensionality and $n$ is the spin dimensionality) has topological phase transitions. In the class of O(3) Heisenberg system Lau and Dasgupta has shown in a numerical study [2] that the phase transition disappears in absence of point defects and the system remains in its low temperature ordered phase.

Another class of O(3) system of interest is where the Hamiltonian is

$$H = -\epsilon \sum_{i,j} P_L(\cos\gamma_{i,j})$$

(1)

where $i,j$ are nearest neighbours and $\cos(\gamma_{i,j}) = (\sigma_i, \sigma_j)$. Chiccoli, Pasini and Zannoni [3] have numerically investigated this system for $L=2$ and found that the order parameter correlation function exhibits a power law decay in the ordered phase and an exponential decay in the high temperature phase. A far more elaborate study in this system (and also in $d=2, n=40$ model) has more recently been made by Kunz and Zumbach [4]. These authors have found strong evidence for a topological phase transition driven by defects. In the $n=3$ case, this transition is associated with a divergence of correlation length and a cusp in the specific heat.

In this Letter we present a Monte Carlo study on a square lattice with 3-dimensional spins interacting with nearest neighbours through the Hamiltonian (1) for $L=4$. The energy and order parameters $<P_2>$ and $<P_4>$ have been computed for $10\times10, 20\times20$ and $30\times30$ systems. We have chosen a $80\times80$ lattice to study the decay of the order parameter correlation function and have found an algebraic decay in the low temperature phase and an exponential decay at high temperatures. To accurately ascertain the order of the phase transition we have employed the Ferrenberg-Swendsen reweighting technique.
[5] on a 120×120 lattice. The study on the 120×120 system shows that transition is of first order nature with the probability distribution function exhibiting a double peak structure.

We start with calculations based on the mean field (MF) theory and the two site cluster (TSC) theory on these systems. This may seem to be of academic interest only because in a strongly fluctuating two dimensional system the MF theory is not expected to perform well, but the TSC calculations, as will be seen, succeed fairly well in explaining the MC results.

The MF approximation [6,7] can be developed for the models defined by the equation (2). In the MF approximation scheme, the singlet orientational distribution function is given by

\[ P(\cos \theta) = \frac{\exp \left[ z \beta S P_L(\cos \theta) \right]}{Z_1} \]  

where

\[ Z_1 = \int_0^\pi d\theta \sin \theta \exp \left[ (z/T^*) S P_L(\cos \theta) \right] \]  

is the single-particle pseudo-partition function with \( L=4 \) for the present model and \( \theta \) is the orientation of the particle axis with respect to the director. Here \( z \) is the lattice coordination number (\( z=4 \) in the present case) and \( S \) is some variational parameter. The difference in the free energy per particle between the ordered and the isotropic phases is given by

\[ \beta F_0^* = (z/2) \beta S^2 - \log Z_1 + \log 2, \]  

where \( F_0^* = F_0/\epsilon \) and \( \beta = 1/T^* \).

The minimization of the free energy with respect to the variational parameter gives \( S = \langle P_M \rangle = \langle P_M \rangle_{Z_1} \) i.e.

\[ \langle P_M \rangle = \frac{\int_0^1 d(\cos \theta) P_M(\cos \theta) P(\cos \theta)}{\int_0^1 d(\cos \theta) P(\cos \theta)} \]  

Solving the above consistency equation one can calculate the energy, specific heat and orientational order parameters \( \langle P_M \rangle \) for \( M=2,4 \) etc. and then the transition can be identified [8].

The cluster variation technique, for improving upon the MF description of an ordered state was first established by Strieb, Callen and Horwitz for Heisenberg ferromagnet [9].
Since then, a number of attempts have been made to utilize this procedure to explain the disordering transition of nematics [10-16]. As applied to nematics, this procedure involves an initial postulate that there exists a mean field which favours orientation along the director, but terms are added to the free energy expression to take account in detail of the interactions between particles within what is called a cluster. For the model potential given by equation (2), the approximate free energy per particle in the TSC theory is given by [15],

$$\beta F_2^* = -(z/2) \log Z_{12} + (z-1) \log Z_1$$

where \(Z_{12}\) is the two-particle pseudo-partition function

$$Z_{12} = \int \int d\omega_1 d\omega_2 \exp[\beta S (z-1) \{P_4(\cos \theta_1) + P_4(\cos \theta_2)\} + \beta P_4(\cos \theta_{12})]$$

and \(d\omega_i = \sin \theta_i d\theta_i d\phi_i\). The condition of minimum free energy with respect to \(S\) gives the consistency requirement

$$\langle P_4 \rangle_{Z_1} = (1/2) \langle [P_4(\cos \theta_1) + P_4(\cos \theta_2)] \rangle_{Z_{12}}$$

The various thermodynamic observables are obtainable from the free energy. The free energy is given by

$$U^* = -(z/2) \sigma_4,$$

where \(\sigma_L\) are the short-range order parameters

$$\sigma_L = \langle P_L(\cos \theta_{12}) \rangle_{Z_{12}}$$

evaluated at \(r=a\), the nearest neighbour separation. The TSC heat capacity can be obtained by differentiating the energy with respect to the temperature for which exact expressions are given in reference [15]. The integrals appearing in the consistency equation were calculated using the 32-point Gaussian formula and convergence was ensured by subdivision of the intervals. The consistency point were located by direct minimization of the free energy in terms of the variational parameter.

The MC simulations reported in this paper have been performed with periodic boundary conditions on a two dimensional square lattice of particles interacting through equation (2) for \(L=4\). In particular we have studied three lattice sizes \(10 \times 10, 20 \times 20\) and \(30 \times 30\) using the standard Metropolis Monte Carlo algorithm [18-20]. The simulation at the lowest temperature studied for each of the cases was started from a completely aligned
system, while for the other temperatures, the final configuration of the equilibration run at the nearby lower temperature was used to start both the production run at the same temperature and the equilibration run at the next higher one. Equilibration runs took between 10000 and 15000 cycles, where one cycle corresponds to N attempted moves (N being the number of particles in the system). Production runs were typically between 15000 and 25000 cycles and longer runs, from 50000 to 100000 cycles, have been taken near the heat capacity anomaly for both the systems. Sub averages of different quantities were calculated after a certain number of cycles, typically between 1000 and 2000. We have calculated for each simulation energy, specific heat, second and fourth-rank order parameters and orientational pair correlation functions.

The second-rank order parameter $\langle P_2 \rangle$ is calculated from the average over cycles of the largest eigenvalue, $\lambda_3$, of the ordering matrix $Q$,

$$Q_{\alpha\beta} = \langle q_{i,\alpha} q_{i,\beta} - (1/3) \delta_{\alpha,\beta} \rangle$$

(11)

where the symbols have their usual meaning. The matrix is computed and diagonalised at every cycle and the average, denoted by the angular bracket, extends to all the particles in the system. The calculation of the fourth-rank order parameter $\langle P_4 \rangle$ was done according to the algorithm proposed in reference [17].

We have also calculated the second-rank pair correlation coefficient $\sigma_2(r)$,

$$\sigma_2(r) = \langle P_2(\cos \theta_{ij}) \rangle_r$$

(12)

which gives the orientational correlation between two particles i and j separated by a distance r. This represents the first coefficient in the expansion of the rotationally invariant angular correlation function [17-18]. This quantity has been computed for a 80×80 at reduced temperatures 0.3, 0.37 and 0.4.

The recently available reweighting technique of Ferrenberg and Swendsen [5] has been used to accurately predict the order of the phase transition and to locate the transition temperature in a relatively larger lattice viz a 120×120 one. The technique involves generating a vast amount of data to obtain the energy-histogram at a temperature estimated to be close to the transition temperature and then use a transformation to obtain the histogram at neighbouring temperatures. Thus the canonical distribution function is directly available at any temperature near the transition. To trust the results the parent histogram will have to be as accurate as possible and we have used more than one million sweeps of MC simulation (per particle) after equilibration has been acheived on the
120×120 lattice at a temperature $T^* = 0.382$. The distribution function clearly has a two peak structure and by using the reweighting technique we find that the two peaks have equal heights at a temperature 0.3827, signalling the precise location of the first order transition temperature. The strength of the Ferrenberg-Swendsen technique lies in the fact that once the distribution function is available at one temperature T, the same at all temperatures in the neighbourhood of T and hence the ensemble averages of any thermodynamic quantity at these temperatures can be calculated. We have calculated $< E >$ in the neighbourhood of transition and from a numerical fit, the peak of the derivative, which gives the specific heat $C_v$ (a very sharp one indeed), has been located at $T^* = 0.3818$ strongly suggesting once again a first order transition.

The reduced energy $U^*$ obtained from MC simulation for the three lattice sizes has been plotted as a function of the reduced temperature $T^*$ in figure 1. As is evident from the figure the results nearly overlap for all three lattice sizes except predictably near the transition region. The prediction of the TSC theory is also depicted in the figure and the agreement with the simulation results is reasonably good. We have computed the specific heat in two ways for these three lattices; one directly from the MC simulation as a fluctuation quantity and the other from a numerical differentiation of the energy-temperature curves. The location of the specific heat maxima obtained by the two methods agrees well while the peak heights do not. A finite size scaling of the transition temperature obtained from the specific heat maximum (including the result for the 120×120 lattice) has been performed and shown in figure 2. The value of $T_c^*(\infty)$ thus obtained is 0.380. In table 1 we present the results along with the predictions of the MF and TSC theories. The agreement with the MF result is expectedly very poor while the TSC results are close to the $T_c^*$ for 10×10 lattice. This may not be surprising because with decreasing lattice size the fluctuations are truncated thus increasing the value of $T_c^*$ and bringing it closer to the meanfield predictions [21].

Figure 3 shows the results for the order parameters $< P_2 >$ and $< P_4 >$. The changes in both quantities at the transition are sharp, the sharpness increasing with the lattice size. The TSC and MF predictions are also shown and their behaviour can again be illustrated by the argument presented in the preceding paragraph. The order parameters show a peculiar behaviour in that, there is a small temperature region where $< P_4 >$ is greater than $< P_2 >$. Similar behaviour, it may be noted, was obtained by [15] for the 3-d $P_4$ model. The MF and the TSC theories predicts this behaviour and is in qualitative
agreement with the MC results.

Figure 4 shows the variations of $\sigma_2$ and $\sigma_4$, computed for the three lattice sizes, with temperature along with the MF and TSC predictions. The latter again is good qualitative agreement with the MC predictions.

The decay of the 2nd rank correlation function $\sigma_2(r)$ at different temperatures for $r$ ranging up to half the lattice size (which is 80×80) has been shown in figure 5. For $T^* = 0.3$ and 0.37 the results could be fitted to a power law with the decay constant $k_p$ being equal to 0.027 and 0.056 respectively. Above the transition, namely at $T^* = 0.4$, the decay is clearly exponential with the decay constant given by 0.843. It must be noted that the value of $k_p$ are significantly smaller than those obtained in the $P_2$-model by Chiccoli, Pasini and Zanoni [3] or that predicted by the Kosterlitz-Thouless theory [22] for the XY model near the pseudo transition temperature.

Finally in figure 6 we show the distribution function obtained for the 120×120 lattice at $T^* = 0.382$ and the transformed distribution function at $T^* = 0.3827$ obtained by using the Ferrenberg-Swendsen technique [5]. In the latter case the two peaks have equal heights signalling the exact transition temperature for this lattice size.

We have therefore presented a detailed a Monte Carlo study of the planar $P_4$ model for various lattice sizes up to $L = 80$ or 120 which seem to be adequate. We are tempted to conclude that the system undergoes a topological phase transition which is clearly first order. The exact nature of the topological defects leading to the phase transition has not been described in the present paper and will be reported later.

Acknowledgements

The present calculations were carried out on a DEC ALPHA 3000/600S workstation in the department of Physics, Jadavpur University. One of us (KM) acknowledges financial support from Council of Scientific and Industrial Research, Government of India.
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| Method | $T^*_c$ | $\langle P_2 \rangle_c$ | $\langle P_4 \rangle_c$ | $T^*_D$ | $\Delta S/Nk_B$ |
|--------|---------|------------------|------------------|---------|----------------|
| MC     |         |                  |                  |         |                |
| a) $10 \times 10$ | 0.397   | 0.502            | 0.521            | 0.391   | $-$            |
| b) $20 \times 20$ | 0.386   | 0.410            | 0.404            | 0.381   | $-$            |
| c) $30 \times 30$ | 0.380   | 0.403            | 0.396            | 0.380   | $-$            |
| d) $120 \times 120$ | 0.3818  | $-$              | $-$              | $-$     | $-$            |
| MF     | 0.501   | 0.430            | 0.561            | $-$     | 1.259          |
| TSC    | 0.404   | 0.503            | 0.604            | $-$     | 1.178          |
Figure Captions

Fig. 1. Energy for the 10 × 10, 20 × 20 and 30 × 30 lattices: a) (Circles): 10 × 10 MC estimates; b) (Squares): 20 × 20 lattice; c) (Solid Circles): 30 × 30 lattice; (d) (Continuous line): TSC results.

Fig. 2. Finite-size scaling of the transition temperatures obtained from the specific heat peaks for four lattice sizes from 10×10 to 120×120. The value of $T^*_c(\infty)$ is 0.380.

Fig. 3. Results for the second and fourth-rank long-range order parameter: a) (Circles): 10 × 10 MC estimates; b) (Squares): 20 × 20 MC results; c) (Solid Circles): 30 × 30 MC results; c) (Continuous line): TSC predictions; d) (Dashed line): MF results.

Fig. 4. Results for the short-range order parameters for a) 10 × 10, b) 20 × 20 and c) 30 × 30 lattices; (Circles): MC estimates for $\sigma_2$; (Squares) MC estimates for $\sigma_4$; (Continuous line): TSC results for $\sigma_2$; (Dashed line): TSC results for $\sigma_4$.

Fig. 5. Second rank correlation function $\sigma_2$ for a) 80 × 80 lattice calculated at a) $T^* = 0.3$, b) $T^* = 0.37$; c) $T^* = 0.4$.

Fig. 6. The probability distribution for energy at $T^* = 0.3827$. The curve shown has been obtained by reweighting of the distribution function originally obtained for $T^* = 0.382$.

Table Captions

Table 1. Transition values of different parameters for $P_4$ model. $T^*_c$ and $T^*_D$ are respectively the temperatures at which the specific heat (obtained from by differentiating the energy-temperature curve) shows the maxima and the derivative of the order parameter-temperature curve have minima. $< P_2 >_c$ and $< P_4 >_c$ are respectively the transition values of the order parameters. $\Delta S/NK_B$ is the reduced entropy change at the transition.