

# Topological defects and its role in the phase transition of a dense defect system

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## Abstract

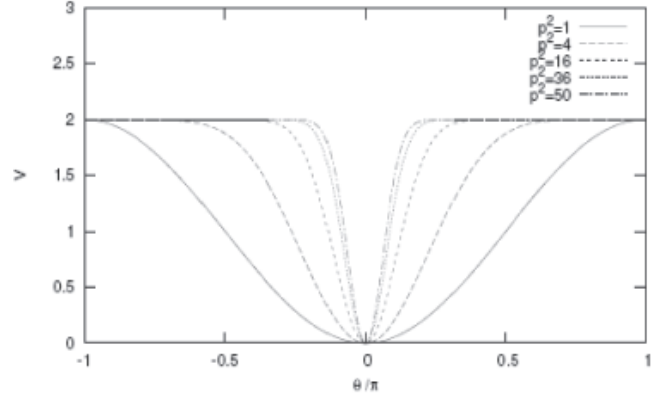
Monte Carlo simulation has been performed on a classical two dimensional XY-model with a modified form of interaction potential to investigate the role of topological defects on the phase transition exhibited by the model. In simulation in a restricted ensemble without defects, the system appears to remain ordered at all temperatures. Suppression of topological defects on the square plaquettes in the modified XY-model leads to complete elimination of the phase transition observed in this model.

## 1. Introduction

In 1984, Domany, Schick and Swendsen [1] proposed an extension of the two-dimensional (2D) XY-model where the classical spins (of unit length), located at the sites of a square lattice and free to rotate on a plane, say the XY plane (having no z-component) interact with nearest-neighbors through a modified potential

$$V(\theta_{ij}) = 2 \left[ 1 - \left( \cos^2 \frac{\theta_{ij}}{2} \right)^{p^2} \right] \quad (1)$$

where  $\theta_{ij}$  is the angle between the nearest neighbor spin and  $p^2$  is a parameter used to alter the shape of the potential or, in other words,  $p^2$  controls the nonlinearity of the potential well. For  $p^2=1$ , the potential reduces to that of a conventional XY-model while with the increase in  $p^2$ , the potential well gets narrower with a width  $\sim \pi / p$  and for  $\theta \geq \pi / p$  it is essentially constant at  $V(\pi) = 2$ . The shape of the potential is shown in Fig. 1 for several of  $p^2$ . The conventional 2D XY-model does not possess any true long range order [2] and it is known that in this model,



**Fig. 1.** The potential energy of Eqn. (1) is shown for different values of  $p^2$ .

non singular spin wave excitation alone cannot destroy the quasi long range order (QLRO). However, the presence of topological defects leads to the QLRO-disorder phase transition, now familiar as the Kosterlitz- Thouless (KT) phase transition. Kosterlitz and Thouless [3, 4] predicted that topological singularities are both necessary and sufficient for the QLRO-disorder phase transition in the 2D XY-model and using a renormalization group (RG)

approach they established that the phase transition is mediated by unbinding of vortices and anti-vortices which are stable topological defects in this system. The phase with QLRO is characterized by a slow algebraic decay of the spin-spin correlation function whereas a fast exponential decay is observed in a disordered system.

The modified XY-model of Eqn. (1) has been analyzed by a number of investigators [1, 5-10] and they found that for strong enough nonlinearity ( $p^2 \sim 50$ ), the KT transition gets converted into a first order phase transition. In a recent work [11] we have shown by performing extensive numerical simulations on relatively large lattice sizes (up to 192 X 192) that the modified XY-model for large values of  $p^2$  behaves like a dense defect system and exhibits first order phase transition as all the finite size scaling rules for a first order phase transition were seen to be obeyed accurately. van Enter and Shlosman [9, 12] provided a rigorous proof of a first order phase transition in various SO(n)-invariant n-vector models which have a deep and narrow potential well and the model under investigation is a member of this general class of systems. van Enter and Shlosman argued that in spite of the order parameter in 2D n-vector model being predicted to vanish by the Mermin-Wagner theorem, long range order prevails in the system via higher order correlation functions. We observed that while the lowest order correlation function decays to zero, the next higher order correlation function has a finite plateau [11] which is in accordance with the statement of van Enter and Shlosman [9].

In the present paper, we investigate the role of topological defects in the phase transition of the modified XY-model under consideration. We are specifically interested in enquiring whether the first order phase transition in the modified XY-model is defect driven or not. In other words, if in the absence of the role played by topological defects, would one observe the same order-disorder phase transition as the one found in the system with topological defects? If suppression of the defects changes the nature of the phase transition or eliminates it altogether, one may conclude that topological defects are necessary to describe the phase transition correctly.

## 2. The Simulation Details

In order to study the behavior of the topological excitations and the role of topological defects in phase

transitions exhibited by the model under investigation, we have used the conventional Metropolis single spin update algorithm [15, 16] with some modifications in our MC simulation. We have found that while simulating a continuous lattice spin model using standard Metropolis algorithm, we need to adjust a parameter very carefully to generate a new configuration. This parameter determines the amplitude of the random angular displacements of the spins and the results become very sensitive to the value of this parameter. In order to get rid of this difficulty of choosing the parameter, we generate a new spin configuration following the prescription of Wolff [17]. We take a random unit vector  $\vec{r}$  and a spin flip  $\vec{s} \rightarrow \vec{s}'$  is defined as  $\vec{s}' = \vec{s} - 2(\vec{s}, \vec{r})\vec{r}$  where  $(\vec{s}, \vec{r})$  is the dot product of  $\vec{s}$  and  $\vec{r}$ . Apart from this method of generating a new configuration, the rest of the algorithm is the standard Metropolis algorithm. Defining a spin flip in that way, our modified Metropolis algorithm is free from tuning any adjustable parameter while simulating a lattice spin model with continuous energy spectrum while the conditions of ergodicity and detailed balance remain fulfilled.

The average defect pair density is calculated in the following way. A vortex (anti-vortex) is a topological defect in which the angle variable  $\theta$ , specifying the direction of the order parameter, changes by  $2\pi(-2\pi)$  in one circuit of any closed contour enclosing the excitation core. In order to trace out the topological defects, we consider a square plaquette in the physical space. Let  $\vec{s}_1, \vec{s}_2, \vec{s}_3$  and  $\vec{s}_4$  be the four spins at the corners of the square plaquette. The angles between these adjacent spins are calculated with proper sign and these are then summed algebraically to find the total angle. The square plaquette is said to enclose a vortex (topological charge  $Q = 1$ ) when the sum equals  $2\pi$ , or more precisely very close to  $2\pi$ , taking into account the possible numerical errors. The square plaquette is said to enclose a anti-vortex (topological charge  $Q = -1$ ) if the sum equals  $-2\pi$ . If the sum is zero, there is no topological defect in the plaquette. Average defect pair density (taking into consideration both vortices and anti-vortices) is calculated as the thermodynamic average of the absolute value of the vorticity summed over the entire lattice divided by the total number of spins. In this method, it is ensured that the net topological charge is always equal to zero in a system with periodic boundary conditions. It

should be mentioned here that the smallest part of the system in real space that enclose a  $Q = \pm 1$  point defect is a triangle. One could thus consider a triangular plaquette in the physical space as well to trace out topological defects. We have tested that the total number of topological charges in the entire lattice remains same whether we choose a square plaquette or a triangular plaquette. Only topological charges of strength  $Q = \pm 1$  are considered since they are energetically favorable. In our investigation of the equilibrium behavior of topological defects near phase transition, we carried out simulations on system sizes with linear dimension  $L = 16, 32, 48$  and  $64$  with periodic boundary conditions.  $10^5$  Monte Carlo sweeps (MCS) were used for equilibration and  $10^6$  MCS were used for calculating thermodynamic averages. One MC sweep is said to be completed when the number of attempted single spin moves equals the total number of spins in the system. The values of  $p^2$  taken to study the variation of average defect pair density with  $p^2$  are 4, 9, 16, 25, 36, 50, 64, 81 and 100.

In order to implement the procedure of the suppression of topological defects in our model, a “chemical potential” term associated with the topological charges is included [13, 14]. The modified Hamiltonian in the simulation is given by

$$H_m = \sum_{(ij)} 2 \left[ 1 - \left( \cos^2 \frac{\theta_{ij}}{2} \right)^{p^2} \right] + \lambda \sum_i Q_i \quad (2)$$

where  $\theta_{ij}$  is the angle between the nearest neighbor spins  $i, j$  and  $|Q_{ijkl}|$  is the absolute value of the charge enclosed by the square plaquette. A positive value of  $\lambda$  ensures that formation of the charges becomes expensive in terms of energy. So for positive  $\lambda$ , this “chemical potential” terms has the effect of suppressing configurations containing defects. In the simulation with this modified Hamiltonian, a calculation of  $\Delta E$ , the energy change associated with an attempted move of a spin, involves calculations of the changes in topological charges associated with four unit square plaquettes which share the spin under consideration. For almost complete suppression of the defects, the value of  $\lambda$  was chosen between 5 and 20 irrespective of temperature. The  $\lambda \rightarrow \infty$  limit of Eqn. (2) indicates an ensemble in which

configuration containing topological defects are not allowed. We started our simulation in that restricted ensemble with a configuration in which all the spins are aligned parallel to one another, i.e., there is no topological defect. The restricted simulations were carried out by using the modified Metropolis spin update algorithm described earlier in this section. We performed our restricted simulations on system sizes with linear dimension  $L = 16, 32, 64$  and  $96$  with periodic boundary conditions. The  $\lambda = 0$  corresponds to an unrestricted simulation, where no suppression of topological defects take place.

For the purpose of calculating various thermodynamic quantities, we have used multiple histogram reweighting technique of Ferrenberg and Swendsen [18]. In the restricted simulations,  $10^6$  MCS were taken for equilibration and  $10^7$  MCS were used for computing the raw energy histograms.

### 3. Results and Discussions

#### A. Behavior of topological excitations near phase transition

We used the method described in Sec. II to determine the average defect pair density ( $\rho$ ) of the system. The variation of the  $\rho$  with the dimensionless temperature  $T$  is shown in Fig. 2 for several values of parameter  $p^2$ . The average defect pair density is found to increase sharply as  $T$  increases through the transition temperature  $T_c(p^2)$  and appears to exhibit a sharp jump at  $T_c(p^2)$ , particularly for  $p^2 \gg 1$ . Fig. 2 indicates that  $T_c(p^2)$  decreases as the value of  $p^2$  increases. It is evident from Fig. 2 that for larger

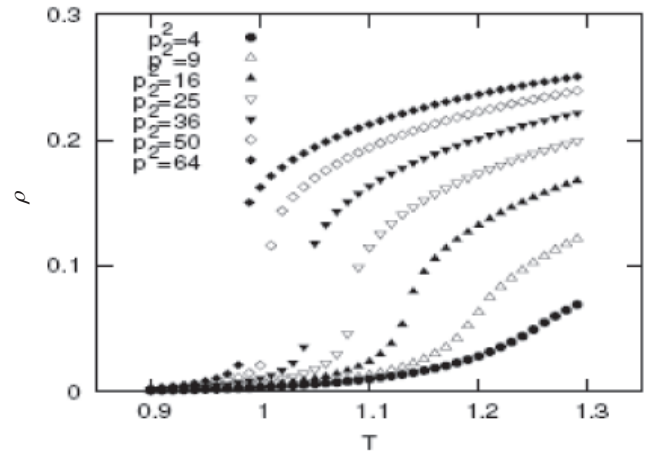
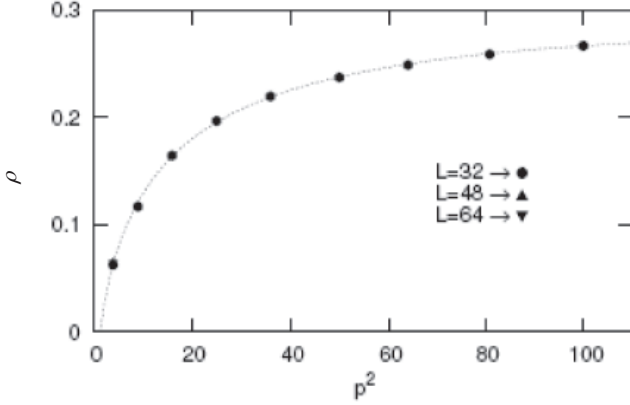


Fig. 2. Average defect pair density  $\rho$  plotted against dimensionless temperature  $T$  for  $L = 64$  for various values of  $p^2$

values of  $p^2$ , at some temperature  $T_c(p^2)$ , vortices suddenly appear in great number and a first order phase transition takes place.

We have also studied the behavior of topological excitations with the parameter  $p^2$ . The average defect pair density ( $\rho$ ) as a function of the parameter  $p^2$  is plotted in Fig. 3 for three different system sizes at a temperature  $T$



**Fig. 3.** Average defect pair density  $\rho$  plotted as a function of  $p^2$  at  $T = 1.28$  for three system sizes. The best fit corresponds to  $L = 64$ . The error bars are smaller than the dimension of the symbols used for plotting.

$= 1.12$  which is above the transition temperature of the model for  $p^2 = 50$ . We observed that above transition temperature, the data for  $\rho$  versus  $p^2$  are nicely fitted by the following expression.

$$\rho(T) = \rho_{\max} - \alpha(T) \exp\left(-\gamma\sqrt{p^2}\right) \quad (3)$$

Eqn. (3) takes into account both vortices and anti-vortices. There is no significant system size dependence of the parameters and it may be noted that  $\rho$  increases with  $p^2$ . In the limit  $p^2 \rightarrow \infty$  the system contains only vortex excitations. This means that in the high  $p^2$  limit, the system must be disordered even at very low temperatures and consequently the transition temperature must be very low. This is the reason behind the decrease in the transition temperature with increase in  $p^2$ .

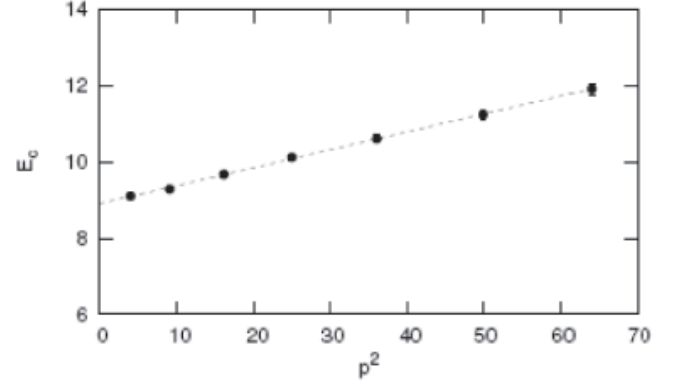
We have also calculated the defect core energy ( $E_c$ ) for various values of  $p^2$ . Because there is always a positive energy cost  $E_c$  associated with the creation of a vortex core, thermally excited vortices in thermal equilibrium always contribute terms proportional to  $\exp(-E_c/T)$  to the partition function. Therefore the total number of topological charges ( $n$ ) shows an exponential behavior  $\exp(-E_c/T)$  at

low temperatures and is given by

$$n = n_0 \exp(-E_c/T) \quad (4)$$

Taking natural logarithm on both sides of Eqn. (4)

$$\ln n = \ln n_0 - \frac{E_c}{T} \quad (5)$$



**Fig. 4.** The defect core energy  $E_c$  plotted against the parameter  $p^2$  with the linear fit represented by the dotted line. The error bars are of the dimension of the symbols used for plotting.

The defect core energy  $E_c$  for each  $p^2$  is determined from the linear fit of the plot  $\ln n$  versus  $1/T$  and Fig. 4 shows the plot of variation of  $E_c$  versus  $p^2$ . Fig. 4 suggests that as the amount of non linearity in the potential well increases, the defect core energy also increases linearly.

#### B. Restricted simulations with no defects

Before presenting our results of restricted simulations, we briefly define the thermodynamic quantities that we have evaluated. The MC simulations were carried out with the modified Hamiltonian given by Eqn. (2) where the new term acts as a ‘‘Chemical potential’’ for the defects. The value of  $p^2$  was taken to be 50 in order to carry out the restricted simulations.

The specific heat  $C_v$  is evaluated from the energy fluctuations

$$C_v = \frac{1}{N} \frac{\left(\langle H^2 \rangle - \langle H \rangle^2\right)}{T^2} \quad (6)$$

where  $T$  is the dimensionless temperature and  $N = L^2$  is the total number of spins. The order parameter is given by

$$\langle P_1 \rangle = \langle \cos \phi \rangle \quad (7)$$

where  $\phi$  is the angle that a spin makes with the preferred direction of orientation and the average is over the entire sample. The first rank pair correlation function is defined as

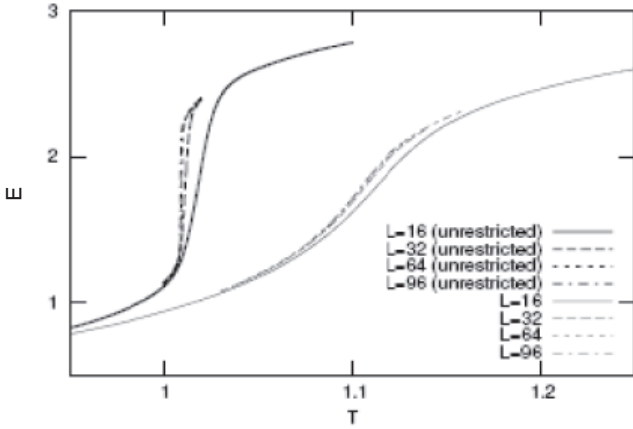
$$G_1(r) = \left\langle \left\langle \cos \theta_{ij} \right\rangle \right\rangle_r \quad (8)$$

where  $i$  and  $j$  are two spins separated by a distance  $r$ . The second rank pair correlation function is defined as

$$G_2(r) = \left\langle P_2(\cos \theta_{ij}) \right\rangle_r \quad (9)$$

where  $P_2$  is the second order Legendre polynomial.

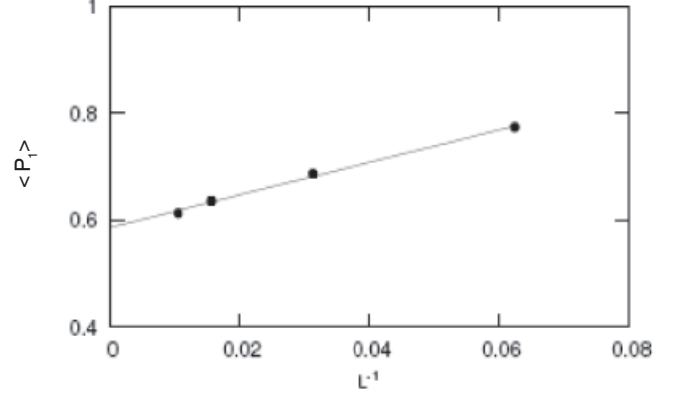
Fig. 5 shows the temperature dependence of the average energy ( $E$ ) for a number of lattices, as obtained by applying the histogram reweighting technique. For comparison, the same plots for unrestricted simulations (where no defect is suppressed) are shown by thick lines in the same figure. It is evident from the figure that the energy changes only gradually and smoothly with temperatures for the restricted simulations while a sharp



**Fig. 5.** The average energy  $E$  per particle plotted against dimensionless temperature  $T$  for different lattice sizes. The thick curves (on left) correspond to unrestricted simulations.

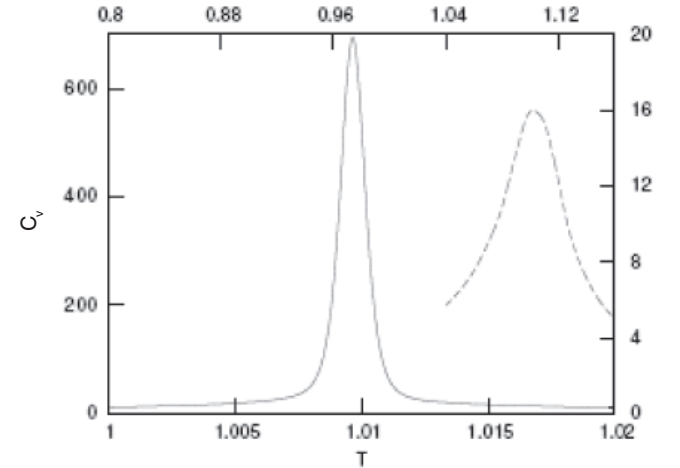
variation of the same with temperature is observed in the unrestricted case. The average value of the order parameter  $\langle P_1 \rangle$  defined in Eqn. (7), is always nonzero for a finite size system. Hence we have studied the system size dependence of  $\langle P_1 \rangle$ . The values of  $\langle P_1 \rangle$  at  $T \rightarrow \infty$  versus  $1/L$  are plotted in Fig. 6 and the system size dependence is, in fact, well fitted by the form  $\langle P_1 \rangle = P_0 + a/L$  with  $P_0 = 0.587 \pm 0.005$  and  $a = 3.3035 \pm 0.141$ . It is clear from

Fig. 6 that there is no indication of  $\langle P_1 \rangle$  extrapolating to zero in the thermodynamic limit  $L \rightarrow \infty$  thereby suggesting a state with long range ferromagnetic order.



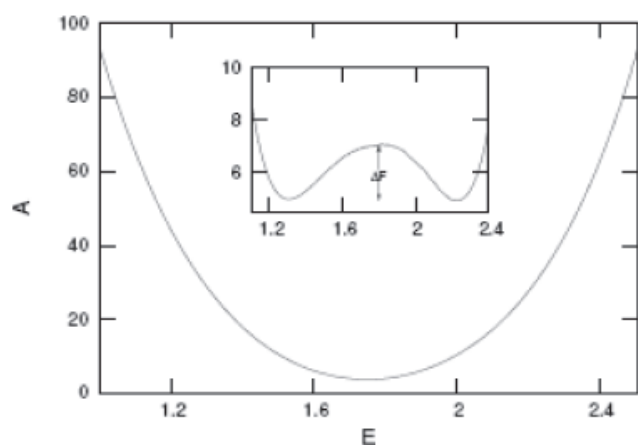
**Fig. 6.** The plot of order parameter  $\langle P_1 \rangle$  at  $T = 1.12$  vs.  $1/L$ . The straight line is the best linear fit to the data. The error bars are smaller than the dimension of the symbols used for plotting.

The specific heat  $C_v$  was obtained from the energy fluctuation relation (Eqn. (6)). The specific heat data for  $L = 64$  in a restricted ensemble are shown by dashed line in Fig. 7 where the results for the unrestricted case are shown by solid line for comparison. For clarity the data for the restricted and the unrestricted simulations are plotted in two different scales. While  $C_v$  has a large peak height ( $\sim 700$ ) at the transition temperature in the unrestricted case, which presumably is a signal of a phase transition in a



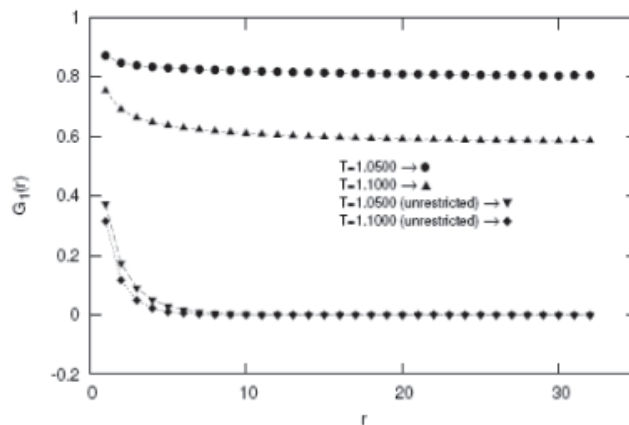
**Fig. 7.** The specific heat  $C_v$  plotted against dimensionless temperature  $T$  for restricted ensemble (represented by dashed line) for  $L = 64$ . The same is plotted for an unrestricted ensemble (shown by solid line). For clarity the graphs are plotted in two different scales. The bottom X-axis are chosen to plot the results for unrestricted simulations while the top X-axis and right Y-axis are chosen to plot the same for restricted simulations.

finite system, in the defect-free case the peak height ( $\sim 16$ ) is drastically reduced and almost disappears in comparison with the normal case (where no defect is suppressed). We would like to argue that, in the restricted ensemble, the existence of a peak in  $C_v$  of insignificant height (compared to that of an unrestricted ensemble) over the temperature range cannot be a sign of a phase transition. These may be attributed to the fact that complete suppression of topological defects is never possible, there always exists a small number of residual charges in the system. We have observed that as the value of  $\lambda$  is increased, the number of residual topological charges decreases and the peak height in  $C_v$  gets reduced. We have run the restricted simulation for different values of  $\lambda$  and confirmed this behavior. However, it may be noted that beyond a certain value of  $\lambda$ , the peak height in  $C_v$  does not change with any further increase in  $\lambda$  which may be attributed to the presence of some residual defects as already mentioned. We have also calculated the free energy like quantity  $A$  from the energy histograms. It is defined as  $A(E; \beta, L, N) = -\ln N(E; \beta, L)$  where  $N(E; \beta, L)$  is the histogram count of the energy distribution. Fig. 8 shows the plot of the quantity  $A$  against  $E$  for  $L=64$ . The inset of Fig. 8 shows the same plot of the original model (Eqn. 1) where a double well structure of equal depth at the transition temperature signals a first order transition. We observe the absence of any such double well structure in  $A$  when defects are suppressed. We are inclined to conclude from



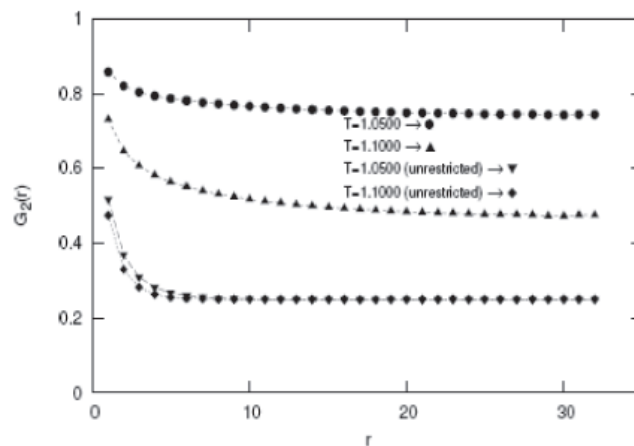
**Fig. 8.** The free energy  $A$  generated by the multiple histogram reweighting technique plotted against energy per particle for  $L = 64$  in the restricted ensemble. Absence of a double well structure is to be noted. The inset shows the same plot for an unrestricted ensemble where the presence of a double well structure is observed.

the results of  $C_v$  and  $A$  that the defect free phase exhibits no phase transition at all. We now turn to pair correlation functions defined earlier in this section. Fig. 9 shows the plot of  $G_1(r)$  against  $r$  for  $L = 64$  in the restricted as well as the unrestricted cases. The first rank pair correlation



**Fig. 9.** The plots of the pair correlation function  $G_1(r)$  against  $r$  for the  $64 \times 64$  lattice for the temperatures indicated. The curves are plotted for  $r$  ranging up to  $L/2$ .

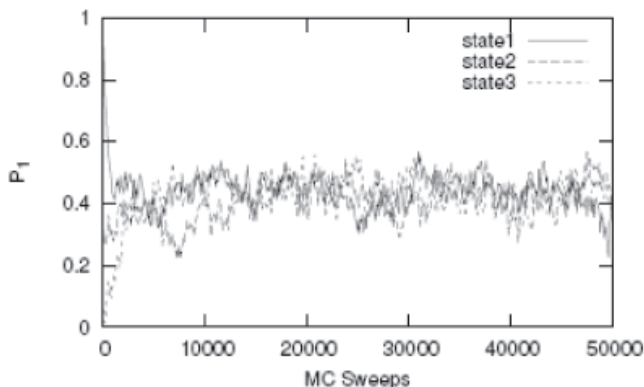
function  $G_1(r)$  for  $p^2 = 50$  at temperatures  $T = 1.0500$  and  $T = 1.1000$ , which is much higher than the transition temperature of the original model, decays exponentially to zero in the unrestricted simulations, as it should, in the complete absence of long range order and a best fit with  $G_1(r) = \alpha \exp(-\delta r)$  shows a nice fit to the data. For the simulation where the defects are suppressed,  $G_1(r)$  decays algebraically and a best fit with  $G_1(r) = ar^{-b} + f$  yields the parameter  $f = 0.806 \pm 0.001$  for  $T = 1.0500$  and  $f = 0.590 \pm 0.001$  for  $T = 1.1000$ . It may be noted that the parameter



**Fig. 10.** The plots of the pair correlation function  $G_2(r)$  against  $r$  for the  $L = 64$  lattice for the temperatures indicated. The curves are plotted for  $r$  ranging up to  $L/2$ .

f is the asymptotic value of the pair correlation function. The next higher order correlation function  $G_2(r)$  against  $r$  for  $L = 64$  is plotted in Fig. 10 at  $T = 1.0500$  and  $T = 1.0100$  for both the cases. The results indicate that  $G_2(r)$  decays algebraically in both cases and long range order prevails in the system via higher order correlation functions.

We now need to address the question of phase space connectivity before arriving at the conclusion that topological defects are indeed necessary for the phase transition. Since we have used large values of  $\lambda$  in our restricted simulations in order to suppress the evolution of topological defects, we have to demonstrate that the observed behavior is not caused by trapping of the system in a small region of phase space with nonzero  $\langle P_1 \rangle$ . Any MC study is guaranteed to generate appropriate ensemble averages if there is a path connecting any two points in the phase space with nonzero transition probability. We have investigated the phase space connectivity by observing the evolution of the order parameter and energy with MC sweeps. The connectedness is satisfied if the observed



**Fig. 11.** The evolution of the order parameter at  $T = 1.1800$  for  $L = 64$  lattice after suppressing the defects using  $\lambda = 20$  for three different initial configurations:  $P_1 = 0.999$ ,  $P_1 = 0.244$  and  $P_1 = 0.012$ . The final values of the order parameter have the same average value.

quantities for different initial states converge to the same final value. In Fig. 11, we have shown that for  $L = 64$ , after suppressing the defects (by using  $\lambda = 20$ ) on the square plaquettes, the final values of the order parameter is same for three different initial configurations. This observation ensures that we can use a value of  $\lambda$  up to 20 without violating the phase space connectivity and the observed nonvanishing of  $\langle P_1 \rangle$  is not a result of trapping of the system in the phase space.

## 4. Conclusions

It is established in this paper that topological defects play a very crucial role in the phase transitions exhibited by the models we discussed. We have observed that the average defect pair density grows rapidly with the increase in  $p^2$  (which increases the nonlinearity of the potential well). For high  $p^2$ , the potential well becomes narrower so that there is an insufficient increase in the defect density at low temperatures and then, at a certain temperature, they suddenly appear in the system in great numbers. Therefore it may be thought that for larger values of  $p^2$  the class of models, we have investigated, behave like a dense defect system and give rise to a first order phase transition as has been predicted by Minnhagen [6-8]. It has also been observed that the first order transition is eliminated totally when configurations containing topological defects are not allowed to occur and the system appears to remain ordered at all temperatures. Hence topological defects are necessary to account for the first order phase transition for larger values of  $p^2$ .

## 5. Acknowledgments

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