

Study of Nematic-Isotropic Phase-Transition Using P_2P_4 Model

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Abstract

Monte Carlo study has been performed in the modified planar Lebwohl Lasher model containing P_2 and P_4 Interaction where P_2 and P_4 are second and fourth order Legendre polynomial having three-dimensional spin. Weakly First order Nematic to Isotropic phase transition is observed using this model. Extensive Monte Carlo simulations using Wolff algorithm are performed to investigate the average energy, order parameter, ordering susceptibility, entropy and specific heat near phase transition. Transition temperature is also estimated.

Keyword: Nematic liquid crystal, Lebwohl-Lasher model, Monte-Carlo simulation, Wolff algorithm, Nematic -Isotropic phase transition

1. Introduction

The Lebwohl-Lasher model [1] consist of a system of rod like molecule placed in a lattice site of three dimensional cubic lattice with interaction potential given by $U_{ij} = -\epsilon_{ij}P_2\cos\theta_{ij}$, where θ_{ij} is the angle between the axis of the i^{th} molecule and j^{th} molecule and ϵ_{ij} is the strength parameter. ϵ_{ij} is equals to ϵ for i equals to j otherwise its value is zero. The model explains the behaviour of Nematic-Isotropic phase transition. The model can also be compared with the Ising and Heisenberg model in the field of magnetism. The basic difference of this model with two dimensional O(3) Heisenberg model for magnetic system is that the direction $\hat{n}$ and $-\hat{n}$ are equivalent, $\hat{n}$ being the director. The nematic P_2 model and XY model exhibit continuous phase transition while O(3) Heisenberg model does not exhibit any transition.

In planar Lebwohl Lasher model, lattice dimension (d) is 2 and spin dimension (n) is 3. This model was first investigated by Chiccoli et.al [2]. They used usual Metropolis's algorithm with the periodic boundary condition ranging from 5×5 to 80×80 . But from their work it was not clear that whether the system exhibits phase transition or not. Kunz and Zumbach [3] execute MC study using cluster algorithm of Wolff [4]. They study 256×256 lattice. They observed continuous transition at dimensionless temperature $T_C = 0.358$, where $T_C = \frac{k_B T}{\epsilon}$ and k_B is the Boltzmann constant. They found the strong topological phase transition and correlation length ξ and susceptibility diverges at transition temperature. They also found a cusp in specific heat curve.

Despite of detailed study by Kunz and Zumbach, some years back we [5] felt necessary to carry out further investigation with the P_2 model. We increase the accuracy of Monte Carlo simulation using cluster algorithm of Wolff at large number of temperatures near T_C . We carry out finite size scaling using the specific heat, order parameter susceptibility and autocorrelation time data. The system exhibits second order phase transition at around $T_C=0.55$, which resembles with Kunz Zumbach observation. Recently S.

Shabnam et al [6] studied the same P_2 model and observed that the system possesses quasi long-range order (QLRO), but they cannot give any conclusion about the order of transition. Another review was done by G.Skacej et.al at his recent work [7].

Zannoni [8] proposed that beside using $P_2 \cos \theta$, higher rank interaction like $P_M \cos \theta$ with $M=4,6$ can be introduced. A. Pal et.al [9] uses pure P_4 term in the potential and observed strongly first order nematic isotropic transition. Chiccoli also [10] used P_4 interaction term in his observation. Heat capacity is insensitive to the system size as observed by Chiccoli et. al. If the system exhibit true phase transition heat capacity should sharpened systematically. Romano [11] gives P_6 term in his potential. Both of their results agree with the observation of Zannoni [7]. Zhang et al and Priezev [12] et al include P_4 term in LL model and observed a weakly 1st order transition.

As the non-negligible higher rank contribution is expected for real molecules After a decade, the model is revisited by me in slightly different approach.. So, it is considered to add even rank term (P_4) term along with P_2 to the potential and the contribution of P_2 and P_4 are equally shared. In this paper, the mixed effect of second and fourth rank term in 1:1 ration in the potential of a nematic is studied systematically. The objective of this paper is to study the nature of transition. At least ten temperatures are investigated around transition temperature for $L=50, 70$ and 100 lattice sizes. The simulation is performed in square lattice using cluster algorithm of Wolff. Periodic boundary condition is also used. Energy, second rank orientational order parameter is calculated. Specific heat and order parameter susceptibility is calculated for modified model by fluctuation technique. Average cluster size using Wolff algorithm is also noted with temperature. Auto correlation time [13] is measured for different lattice sizes. Pair correlation time is also calculated.

2. Computational Method

In this section we will discuss different mathematical treatment that are used in this paper to study this model.

2.1 Wolff Algorithm for Monte Carlo method

In context with liquid crystalline system, we consider the Hamiltonian of modified Lebwohl-Lasher model is

$$H = -\epsilon \sum_{\langle x,y \rangle} \left[\frac{3\{(\vec{\sigma}_x, \vec{\sigma}_y)^2 - 1\}}{2} + \left[\frac{3\{(\vec{\sigma}_x, \vec{\sigma}_y)^2 - 30(\vec{\sigma}_x, \vec{\sigma}_y) + 3\}}{8} \right] \right] \quad (1)$$

We choose a random vector $\vec{\sigma}_x$ in a random lattice site at first point. We flip $\vec{\sigma}_x$ by

$$\vec{\sigma}'_x = \hat{R}(x)\vec{\sigma}_x = \vec{\sigma}_x - 2(\vec{\sigma}_x, \vec{r})\vec{r}. \quad (2)$$

We link all nearest neighbour y connecting x . The bond $\langle x, y \rangle$ is activated by the probability

$$p(x, y) = 1 - \exp \left(\min \{0, \beta \vec{\sigma}'_x, [1 - \hat{R}(x)]\vec{\sigma}_y\} \right) \quad (3)$$

If the property is satisfied $\vec{\sigma}'_y$ is flipped. y is marked and adjoined in the cluster. The process continues iteratively in the same way for all bonds leading to unmarked neighbours of adjoined sites until the process stops.

2.2 Determination of thermodynamic quantities by fluctuation

Potential used in this model is given by,

$$E = -\epsilon \left[\left(\frac{3\cos^2 \theta - 1}{2} \right) + C \left(\frac{35\cos^2 \theta - 30\cos \theta + 3}{8} \right) \right] \quad (4)$$

Where C is the strength parameter. In this model, we choose $C=1$ and strength of interaction $\epsilon = 1$.

The P_2 and P_4 are potential contribute to the Hamiltonian equally (50%).

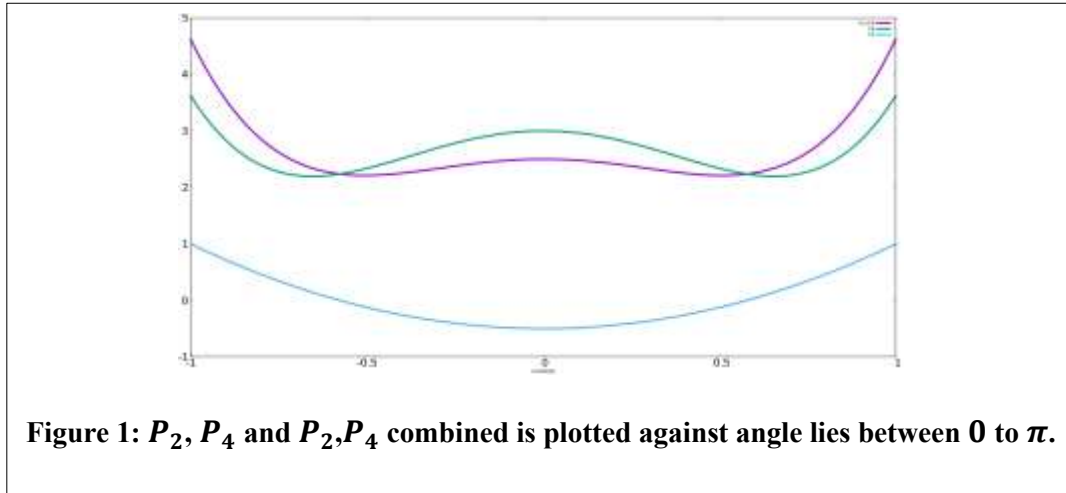


Figure 1: P_2 , P_4 and P_2, P_4 combined is plotted against angle lies between 0 to π .

In Figure 1 we plot the mean field potential which is proportional to $P_M \cos \theta$ with varying value of θ from 0 to π for $M=2$ and 4. The mean field potential possesses $\frac{M+2}{2}$ minima for θ lying between $[0, \pi]$. When M is even

the minima are at $\theta = 0$ and $\theta = \pi$ and becomes narrower and steeper with increasing value of M . So, if we increase the rank of interaction there may be a chance of a particle to be trapped inside the minima rather than inclined towards the director. The P_4 model has three minima within $[0, \pi]$ and magnitude of minima is steeper than mixture of P_2, P_4 .

The average energy per particle of the system is given by

$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^N E_i \quad (5)$$

N being the total number of particles in the system ($N = L^2$) and the reduced specific heat per particle is given by $C_v = \frac{1}{L^2} \frac{d}{dT} \langle E \rangle = \frac{d}{dT} \langle E \rangle$,

(6)

where the angular brackets represent the ensemble average and T is the dimensionless temperature. Specific heat can also be evaluated from the fluctuation of energy

$$C_v = \frac{1}{T^2} (\langle E^2 \rangle - \langle E \rangle^2). \quad (7)$$

The usual long range order parameter is defined as

$$\langle P_2 \rangle = \frac{1}{2} \langle 3 \cos^2 \theta - 1 \rangle \quad (8)$$

which is obtained by maximizing $\langle P_2 \rangle$.

The order parameter susceptibility defined as the fluctuation of order parameter

$$\chi_0 = \frac{1}{T} (\langle P_2^2 \rangle - \langle P_2 \rangle^2) \quad (9)$$

The second rank pair correlation function is defined as

$$G_2(r) = \langle P_2(\cos \alpha_{ij}) \rangle_r, \quad (10)$$

where α_{ij} is the angle between two spins i and j separated by a distance r .

3. Result and discussion

We use planar $P_2 P_4$ model having nearest neighbour interaction, where P_2 and P_4 are the second and fourth order Legendre Polynomial. The model describes a two dimensional nematic having three-dimensional

spin. Monte Carlo simulation were performed on planar model of lattice size $L=50, 70, 90$ and 100 using the cluster algorithm of Wolff [4] instead of spin flip algorithm of Metropolis. Ergodicity and detailed balance condition are maintained in this technique. Periodic boundary condition is used. For each lattice size ten to eleven temperatures close to the transition were used. Three million of Monte Carlo (MC) steps are generated to reach in equilibrium and averages of thermodynamic quantities are measured with 3 million.

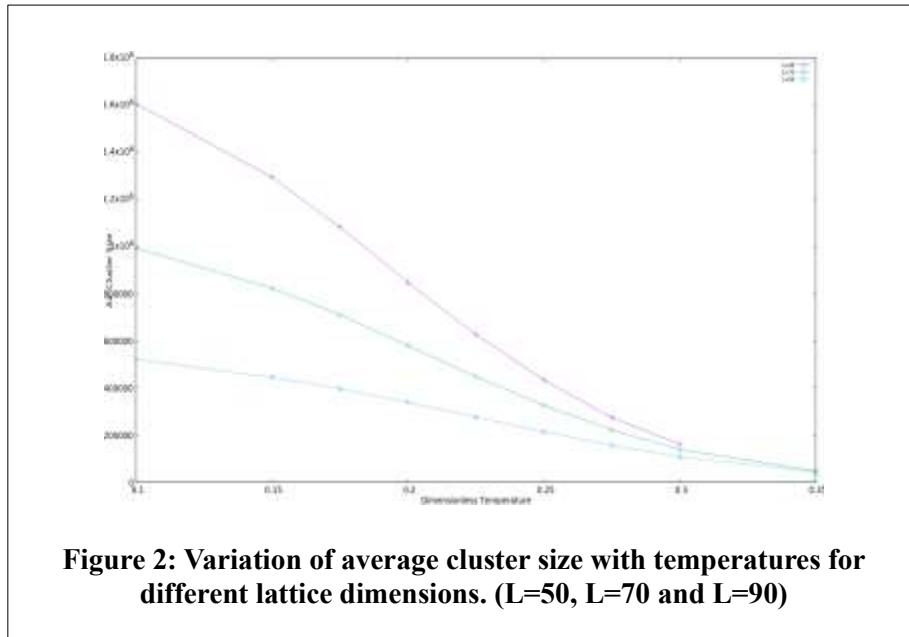


Figure 2: Variation of average cluster size with temperatures for different lattice dimensions. ($L=50, L=70$ and $L=90$)

It is seen from the Figure 2 that the average size of Wolff cluster decreases with temperature. At any temperature average cluster size of higher lattice size should be large. It is plotted for $L=50, L=70$ and $L=100$ lattice size. The nature is same for all lattice sizes.

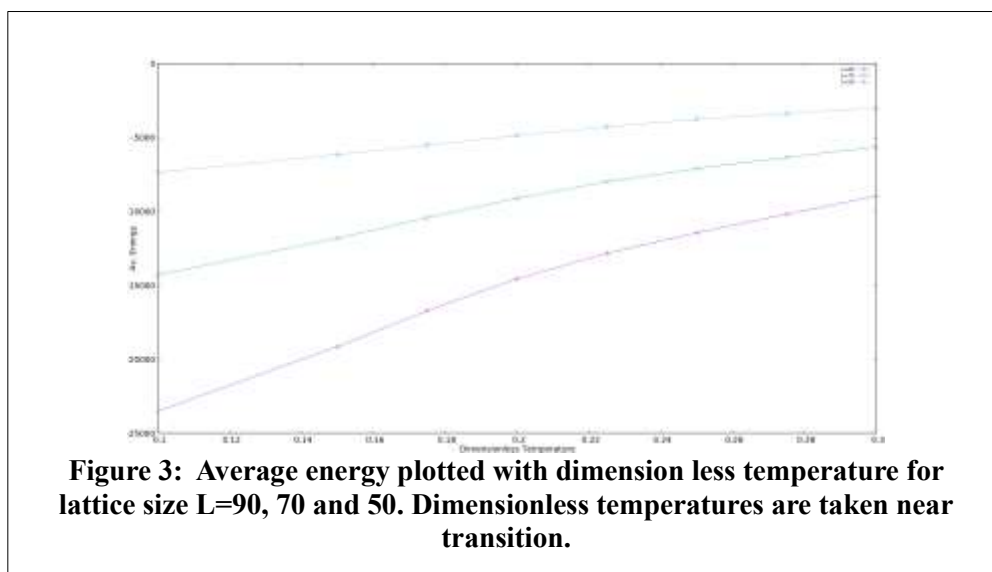
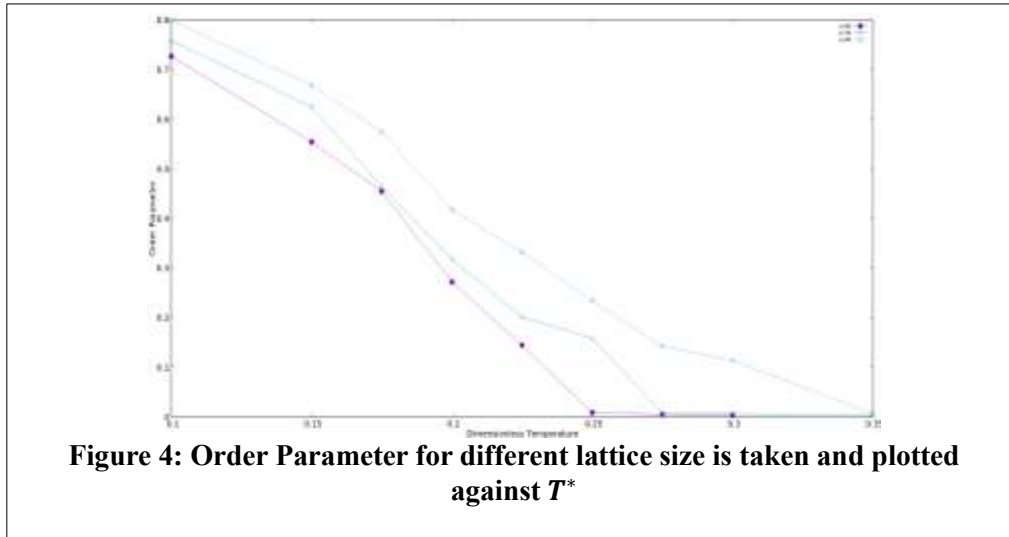


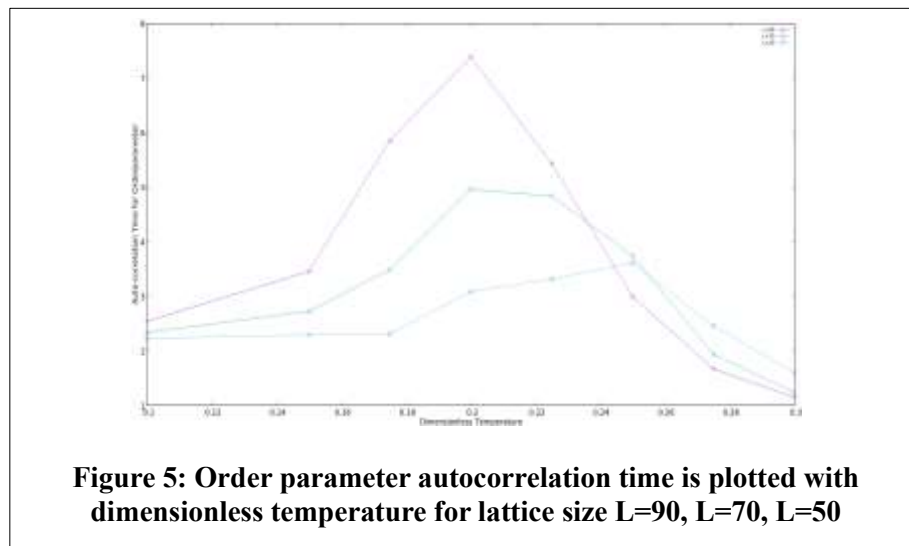
Figure 3: Average energy plotted with dimensionless temperature for lattice size $L=90, 70$ and 50 . Dimensionless temperatures are taken near transition.

The average energy is plotted with temperature in Figure 3. It is seen from the graph that there is continuous increase in energy between $T^* = 0.1$ to $T^* = 0.3$. In case of pure P_4 model, there was a sharp

transition [6] of average energy which indicates the first order transition. In P_2 model, increase in energy is continuous [5].



The orientational order parameter is plotted near transition and rapid fall of order parameter from nematic phase to isotropic phase is clearly seen in Figure 4. From the graph it can be concluded that transition takes place in between the dimensionless temperature 0.15 to 0.25. The nature of the graph shows the evidence of first order transition.



The autocorrelation of energy and order parameter are observed. Autocorrelation of order parameter has definite peak, but autocorrelation of energy does not show any peak. In Figure 5 the autocorrelation time for order parameter is plotted for sizes $L=50$, 70 , 90 . The peak shifts to lower temperature side as the lattice size increases. In pure P_2 model we also get the peak in auto correlation time of order parameter and concluded Wolff cluster algorithm is more efficient than Metropolis as the critical exponent is low for this technique [5].

In Table1 auto correlation of energy and specific heat at different temperatures are given for lattice sizes $L=50$, 70 and 90 around transition temperature. The data shows that there is no peak for energy auto-

correlation time. Specific heat also shows continuous decrease in values. Specific heat at constant volume is also noted from fluctuation.

	L=50		L=70		L=90	
T^*	τ_{energy}	C_V	τ_{energy}	C_V	τ_{energy}	C_V
0.09	3.66	427.99	4.61	788.85	4.72	935.68
0.095	3.83	414.33	3.91	631.39	4.52	916.81
0.1	3.60	398.09	3.98	623.92	4.73	904.71
0.15	3.90	331.35	4.62	534.97	5.58	780.138
0.175	3.83	282.80	5.10	397.86	6.70	461.97
0.2	4.68	195.96	5.34	213.58	6.10	201.90
0.225	4.49	117.72	5.08	42.53	5.86	99.68
0.25	4.67	70.47	5.87	63.32	8.15	58.93
0.275	5.33	45.70	9.28	42.53	15.85	40.70
0.3	7.61	33.33	16.43	31.44	27.67	30.12
0.35	23.25	21.53	38.8	18.51	-	-

Table 1: Autocorrelation of energy and specific heat are given for eleven temperatures around transition for three different lattice sizes

No peak but rapid decrease in C_V is observed from fluctuation data but if the derivative of average energy is taken, peak is observed. (Figure 6)

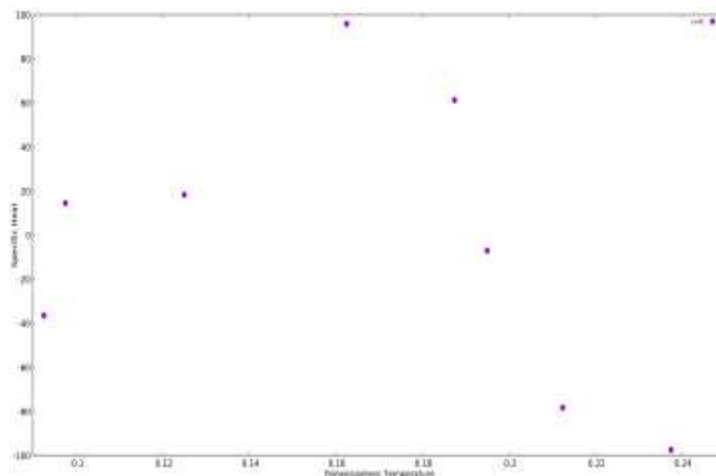


Figure 6: Specific heat is plotted with temperature for L= 90, from derivative of average energy.

System entropy is calculated for ten to eleven temperatures around transition for $L=90, 70$ and 50 . It increases with lattice size but for all lattice sizes the variation of entropy with temperature is nearly equal.

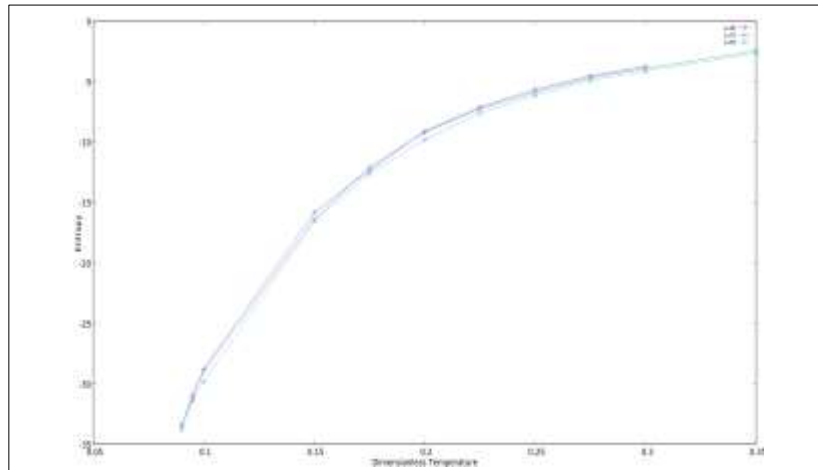


Figure 7: Entropy changes with temperatures for different lattice sizes ($L=90, 70$ and 50)

Ordering susceptibility is plotted with temperature for varying lattice sizes in Figure 8. It shows a peak, whereas in our earlier work with P_2 model [5] the peak is sharper. Specific heat from fluctuation is also plotted for different temperatures. Here also flatten peak is observed.

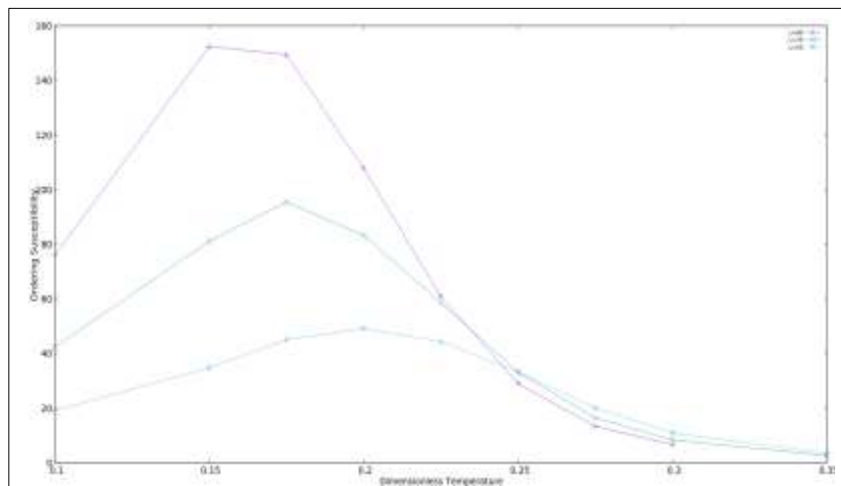


Figure 8: Order parameter susceptibility is plotted with T^* for three lattice sizes

For plotting pair correlation, the range of r has been chosen as half of the lattice size. For the system exhibiting true long-range order, the correlation function decays to a plateau for large r and the limiting value is close to $\langle P_2 \rangle^2$. If the system exhibits quasi long range order the correlation decays like power law as it happens in XY model. In disordered system it dies of exponentially. In Figure 9 pair correlation function is plotted for above, below and near transition temperature.

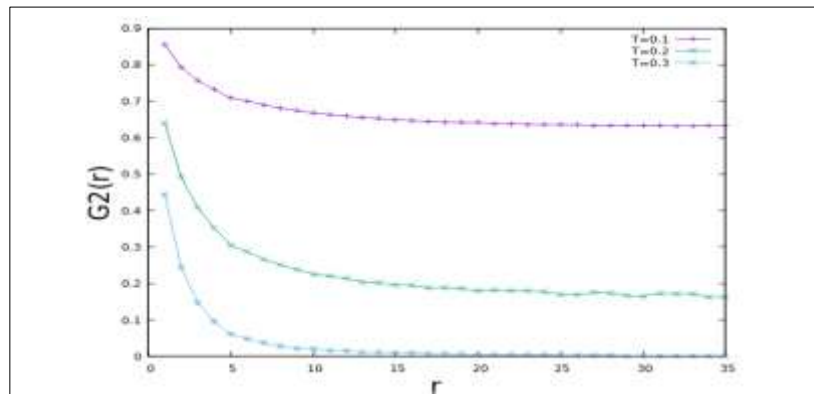


Figure 9: Pair correlation functions are plotted for lattice size $L=70$ for r upto $L/2$ at temperature $T^* = 0.1, 0.2, 0.3$.

For temperature below T_c ($T^*=0.1$) the angular correlation fits with power law $f(x) = a + bx^{-p}$, where $a=0.5677$, $b=0.2964$, $c=0.4574$. This is shown in Figure 10. This implies the system exhibits quasi long-range order (QLRO). For the temperature lower than transition temperature $T^* = 0.1$, $G_2(r)$ could be fitted accurately with a power law decay to a plateau.

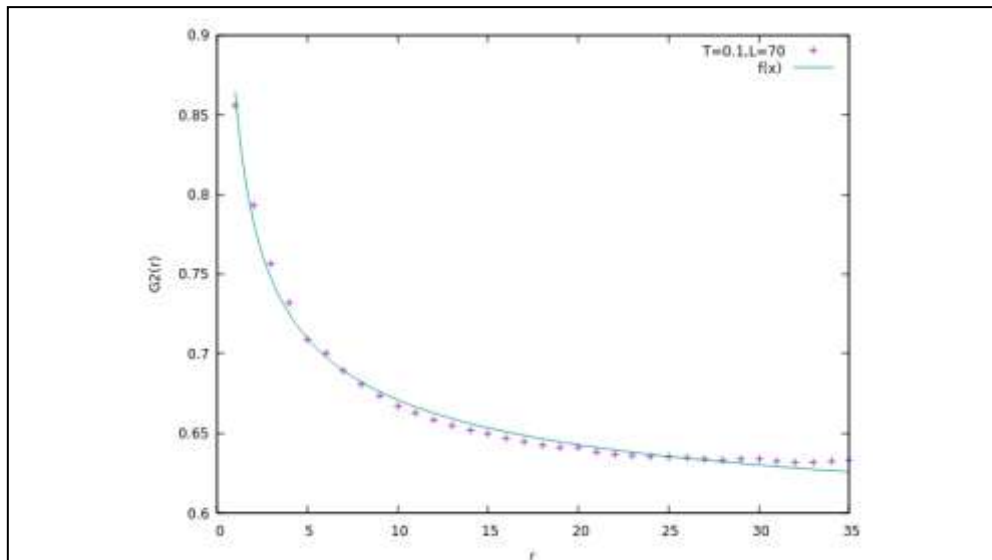


Figure 10: Fit of pair correlation function with power law for $L=70$ for temperature lower than transition temperature.

In Fig 11 exponentially fit agrees reasonably well at temperature above T_c ($T^*=0.3$). For more higher temperature may be exact fit is possible. The fit parameter c is equals to 1.31826. It implies the system reaches to disordered state. It clearly signifies that system goes to QLRO to ordered state transition.

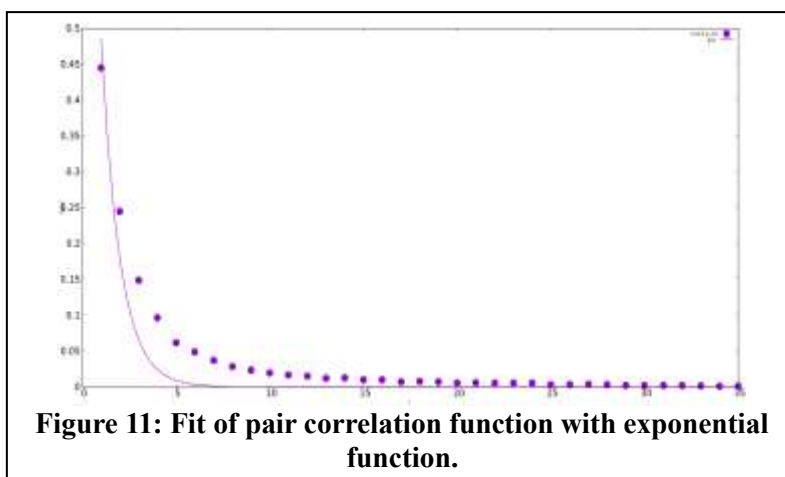


Figure 11: Fit of pair correlation function with exponential function.

Conclusion

The objective of the paper is to study the effect of P_2 and P_4 potential with equal contribution in Nematic Isotropic transition. Planar Lebwohl Lasher model is used with 3 dimensional spin interacting via combination of P_2 and P_4 potential. Monte Carlo simulation is used to study at least 10 temperature around transition temperature. Monte Carlo study of P_2 P_4 model reveals that the system exhibits QLRO to disordered transition. The nature of transition is very weakly first order. The range of transition temperature is within 0.15 to 0.2

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