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One Dimensional Lattice Models of Plane Rotators

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The order-disorder properties of two one-dimensional lattice models of plane rotators are investigated. The first is a 256 particle-system and the anisotropic interaction is of the $T_2(\cos\theta_{ij})$ type (where $T_2(\cos\theta_{ij})$ is the second Tchebyshev polynomial $\cos 2\theta_{ij}$ and $\theta_{ij} = \theta_i - \theta_j$ is the angle between molecular symmetry axes), confined to the nearest neighbours. In the other system the interaction is long-range, of the $r^{-3/2}$ type, the anisotropic part being $T_2(\cos\theta_{ij})$ again. The system size is 512 with the range of interaction extending to 64-neighbours on each side. We have performed Monte Carlo studies of both systems and find that at low temperatures Faber's theory of nematic order accurately describes both systems. Comparison with the work of Romano[8] reveals that for the system with long-range interaction, the transition temperature changes with the truncation distance of the potential.

Keywords: Lattice models, monte carlo.

1. INTRODUCTION

Nematics are composed of rod-like molecules which are partially aligned about the director, conventionally denoted by the unit vector $\hat{n}$. The degree of alignment is described by an order parameter $S_2 = \langle P_2(\cos\theta_i)\rangle$ where θ_i is the angle between the director and the symmetry axis of the i-th molecule and the average is taken over the macroscopic volume. Faber[1] has developed a theory of nematic disorder in which the misalignment of the molecules is described in terms of thermally excited modes of distortion in the director field. He has applied the theory[2] to the simple cubic lattice model which is associated with the names of Lasher and Lebwohl[3]. Later Roy[4] applied this theory to several two- and three-dimensional lattice models and comparison was made with results of the Monte Carlo simulation. They demonstrated that except at temperatures close to the nematic-isotropic transition, the theory, in all cases, provides an accurate description of results generated by the Monte Carlo simulation.

In the present paper, Faber's theory is applied to two other lattice models:

a) A linear chain of plane rotators interacting with the nearest neighbours via a $T_2(\cos\theta_{ij})$ interaction where $T_2(\cos\theta_{ij})$ is the second Tchebyshev polynomial $\cos 2\theta_{ij}$ and θ_{ij} is the angle between molecular symmetry axes, and
b) A linear chain of plane rotators having a long-range interaction of the type $r_{ij}^{-3/2}$ $T_2(\cos\theta_{ij})$.

The linear chain with nearest neighbour interaction has an exact solution[5,6]. Also Denham *et al.*[7] have performed a Monte Carlo simulation on such a chain of 256 rotators. We too have done a Monte Carlo simulation on such a model of identical size primarily to generate the short-range order parameters $\sigma_2(l) = \langle T_2(\cos\theta_{ij})\rangle$ where θ_{ij} is the angle between the i-the and j-th molecules separated by a distance la, a being the lattice spacing. As is well known this system is orientationally disordered at all finite temperatures and therefore does not exhibit an order-disorder transition.

The linear chain of plane rotators with long-range interaction does not possess an exact solution and Romano[8] has carried out the Monte Carlo simulation of a system consisting 1024 particles with the $r^{-3/2}\ T_2(\cos\theta_{ij})$ interaction extending over the entire system. The reason for choosing the particular power of r, namely $-3/2$, however, does not have a deep physical significance. Romano[8] argues that a linear chain with a r^{-1} potential produces a ground state with an infinite energy per particle while the one with a r^{-2} potential is disordered at all finite temperatures. It therefore seems both simple and reasonable, in view of Romano, to choose a mid point value of $-3/2$ for the exponent of r with the expectation that the system would exhibit a transition from an ordered to a disordered phase at a finite temperature, which it indeed does.

According to Romano, the linear chain exhibits a second order transition at $T_c = 2.16 \pm 0.01$. It is to be expected that the degree of order present in the system and hence the transition temperature, too, would depend significantly upon the range of interaction. To test this conjecture we have carried out a Monte Carlo simulation in a 512 particle system, with the interaction truncated beyond the 64-th neighbour and indeed have observed a different transition temperature, predictably a lower one.

In the Section 2.1 we present a discussion of the linear chain with nearest neighbour interaction in the light of Faber's theory. We also point out the features which distinguish the one-dimensional case from the three-dimensional one. The linear chain with long-range interaction is also discussed. In Section 2.2 the equations relevant to the nearest neighbour model are developed and those for the long-range interaction are developed in Section 2.3. The computational details and the results and discussions follow in Sections 3 and 4.

2. THEORY

2.1 Linear Chain Models in the Light of Faber's Theory

Faber assumes that all orientational disorder is due to mode excitation. In the idealized ground state the director $\hat{n}$ is parallel everywhere to the Z-axis and the system is perfectly aligned with $S_2 = 1$. As each the distortion mode is excited, $\hat{n}$ is tilted further away from the Z-axis thereby reducing the degree of order S_2. The alignment is bound to disappear at high temperatures and, when the disorder is complete, we must have $S_2 = 0$ if the system is of infinite extent. In a completely disordered system of finite size, however, the average value of S_2, defined with respect to a director which maximizes the apparent degree of alignment and which may fluctuate in direction from one instant to the next, is not zero but $N^{-1/2}$, N being the number of particles in the system[7]. In a three-dimensional system, the change from $S_2 = 1$ to $S_2 = 0$ which occurs on heating involves a weakly first order phase transition, but phase transitions are not expected in

any one-dimensional system with short-range interactions. Faber's theory, in a simple manner, provides one route to understanding the difference between the one- and three-dimensional cases. The mean square amplitude of a single twist mode is proportional in thermal equilibrium to T/Nq^2. In three-dimensions the smallest allowed value of the wave vector q is $(2\pi/a)N^{-1/3}$, (a being the lattice spacing) and the mean square amplitude associated with this, being proportional to $TN^{-1/3}$ is infinitesimal in a system of infinite extent. In one dimension, however, the smallest allowed value of q is $(2\pi/a)N^{-1}$ and its mean square amplitude being proportional to TN, is large. Inevitably, there can be no long-range order in the one-dimensional case unless T is precisely zero, for the smallest conceivable degree of heating introduces long-range fluctuations into the orientation of the (local) director which suffice to reduce S_2 to zero. As the temperature increases the range of these fluctuations diminishes and hence the short-range correlations of orientations which determine the energy and entropy of the system diminish too. It is scarcely surprising that they do so in a continuous rather than a discontinuous manner. The short-range correlations are expressed by the quantities $\sigma_2(l)$ for which exact expressions[6] have been available since 1973. They are such that $\sigma_2(l) = \sigma_2(1)^l$.

If the T_2 interaction potential is not confined to the nearest neighbours but decreases like $1/r^n$, the mean square amplitude in thermal equilibrium associated with the smallest allowed value of q in a one-dimensional lattice is proportional to $TN^{(n-2)}$. This implies that long-range order, with a non-zero value for S_2, is to be expected at low T, even in a system of infinite extent, provided that $n < 2$. Romano[8] has confirmed this by Monte Carlo calculations for the case $n = 3/2$. Faber's theory is reasonably successful in matching Romano's result also.

2.2 One-dimensional Lattice with Nearest Neighbour Interaction

The model studied is a linear chain of length $L = Na$ in which N molecules are arranged with lattice spacing a. The molecules are constrained to lie in a plane and are referred to as plane rotators. The anisotropic interaction is restricted to the nearest neighbours and takes the form

$$u_{ij} = -\varepsilon T_2(\cos\theta_{ij}), \tag{1}$$

where, ε is a positive constant. Cyclic boundary conditions are imposed in that the first and N-th particles are neighbours.

The short-range order parameter for this model is defined by

$$\sigma_2 = \langle \cos 2(\theta_i - \theta_j) \rangle, \tag{2}$$

and the long-range order parameter is

$$S_2 = \langle \cos 2\theta_i \rangle. \tag{3}$$

Following the assumptions and procedures which Faber[2] has fully explained, we first evaluate a quantity $\alpha(l)$, which is defined by the relation

$$\sum_{q\neq 0} \langle(\Delta\psi)_l^2\rangle = \alpha(l) \sum_{q\neq 0} \langle\psi^2\rangle, \tag{4}$$

where $\langle\psi^2\rangle$ is the mean square angle through which the molecular symmetry axes are rotated when a single mode is thermally excited, $\langle(\Delta\psi)_l^2\rangle$ is the mean square value of $(\psi_i - \psi_j)$ for two molecules separated by $r_{ij} = la$, and the sums are over all possible values other than zero for the wave vector $\mathbf{q}$ of the periodic distortion modes of the director field. We exclude the $q = 0$ mode since it costs no energy and affects only the orientation of the director for the specimen as a whole.

It follows that if, $X = \sum_{q\neq 0} \langle\psi^2\rangle$ then,

$$S_2 = \exp(-2X), \tag{5}$$

and that with $\alpha(l)$ defined in (4)

$$\sigma_2(l) = S_2^{\alpha(l)}. \tag{6}$$

Equation (6) is approximately true in the three-dimensional case as Faber[1] has pointed out, but in two and one dimensions it is exact, which simplifies the calculation of the order parameter.

The energy of the system is calculated as a sum of pair interactions as in Equation (1). Thus

$$\langle U\rangle = -(1/2)\varepsilon \sum_{i=1}^{N} \langle T_2(\cos\theta_{ij})\rangle, \text{ with } i \neq j$$

$$= -(N/2)\varepsilon z \sigma_2, \tag{7}$$

where $z = 2$ is the coordination number and $\sigma_2 = \langle T_2(\cos\theta_{ij})\rangle$ is the short-range order parameter averaged over neighbouring particles. Therefore, the average dimensionless reduced energy per molecule $U^* = \langle U\rangle/N\varepsilon$ is given by

$$U^* = -\sigma_2(1). \tag{8}$$

The increase in energy when a single mode is excited is given by

$$-N\varepsilon\Delta\sigma_2(1) = 2N\varepsilon\alpha(1)\sigma_2(1)\Delta X.$$

The approximation in this context is that the distinction between energy and free energy is negligible. Equating this with $(1/2)\,k_B T$ and summing over $(N-1)$ modes we get

$$4N\varepsilon\alpha(1)\sigma_2(1)X = (N-1)k_B T,$$

or,

$$-2\left(\frac{N}{N-1}\right)\sigma_2(1)\ln\sigma_2(1) = k_B T/\varepsilon = T^*. \tag{9}$$

It may be noted that $\sigma_2(1)$ is independent of $\alpha(1)$ and hence of L (except in so far as $(N/N-1)$ varies), which is not the case in three dimensions.

One may then calculate $\sigma_2(1)$ as a function of the reduced temperature from Equation (9) and then use Equation (6), given a set of values for $\alpha(l)$, to infer both S_2 and $\sigma_2(l>1)$. The permitted values of q satisfy,

$$\mathbf{q} = (2\pi/Na)g\hat{x}, \quad \text{with } -N < 2g \leqslant N. \tag{10}$$

The values of $\alpha(1)$ are evaluated using the following equation which is a straightforward extension of one of Faber's result.[1]

$$\alpha(l) = 2\sum_{q\neq 0}\left(\frac{C_l}{C_1}\right)\Big/\sum_{q\neq 0}\left(\frac{1}{C_1}\right), \tag{11}$$

where,

$$C_l = 1 - \frac{1}{2}\sum_j \cos(\mathbf{q}\cdot\mathbf{r}_{ij})_l. \tag{12}$$

The summation on the right hand side of Equation (12) is over all neighbours of i-th molecule which are separated from it by la. Table 1 lists computed results for different values of l. The values of σ_2 to which they lead are discussed below.

2.3 One-dimensional Lattice with Long Range Interaction

This is a straightforward elaboration of the model considered in the previous section, but the interaction is described by

$$u_{ij} = -\varepsilon\left(\frac{a}{r_{ij}}\right)^{3/2} T_2(\cos\theta_{ij}), \tag{13}$$

where $r_{ij} = la$ is the separation between i-th and j-th molecules with $l = 1, 2, 3$ etc. Each molecule interacts with 64 others.

TABLE 1

Variation of $\alpha(l)$ with l for the nearest neighbour interaction

$\alpha(1)$	$\alpha(2)$	$\alpha(3)$	$\alpha(4)$	$\alpha(5)$	$\alpha(6)$	$\alpha(7)$
0.0468	0.0930	0.1392	0.1846	0.2299	0.2746	0.3193
$\alpha(8)$	$\alpha(9)$	$\alpha(10)$	$\alpha(11)$	$\alpha(12)$	$\alpha(13)$	$\alpha(14)$
0.3633	0.4072	0.4504	0.4936	0.5361	0.5786	0.6203

The reduced energy per molecule is given by

$$U^* = -\sum_l (l)^{-3/2}\sigma_2(l). \tag{14}$$

Once $\alpha(l)$ is known, we can evaluate the long-range order parameter S_2 as a function of the reduced temperature from the equation

$$T^* = -2\left(\frac{N}{N-1}\right)\ln S_2\left(\sum_l (l)^{-3/2}\alpha(l)S_2^{\alpha(l)}\right). \tag{15}$$

Then we can calculate the values of σ_2 (l) using Equation (6) with a set of values of $\alpha(l)$. The boundary conditions for q are same for the model in Section 2.2.

The values of $\alpha(l)$ can be evaluated from the equation:

$$\alpha(l) = 2\sum_{q\neq 0}\left(\frac{C_l}{\sum_{l'}(l')^{-3/2}C_{l'}}\right)\Big/\sum_{q\neq 0}\left(\frac{1}{\sum_{l'}(l')^{-3/2}C_{l'}}\right) \tag{16}$$

There are sixty four times to be included when summing over l' to obtain $\alpha(l)$ from Equation (16). Here

$$C_l = 1 - (1/2)\sum_j \cos(\mathbf{q}\cdot\mathbf{r}_{ij})_l. \tag{17}$$

The sum on the right hand side of Equation (17) again over all neighbours of i-th molecule which are separated from it by la. Computed results for $\alpha(l)$ are given in Table 2.

3. COMPUTATIONAL ASPECTS

The Monte Carlo calculations of the systems described in Sections 2.2 and 2.3 were performed using periodic boundary conditions and the Metropolis algorithm[9-13]. We considered a periodically repeated sample consisting of N particles. Starting from a perfectly ordered state, configurations were generated with a Boltzmann distribution in phase space, keeping the acceptance to rejection ratio of the Monte Carlo moves nearly equal to one.

TABLE 2

Variation of $\alpha(l)$ with l for interaction ranging upto 64 neighbours

$\alpha(1)$	$\alpha(2)$	$\alpha(3)$	$\alpha(4)$	$\alpha(5)$	$\alpha(6)$	$\alpha(7)$
0.9958	1.1401	1.2168	1.2602	1.2977	1.3208	1.3459
$\alpha(8)$	$\alpha(9)$	$\alpha(10)$	$\alpha(11)$	$\alpha(12)$	$\alpha(13)$	$\alpha(14)$
1.3608	1.3803	1.3910	1.4072	1.4155	1.4298	1.4364

Both the reduced energy and configurational specific heat were evaluated for both the cases. Reduced energy was evaluated as $U^* = -\langle u_{ij}\rangle/N\varepsilon$ for a particular reduced temperature $T^* = k_B T/\varepsilon$. The configurational specific heat was evaluated from fluctuations in internal energy as

$$C_V^* = C_V/N\,k_B = (\overline{U^2} - \bar{U}^2)/N(T^*)^2.$$

Calculations for both the short-range and long-range order parameters defined as the ensemble average of $T_2(\cos\theta_{ij})$ and $T_2(\cos\theta_i)$ respectively were carried out to characterize the short and long-range orientational order which might be exhibited by the system. Here θ_{ij} is the angle between the molecular symmetry axes and θ_i is the angle between the molecular axis and the so-called director. Since the orientation of the director is not known in advance and can change in the course of simulation, we had to follow a more elaborate procedure in order to compensate for the director fluctuations. Calculations are performed for each macrostep[13-15] and the traceless and symmetric second rank ordering tensor

$$Q_{ab} = 2\overline{l_a l_b} - \delta_{ab}$$

is taken, where, l_a is the direction cosine of the molecular symmetry axis with respect to the laboratory axis a. The bar indicates an average over a number of configurations which are sufficiently small, so that the director orientation does not change. The Q tensor is then diogonalised and the largest eigenvalue is the order parameter S_2 which is averaged over the production run.

For nearest neighbour interactions, all the calculations were performed with a sample of 256 particles. About 2×10^6 configurations were employed to equilibriate the system at a particular value of the reduced temperature. The various averages were then taken over a production run of typically 2×10^6 configurations. The same procedure was followed for the long-range interaction model with 512 particles and each particle was allowed to interact with 64 others on each side. Near the transition region about 5×10^6 runs were needed to reach equilibrium.

4. RESULTS AND DISCUSSIONS

Predictions for the model considered in the Section 2.2 are compared with the results of computer simulations as well as with exact solution[5,6]. The reduced energy is determined from the short-range order parameter $\sigma_2(1)$ [Eq. (8)]. It has already been argued that the theory is bound to be correct in the limit $T^* \to 0$, where the magnitude of U^* is determined in a simple fashion by the coordination number $z = 2$. Figure 1 shows that this expectation is fulfilled. But at high temperatures, as expected, disagreement with simulation results as well as with exact results is much pronounced. The agreement, which seems satisfactory except at high temperatures, is not surprising: it reflects a similar agreement which Faber[2] and Roy[4] have already demonstrated for several models.

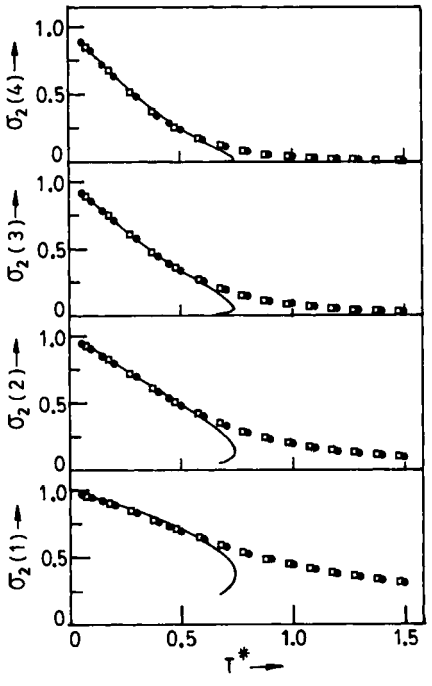

FIGURE 1 Variation of short-range order parameter as a function of temperature for the nearest neighbour interaction model; the smooth curves are the theoretical predictions, the solid circles represent the simulation results, and the squares are the data taken from Ref. 6.

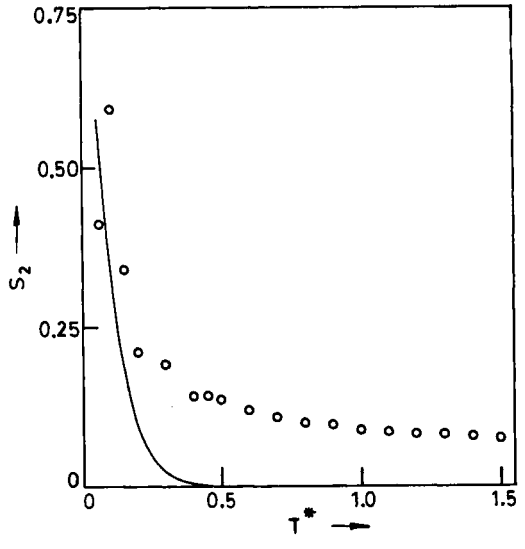

FIGURE 2 Variation of long-range order parameter with reduced temperature for the nearest neighbour interaction; the solid curve is the theoretical prediction; the circles represent simulation data.

The long-range order parameter S_2, calculated for various reduced temperatures, is plotted in Figure 2. For an ensemble of 256 particles, the simulation result for order parameter is found to be about 0.076 at $T^* = 1.5$. This is close to the value of $N^{-1/2}$ expected for a disordered system of finite size. As the temperature is lowered, S_2 increases until at $T^* = 0.2$ it is as large as 0.21 which indicates an orientationally ordered phase. The real system is known to remain disordered at all temperatures. As Denham *et al.*[7] have pointed out, we attribute this discrepancy to the small number of particles employed in the simulation. It is also apparent from Figure 1 that for reduced temperatures upto about 0.5 the theory correctly describes the temperature dependence of $\sigma_2(l)$ for $l = 1$ to 4. It may be noted that higher the value of l larger is the temperature range over which the agreement between predicted $\sigma_2(l)$ and the exact results[6] holds good. Table 3 shows that Faber's theory nearly correctly predicts the variation of $\sigma_2(l)$ with l at $T^* = 0.15$ and $T^* = 0.45$.

The results for the model considered in Section 2.3 are plotted in Figures 3 to 7. Similar procedures are followed in calculating the reduced energy, the specific heat and the order parameters. Since the interaction is long-range, the calculation of $\sigma_2(l)$ for $l > 1$ is also relevant here. The same behaviour was obtained for temperature dependences of reduced energy and order parameters as shown in Figures 3, 5 and 6. Those figures reflect a similar agreement with the analytical results described in Section 2.2. Figures 3 to 5 clearly indicate a disordering transition taking place close to the temperature $T^* = 1.6$ where the specific heat curve shows a peak. The computer simulation results of energy and order parameters show a continuous change across the transition. In Figure 4 we have also plotted C_V^* obtained from dU^*/dT^* using a least square fitting of the energy.

All the short-range correlation functions were found to decrease with increasing l and tend to saturate at a value dependent on the temperature [Fig. 7].

Our simulation results clearly differ from the results obtained by Romano[8] and in particular our transition temperature ($T_c^* = 1.6$) is significantly smaller than that obtained by Romano ($T_c^* = 2.16$). We attribute this disagreement to the range of

TABLE 3

Comparison for the variation of short-range order parameters $\sigma_2(l)$ with l for nearest neighbour interaction model. a) AT $T^* = 0.15$ and b) at $T^* = 0.45$

l	Exact results [Ref. 6]		Faber's theory		Similation results	
	a	*b*	*a*	*b*	*a*	*b*
1	0.922	0.731	0.922	0.738	0.922	0.730
2	0.849	0.534	0.851	0.547	0.849	0.533
3	0.783	0.391	0.786	0.406	0.781	0.387
4	0.721	0.286	0.727	0.303	0.719	0.282
5	0.665	0.209	0.672	0.225	0.660	0.205
6	0.613	0.153	0.622	0.169	0.606	0.149
7	0.565	0.112	0.576	0.126	0.557	0.108
8	0.520	0.082	0.534	0.095	0.511	0.078
9	0.479	0.059	0.495	0.072	0.469	0.055
10	0.442	0.044	0.459	0.054	0.430	0.039

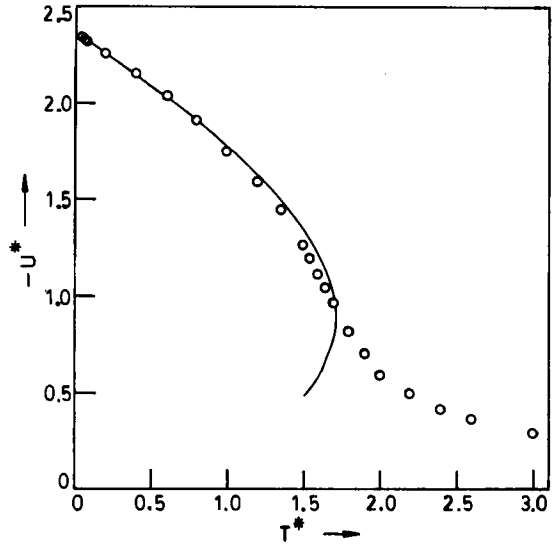

FIGURE 3 Variation of reduced energy per particle with reduced temperature for the long-range interaction model; the smooth curve represents the theoretical prediction and the circles represent simulation data.

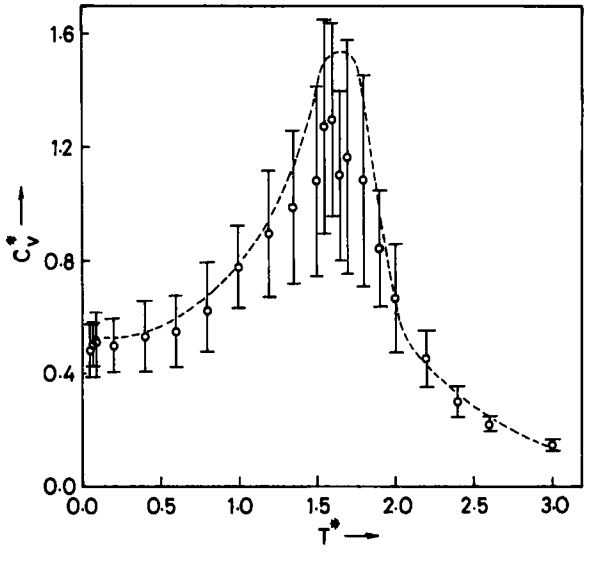

FIGURE 4 The specific heat $C_V^* = C_V/Nk_B$ versus reduced temperature T^* for long-range interaction model. The circles represent the simulation data. The dashed curve obtained by taking derivative of energy and least square fitting of simulation results.

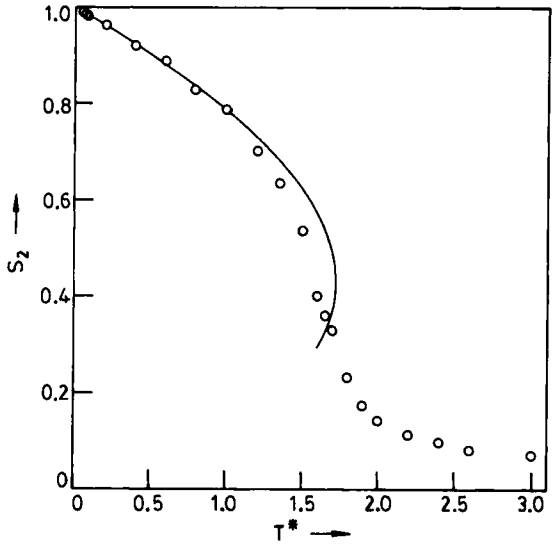

FIGURE 5 Variation of long-range order parameter with reduced temperature for long-range interaction model. The smooth curve is the theoretical prediction and the circles are the data taken from the simulation experiment.

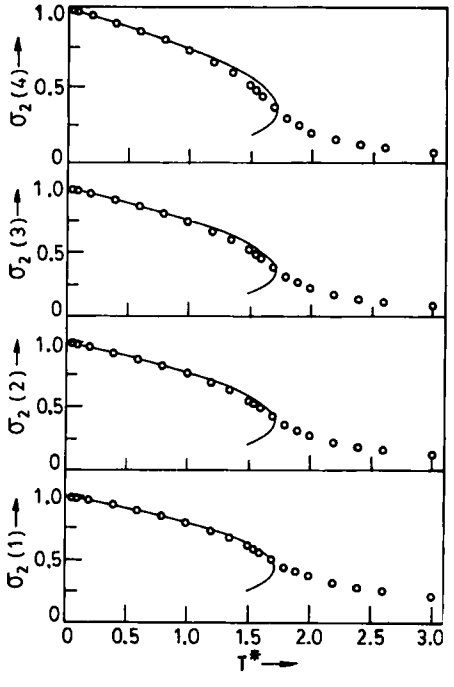

FIGURE 6 Variation of short-range order parameter with reduced temperature for long-range interaction model. The solid curve is the theoretical prediction and the circles are simulation data.

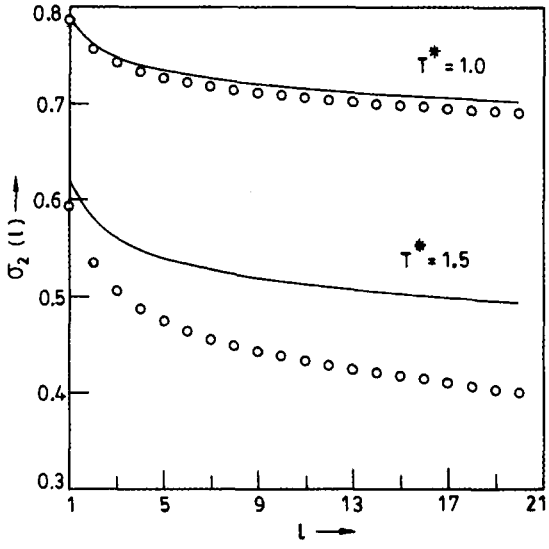

FIGURE 7 Variation of short-range order parameter $\sigma_2(l)$ with l at $T^* = 1.0$ and $T^* = 1.5$; the solid curves are the theoretical predictions and the circles are simulation data.

TABLE 4

Comparison of various parameters obtained by computer simulation for interaction ranging a) upto 64 neighbours, (b) upto 256 neighbours, (c) upto 512 neighbours and (d) data taken from Ref. 8

T^*		U^*	S_2	C_V
	(a)	−1.11	0.40	1.30
	(b)	−1.33	0.65	1.23
1.6	(c)	−1.38	0.67	1.10
	(d)	−1.52	0.68	1.17
	(a)	−0.51	0.12	0.49
	(b)	−0.54	0.17	0.62
2.16	(c)	−0.55	0.18	0.67
	(d)	−0.58	0.20	—

interaction assumed. The transition temperature would be shifted towards a higher value if the interaction was taken with a larger number of neighbours as Romano did.[8] To test the conjecture we have performed simulations at $T^* = 1.6$ and 2.16 with interactions ranging upto 64, 256 and 512 neighbours and in Table 4 the results are displayed and compared with those of Ref. 8. The results clearly support our surmise.

In Table 5 we have depicted the changes in the values of various parameters with the range of interaction, as predicted by Faber's theory, within its range of validity. As is evident from the Table, this theory too points towards our conjecture that an increase

TABLE 5

Comparison of various parameters obtained from Faber's theory for interaction ranging a) upto 64 neighbours, b) upto 128 neighbours, c) upto 256 neighbours, d) upto 512 neighbours and e) data taken from Ref. 8

T^*		U^*	S_2	$\sigma_2(1)$
	(a)	− 2.098	0.904	0.904
	(b)	− 2.171	0.923	0.907
0.5	(c)	− 2.223	0.931	0.909
	(d)	− 2.259	0.933	0.910
	(a)	− 1.785	0.787	0.788
	(b)	− 1.862	0.830	0.795
1.0	(c)	− 1.916	0.846	0.800
	(d)	− 1.954	0.852	0.803
	(a)	− 1.354	0.621	0.622
	(b)	− 1.448	0.697	0.641
1.5	(c)	− 1.512	0.726	0.653
	(d)	− 1.557	0.739	0.661
	(e)	− 1.611	0.704	—

in the number of interacting neighbours helps to increase the magnitude of the internal energy and both long-range and short-range orders.

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References

1. T. E. Faber, *Proc. Roy. Soc.* **A 353**, 247 (1977); *Proc. Roy. Soc.* **A 353**, 261 (1977).
2. T. E. Faber, *Proc. Roy. Soc.* **A 370**, 509 (1980); *Proc. Roy. Soc.* **A 396**, 357 (1984).
3. P. A. Lebwohl and G. Lasher, *Phys. Rev.* **A 6**, 426 (1972).
4. S. K. Roy, *Mol. Cryst. Liq. Cryst.* **133**, 297 (1986).
5. B. C. Freasier and L. K. Runnels, *J. Chem. Phys.* **58**, 2963 (1973).
6. P. A. Vuillermot and M. V. Romerio, *J. Phys.* **C 6**, 2922 (1973).
7. J. Y. Denham, R. L. Humphries and G. R. Luckhurst, *Mol. Cryst. Liq. Cryst.* **41**, 67 (1977).
8. S. Romano, *Liq. Crystals* **3**, 1215 (1988).
9. C. Zannoni, *The Molecular Physics of Liquid Crystals*, Eds. G. R. Luckhurst and G. W. Gray, Academic, New York, (1979), Chap 9.
10. G. P. Landau, *Applications of the Monte Carlo Method in Statistical Physics*, Ed. K.Binder, Springer, Berlin, (1984), Chap. 3.
11. K. Binder, *Monte Carlo Method in Statistical Physics*, Ed. K. Binder, Springer, Berlin, (1979), Chap. 1.
12. O. G. Mouritsen, *Computer Studies of Phase Transitions and Critical Phenomena*, Springer, Berlin, (1984).
13. K. Binder, *J. Comput. Phys.* **59**, 1 (1985).
14. C. Zannoni, *The Molecular Physics of Liquid Crystals*, Eds. G. R. Luckhurst and G. W. Gray, Academic, New York, (1979), Chap. 3.
15. U. Fabbri and C. Zannoni, *Mol. Phys.* **58**, 763 (1986); S. Romano, *Nuovo Cim.* **D 9**, 409 (1987).