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Study of an anisotropic lattice model with interactions of rank higher than four

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We have considered a classical system, consisting of cylindrically symmetric particles, associated with a three-dimensional, simple cubic lattice, and interacting via nearest neighbour pair potentials of the form

$$W = W_{jk} = -\varepsilon P_L(\mathbf{u}_j \cdot \mathbf{u}_k), \quad L = 6, 8;$$

here P_L is a Legendre polynomial of order L , ε is a positive constant setting the temperature and energy scales, and \mathbf{u}_j and \mathbf{u}_k denote the unit vectors defining particle orientations. These potential models have been studied previously in the literature by means of molecular field theory; we report here two-site cluster results for $L = 6, 8$ and Monte Carlo simulation results for $L = 6$. Comparison shows that the two-site cluster approximation produces an overall qualitative improvement over molecular field theory.

1. Introduction

When developing the statistical mechanical formalism for mesogenic systems, one often starts from some simple and somehow reasonable functional form of the pair potential, since the pair potential in a real system is usually unknown; as additional simplifications, particles are usually assumed to be rigid and often to possess cylindrical symmetry. In addition to this approach, which has proved to be quite fruitful, in the last few years another line of research has emerged, i.e. the production of realistic potential models for specific molecules (including atom–atom interactions and intramolecular terms), and their usage in simulation studies [1–4], although, at present, at heavy computational costs.

A few classes of potential models have proved to be mathematically and computationally tractable, possibly at various levels of approximation (sometimes at the cost of drastic simplifications) and yet capable of reproducing at least salient features of mesophasic behaviour: these are lattice models, hard non-spherical bodies (see, for example, [5–13]), and the potential model proposed by Gay and Berne [14], also extensively used in simulation studies (see, for example [15–17]). Lattice models (which are more easily tractable) have mostly been used for nematogens only, whereas the other two kinds of model can produce a rich variety of structural behaviour [9, 11, 12, 14–17]. Among lattice models, the nearest-neighbour potential defined by

$$W = W_{jk} = -\varepsilon P_2(\cos \gamma), \quad \cos \gamma = \mathbf{u}_j \cdot \mathbf{u}_k, \quad \varepsilon > 0, \quad (1)$$

was proposed by Lebwohl and Lasher some 20 years ago [18, 19], and since then it has been extensively studied; here P_2 is a second order Legendre polynomial, \mathbf{u}_j and \mathbf{u}_k

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denote three-component unit vectors defining particle orientations, and ε is a positive quantity setting both energy and temperature scales (i.e. $T^* = k_B T/\varepsilon$). The underlying lattice is considered to be a three-dimensional, usually simple-cubic, one.

The system is rigorously known to possess an orientational ordering transition at finite temperature [20], and has been extensively studied using computer simulation (for example, [21–24]) and a number of other theoretical techniques [25–28]; the transition has a weak first order character, and the transition temperature is estimated to be $T_c^* = 1.1232$, with an uncertainty of the order of 0.0001 [23, 24]. Extensions of the Lebwohl–Lasher model to higher-rank interactions of the form

$$W = W_{jk} = -\varepsilon P_L(\cos \gamma), \quad L = 4, 6, 8, \quad (2)$$

have been proposed and studied using the molecular field (MF) approximation [29] and, for $L = 4$, also by two-site cluster (TSC) theory and Monte Carlo simulation (MC) [30]. Moreover, both MF [31] and MC [32] results indicate that, using a potential model defined by a linear combination of a predominant P_2 and a minor P_4 term, one can modulate (both strengthen or weaken) the first order character of the transition by a suitable choice of the parameters: for example, the order parameter \bar{P}_2 at the transition may be made to range between 0.3 and 0.6 [31]. As for the potential models in equation (2), MF results indicate that, upon increasing L , the transition temperature is reduced, whereas transition entropy and order parameters at the transition increase, i.e. the first-order character of the transition is strengthened. This trend can be qualitatively understood [29] by recalling that, in MF theory, the single particle pseudo-potential is proportional to an even L th rank Legendre polynomial $P_L(t)$, ($t = \cos \theta$, where θ is the angle between the individual molecule and the director), and thus it possesses $(L + 2)/2$ minima over the argument range $[0, \pi]$; as L increases, the potential well corresponding to $t = \pm 1$ deepens and narrows. For the system, it becomes more and more difficult to order along the director because of the existence of these local minima, but, on the other hand, when it does eventually order, it suddenly goes to a situation of nearly complete alignment [29]. For each potential model, MF theory yields orientational order parameters of various even orders \bar{P}_M , and, for the P_4 model, it predicts the existence of a temperature range where $\bar{P}_4 > \bar{P}_2$ [29], as can be understood by recalling that $P_2(0) = -(1/2)$, $P_4(0) = +(3/8)$, i.e. mutual orthogonal orientation of two particles (and hence orthogonal orientation of a single particle with respect to the director) can be energetically favoured, but gives a negative contribution to \bar{P}_2 ; this prediction was confirmed by TSC and MC results [30]. For the P_4 model, MF theory predicts $T_c^* = 0.751$, versus a TSC result of 0.663, and a MC estimate of 0.645 ± 0.005 [29, 30]. Purely sixth- and eighth-rank models produce sizeable order parameters at transition (see [29]), in marked contrast to the behaviour found for usual thermotropic nematics and for pure P_2 or P_4 models, where \bar{P}_2 ranges between 0.3 and 0.5 [23, 24, 30]. The present paper reports TSC calculations for the sixth- and eighth-rank models, and MC results for $L = 6$.

2. Molecular field and two site cluster treatment

The MF treatment [31, 33] can be developed for an arbitrary pair potential [34], and for the models defined by equation (2) it gives [29, 31] the following expression for the difference in free energy per particle between ordered and isotropic phases:

$$\beta A_1^* = (c/2)\beta b_1^2 - \log Z + \log 2, \quad (3)$$

$$Z = Z_1 = \int_0^\pi E_L(\theta) \sin \theta d\theta = \int_{-1}^{+1} \exp(c\beta b_L P_L(t)) dt, \tag{4}$$

$$E_L(\theta) = \exp(c\beta b_L P_L(\cos \theta)). \tag{5}$$

Here $A^* = A/\varepsilon$, $\beta = 1/T^*$, c is the lattice coordination number ($c = 6$ in our case), and $Z = Z_1$ is the single-particle pseudo-partition function; minimization of the free energy with respect to the variational parameter b_L gives $b_L = \langle P_L \rangle_Z$, i.e.

$$b_L = \frac{\int_{-1}^{+1} P_L(t) \exp(c\beta b_L P_L(t)) dt}{Z}, \tag{6}$$

after solving the consistency equation, energy, specific heat, and orientational order parameters can be calculated, and the transition can be identified [29].

The molecular field treatment can be refined by using various cluster-variational techniques [25, 26, 35–37], whereby interactions within a finite cluster are treated exactly, and those with the rest of the system are accounted for in some molecular field way, according to different possible procedures; such approaches were first developed for magnetic systems [35–37], and later applied to nematics (for example, [25, 26]). For the potential model defined by equation (2), the approximate free energy per article at the two-site cluster level is given by [30]

$$\beta A_2^* = -(c/2) \ln \zeta + (c-1) \ln Z, \tag{7}$$

where $\zeta = \zeta_{12}$ is the two-particle pseudo-partition function

$$\zeta = \int d\Omega_1 d\Omega_2 \exp[\beta b_L (c-1)(P_L(\cos \theta_1) + P_L(\cos \theta_2)) + \beta P_L(\cos \gamma)], \tag{8}$$

and $d\Omega_j = \sin \theta_j d\theta_j d\phi_j$. The condition of minimum free energy with respect to b_L gives the consistency requirement

$$\langle P_L \rangle_Z = (1/2) \langle [P_L(\cos \theta_1) + P_L(\cos \theta_2)] \rangle_\zeta. \tag{9}$$

After solving for b_L , various thermodynamic quantities can be obtained from the free energy; for example, the energy per particle is obtained by differentiating the free energy with respect to β and reads

$$U^* = -(c/2) \sigma_L; \quad \sigma_L = \langle P_L(\cos \gamma) \rangle_\zeta, \tag{10}$$

where the short range order parameter σ_L is equal to the appropriate orientational correlation function at nearest neighbour separation; it is also possible to calculate various other short range order parameters σ_M , even M . The expression for the TSC heat capacity is obtained by differentiating the energy with respect to temperature, and can be found in [30]; alternatively (and as a valuable check) the specific heat can be obtained from the energy by numerical differentiation.

After solving the consistency equation, one finds a transition where b_L goes discontinuously to zero, producing a finite jump in energy, specific heat and long range order parameters, defined in this context by

$$\bar{P}_M = \frac{1}{2} \langle [P_M(\cos \theta_1) + P_M(\cos \theta_2)] \rangle_\zeta, \quad \text{even } M. \tag{11}$$

At each temperature, the value of b_L which minimizes the free energy was determined numerically, by means of computer routines of the NAG library, which actually took into account both the function (equation (7)) and its derivative (equation (9)); for each

value of b_L examined, and after an appropriate transformation, calculation of ζ requires an integration over three variables, which was carried out using a 32-point gaussian formula for each dimension.

3. Simulation aspects

Simulations were carried out on a cubic lattice, using periodic boundary conditions, and different sample sizes ($N = n^3$, $n = 8, 10, 12$). Calculations were carried out in cascade, in order of increasing temperature, i.e. at each temperature the final configuration of the equilibration run 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 25 000 and 50 000 cycles (where one cycle or sweep corresponds to N attempted moves), and production runs took between 50 000 and 100 000; sub averages for evaluating statistical errors were calculated over macro-steps consisting of 1000 cycles. Calculated quantities include potential energy, and configurational heat capacity from potential energy results, by polynomial least-square fit and analytical differentiation of the interpolating function; the statistical errors in the specific heat were estimated using the simulation procedure outlined in [30]. We also evaluated long range order parameters of various ranks, \bar{P}_L , $L = 2, 4, 6, 8$; orientational correlation functions (OCF) and singlet orientational functions (SODF) were calculated at selected temperatures. Long range order parameters are defined by [38]

$$\bar{P}_L = \langle P_L(\cos \theta) \rangle \quad (12)$$

where θ is the angle between the individual molecule and the director. Since the system is highly ordered, quantities such as \bar{P}_6 and \bar{P}_8 had to be calculated, and were obtained in the following way: along the MC chain we calculated both the second-rank tensor

$$Q_{\lambda\mu} = (3\langle u_\lambda u_\mu \rangle_{\text{loc}} - \delta_{\lambda\mu})/2 \quad (13)$$

and its fourth rank counterpart [23, 30, 39]; here the subscript loc refers to the current configuration; these quantities were accumulated to give macro-step averages, then used to calculate \bar{P}_2 and \bar{P}_4 , as discussed elsewhere [23, 30, 39, 40]. Moreover, for every sweep we diagonalized the current second-rank ordering tensor, and defined the instantaneous director \mathbf{v} by the eigenvector associated with the eigenvalue possessing the largest magnitude; we then calculated the quantities $\langle P_L(\mathbf{u} \cdot \mathbf{v}) \rangle_{\text{loc}}$ and averaged them. Both for \bar{P}_2 and \bar{P}_4 , estimates obtained according to the two procedures were found to agree to within the statistical uncertainties. Since its director is known, the analysed configuration can also be used to calculate the SODF [38–40]; owing to the underlying symmetry, this quantity is an even function of $\cos \theta$, and the angle can be restricted between 0 and $\pi/2$; the SODF can thus be expanded as

$$S(\theta) = \frac{1}{2} \left[1 + \sum_{m \geq 0} (4m+1) \bar{P}_{2m} P_{2m}(\cos \theta) \right], \quad (14)$$

or

$$\log S(\theta) = \sum_{m \geq 0} h_{2m}(\cos \theta); \quad (15)$$

we produced a 1001 bin histogram of $S(\theta)$ versus $\cos \theta$, from which coefficients \bar{P}_{2m} and h_{2m} were calculated; as a double check, they were also recalculated by a linear least square fit.

Oriental correlation functions [38, 39] are defined by

$$G_L(r) = \langle P_L(\mathbf{u}_j \cdot \mathbf{u}_k) \rangle, \quad \text{as functions of } r = |\mathbf{x}_j - \mathbf{x}_k|, \quad L = 2, 4, 6, 8, \quad (16)$$

where x_k are the dimensionless coordinates of the lattice sites; their values at nearest neighbour separation define the short range order parameters, i.e. $\sigma_L = G_L(1)$. These quantities were calculated at selected temperature, by analysing one configuration every two sweeps; their plots (see following figures) showed a rapid decay to a limiting value consistent with the corresponding order parameter, i.e.

$$\lim_{r \rightarrow \infty} G_L(r) = \bar{P}_L^2. \quad (17)$$

4. Results

MC results obtained with different sample sizes were found to agree with each other, to within the combined statistical uncertainties. Simulation results for potential energy, configurational specific heat and order parameters are plotted in figures 1 to 3, where they are compared with TSC predictions, and show evidence of a strong first-order transition; the transitional properties are summarized in the table. As for the transition temperature and the associated entropy change, there is an ordered phase up to $T_1^* = 0.545$ and a disordered one at $T_2^* \geq 0.550$, and we use U_1^* and U_2^* to denote the corresponding energies. We thus defined $T_c^* = 0.5(T_1^* + T_2^*) \pm 0.5(T_2^* - T_1^*)$, and

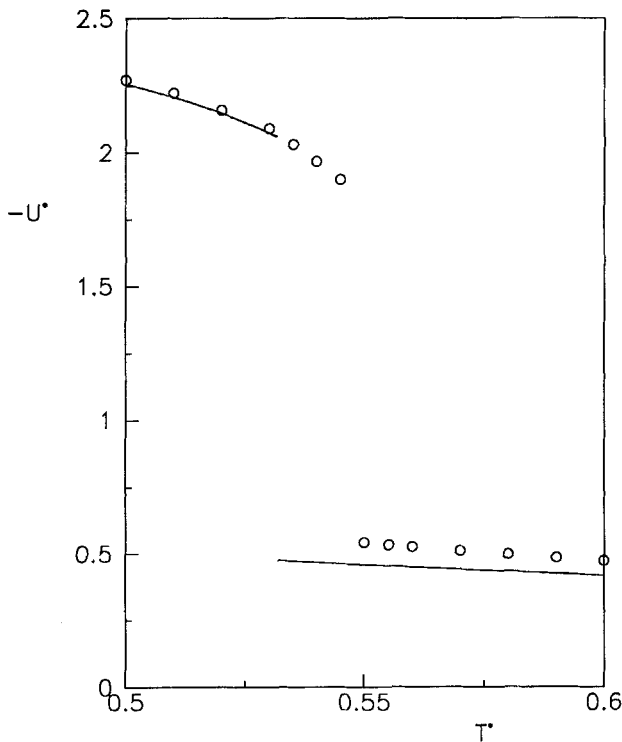


Figure 1. Potential energy: (a) (circles): MC estimates; (b) (continuous line): TSC results; the relative statistical errors on MC estimates are usually smaller than 0.5 per cent.

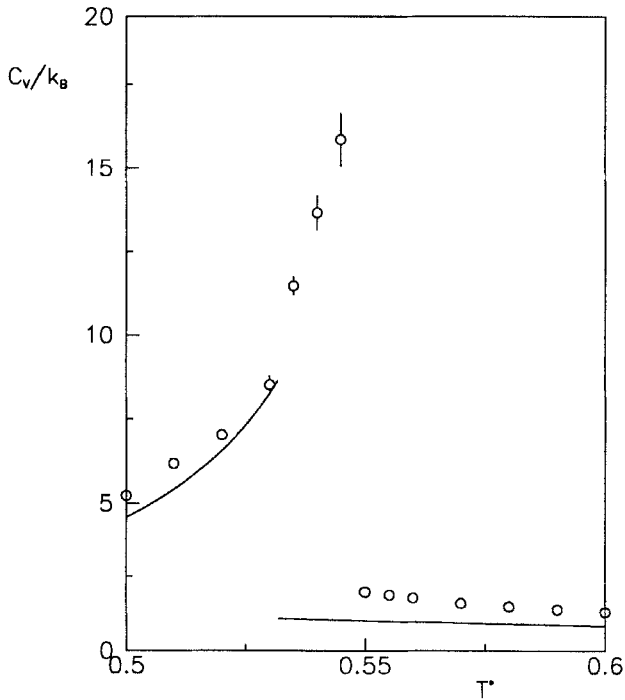


Figure 2. Configurational specific heat; same meaning of symbols as in the previous figure.

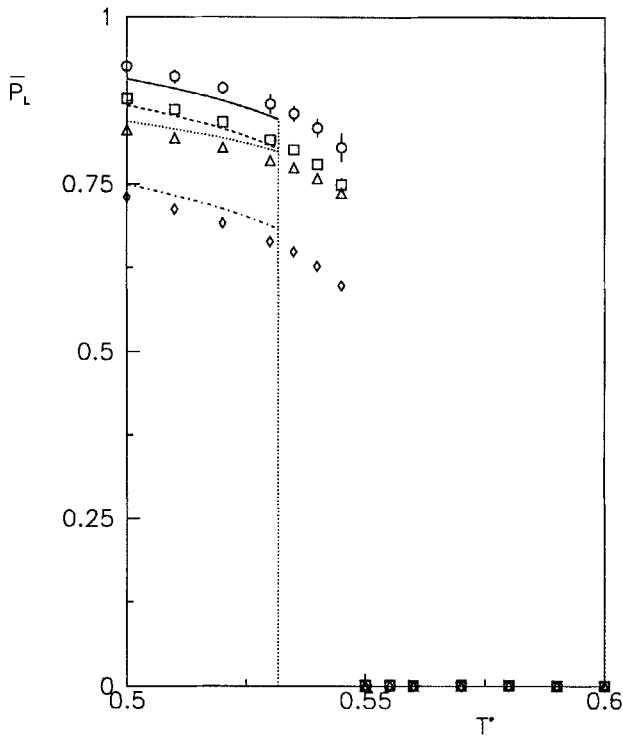


Figure 3. Results for the long range order parameters: (a) (circles): \bar{P}_2 , MC estimates; (b) (squares): \bar{P}_4 , MC estimates; (c) (triangles): \bar{P}_6 , MC estimates; (d) (diamonds): \bar{P}_8 , MC estimates; (e) (continuous line): \bar{P}_2 , TSC results; (f) (dashed line): \bar{P}_4 , TSC results; (g) (dotted line): \bar{P}_6 , TSC results; (h) (dashed-dotted line): \bar{P}_8 , TSC results.

Results for transition temperature, order parameters and entropy variation at the transition, obtained by MF and TSC treatments, together with their MC estimates and associated error bars; MF results were taken from [29].

L		T_c^*	\bar{P}_2	\bar{P}_4	\bar{P}_6	\bar{P}_8	$\Delta S_c/k_B$
6	MF	0.581	0.825	0.781	0.786	0.664	3.187
6	TSC	0.532	0.847	0.804	0.799	0.683	2.980
6	MC	0.548	0.81	0.75	0.737	0.598	2.48
	err.	0.003	0.02	0.01	0.006	0.006	0.09
8	MF	0.508	0.926	0.899	0.872	0.854	4.311
8	TSC	0.464	0.861	0.824	0.794	0.791	3.527

$\Delta U_c^* = (U_2^* - U_1^*)$, $\Delta S_c/k_B = \Delta U_c^*/T_c^*$; the value found for $\Delta S_c/k_B$ had an associated statistical error of ± 0.03 , which we conservatively trebled (as a very crude estimate, assuming a specific heat $C_v/k_B \approx 20$ in the ordered region $T_1^* < T^* < T_c^*$, the uncertainty on the transition temperature could produce an additional uncertainty on ΔU_c^* as large as 0.1).

In contrast to other potential models (for example, [30]), we observed a pronounced hysteresis: the final configuration of the equilibration run at T_2^* was used as starting point for simulation at T_1^* , and after 400 000 cycles, the system was still found to be in the disordered phase; we lowered the temperature to $T^* = 0.540$, ran simulation for further 400 000 macro-steps, and still failed to restore orientational order.

Comparison between MF and TSC treatments (see the table) shows that the TSC correction lowers both transition temperature and transition entropy; for $L=6$, it produces an increase of order parameters at transition, whereas it decreases them for $L=8$. Comparison with simulation results shows that the TSC treatment underestimates the transition temperature by 3 per cent, whereas MF overestimates it by 5 per cent; both approaches overestimate entropy and order parameters at the transition, but TSC treatment changes ΔS_c in the right direction, and, on the whole, produces a qualitative improvement over the MF approach.

MF, TSC and MC results predict that order parameters \bar{P}_L at the transition decrease with increasing L , in contrast to with the fourth-rank model [29, 30]. TSC results for the short range order parameters σ_L are reported in figure 4; orientational correlation functions were calculated at two typical temperatures T_1^* and T_2^* , i.e. just below and just above the transition, and are plotted in figures 5 and 6. Both TSC and MC results show that, in the ordered region the sequence of short range order parameters is $\sigma_2 > \sigma_4 \gtrsim \sigma_6 > \sigma_8$ and parallels the sequence at their long range counterparts; in the disordered phase this becomes $\sigma_6 > \sigma_2 > \sigma_4 > \sigma_8$. Here TSC underestimates σ_6 by roughly 15 per cent, and other short range order parameters by as much as 30 per cent; G_6 correlation survives over a few lattice separations. Values of σ_L were also calculated for the P_8 model, and exhibited a similar behaviour: in the ordered region, the sequence of short range order parameters was $\sigma_2 > \sigma_4 > \sigma_6 \gtrsim \sigma_8$, again the same as for their long range counterparts, and became $\sigma_8 > \sigma_2 > \sigma_4 > \sigma_6$ above the transition temperature: in the disordered phase, the predominance of σ_6 or σ_8 , respectively, can be expected from the form of the two-particle pseudo partition function (see equations (7) to (10)).

Since the system was highly ordered, we also tried to calculate the order parameters using the single parameter (gaussian) approximation described in [41], but is turned

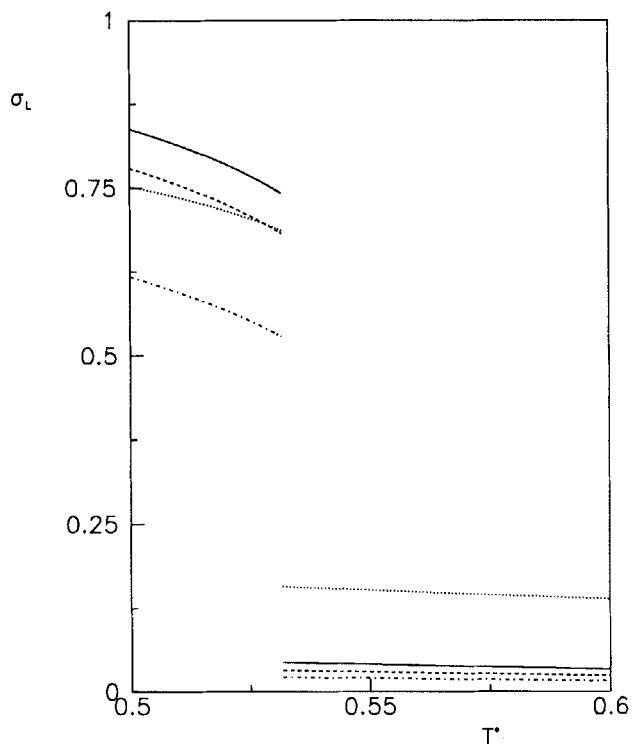


Figure 4. TSC results for the short range order parameters of the P_6 model: (a) (continuous line): σ_2 ; (b) (dashed line): σ_4 ; (c) (dotted line): σ_6 ; (d) (dashed-dotted line): σ_8 .

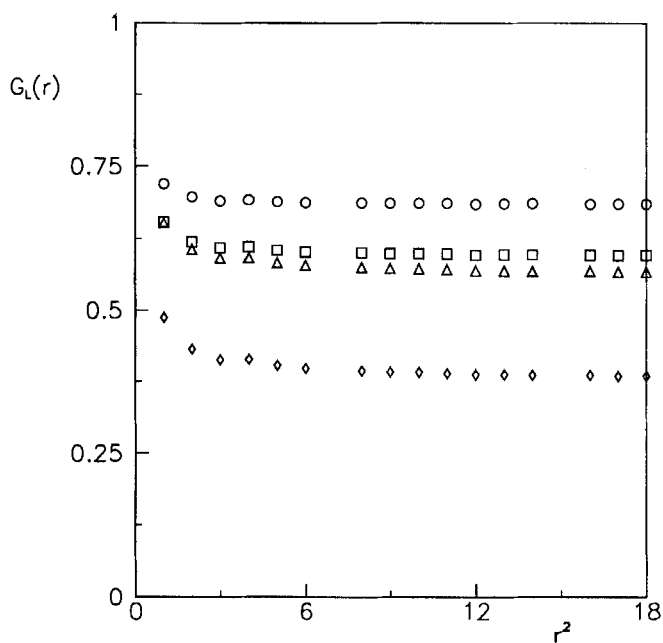


Figure 5. Orientational correlation functions calculated at $T^* = 0.545$: (a) (circles): $G_2(r)$; (b) (squares): $G_4(r)$; (c) (triangles): $G_6(r)$; (d) (diamonds): $G_8(r)$.

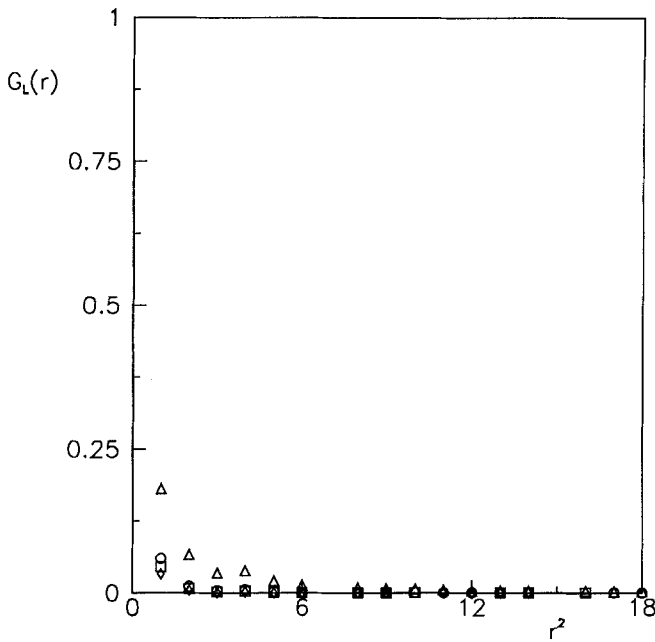


Figure 6. Orientational correlation functions calculated at $T^*=0.550$; same meaning of symbols as in the previous figure.

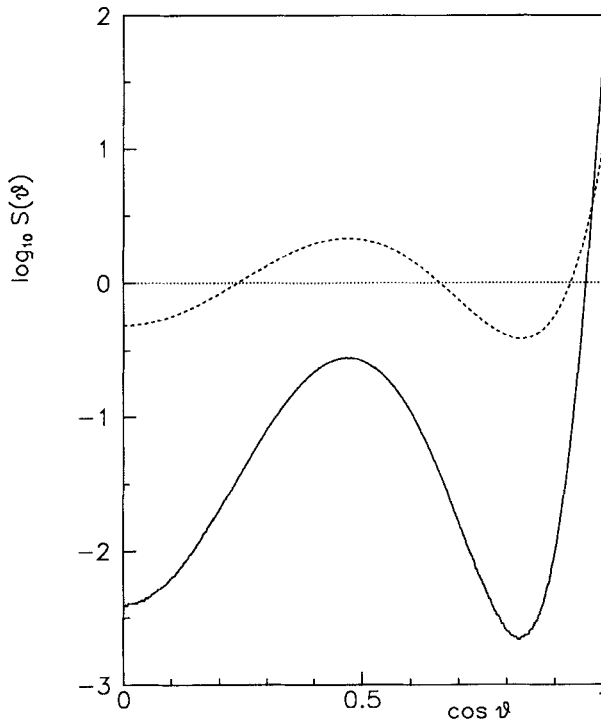


Figure 7. Plots of $\log_{10}S(\theta)$ (continuous line) and $P_6(\cos \theta)$ (dashed line) versus $\cos \theta$; the SODF was calculated at $T^*=0.545$.

out that, whether for MF, TSC or MC results at transitions, no single parameter could simultaneously fit their four values.

The SODF was calculated at T_1^* , and is shown in figure 7, together with $P_6(\cos \theta)$ (we chose to plot $\log_{10} S(\theta)$ for better visualization); comparison indicates that maxima and minima of the two curves fall at the same abscissae, and thus suggests that the h_6 term in equation (15) is predominant (in the MF treatment defined by equation (3) to (6), only $h_6 = b_6$ is different from zero, and h_0 accounts for the normalization factor). This was confirmed by the coefficients h_{2m} and \bar{P}_{2m} in the expansion of $S(\theta)$ (see equation (14) and (15)), calculated up to $m = 10$: h_6 was found to dominate over all others (apart from h_0) by a factor as large as one hundred, and the order parameters showed a slow decrease with increasing m (for example, $\bar{P}_{10} = 0.52$ and $\bar{P}_{20} = 0.14$); on the other hand, the quantities h_{2m} did not show a monotonic trend with increasing m ; the least square approximation to $\log S(\theta)$ obtained by truncating the expansion at $m = 10$ was found to be virtually indistinguishable from the original histogram. The sizeable orientational order at the transition is reflected by its strong first order character and by the observed hysteresis.

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