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Computer simulation study of plane rotators on a three dimensional lattice

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We have considered a classical system, consisting of two component unit vectors (plane rotators) associated with a three dimensional, simple cubic lattice, and interacting via the nearest neighbour pair potential

$$W_m = c\varepsilon \cos(m(\phi_j - \phi_k)), c = \pm 1,$$

where m is a positive integer, ε is a positive constant setting the temperature and energy scales, and $\{\phi_k\}$ are the angles defining the orientation of the plane rotators in an arbitrary reference frame (which can be identified with the lattice frame). The two potential models W_m and $-W_m$ possess essentially the same properties in the absence of an external field (spin-flip symmetry); moreover, all of the potential models W_m have the same partition function, and several mean values can be defined in a way which is independent of m . This model is known rigorously to possess a low temperature ordering transition, extensively simulated in the magnetic language ($m=1$); we examined here the nematic interpretation ($c=-1, m=2$), and compare with molecular field and two site cluster predictions; we have also investigated director fluctuations.

1. Introduction

This paper reports computer simulation results for a certain classical lattice spin system already extensively studied in the literature as a magnetic model; because of the underlying symmetry, it can also, and equally well, be interpreted and investigated as a nematogenic lattice model, i.e. the plane rotator counterpart of the well-known Lebwohl-Lasher model. We consider here a system consisting of two component unit vectors (planar rotators) $\{\mathbf{u}_k\}$ associated with a d dimensional lattice Z^d ; let \mathbf{x}_k denote their coordinates, and let U_{jk} be their translationally invariant pair potential, restricted to nearest neighbours, and having the general form, anisotropic in spin space

$$U = U_{jk} = c\varepsilon(au_{j,1}u_{k,1} + bu_{j,2}u_{k,2}), \quad (1)$$

$$\varepsilon > 0, c = \pm 1, a \geq |b|. \quad (2)$$

Here ε is a quantity setting the energy and temperature scales (i.e. $T^* = k_B T/\varepsilon$), and $u_{j,\lambda}$ denote the cartesian components of the unit vectors, which can be expressed in terms of polar angles $\{\phi_k\}$; when $a=b$ the interaction is isotropic in spin space. Without any loss of generality, the reference axes in spin space can be identified with lattice axes. There exist two important symmetry properties for potential models of this kind.

- (i) Spin-flip symmetry for a bipartite lattice: for any \mathbf{x}_k , a site parity $\sigma_k = \pm 1$ can be defined, depending on the sum of its d coordinates being even or odd; the lattice consists of two disjoint (even and odd) sublattices, and each node is surrounded by nearest neighbours belonging to the other sublattice, then next nearest neighbours belonging to its own, and so on. In the absence of an external field,

the two potential models defined by $c = -1$ and $c = +1$, respectively, have the same partition function and essentially the same structural properties.

- (ii) We rewrite the pair potential in the slightly more general form

$$W_m = \varepsilon(a \cos(m\phi_j) \cos(m\phi_k) + b \sin(m\phi_j) \sin(m\phi_k)), \quad \forall m \geq 1, \quad (3)$$

where m is an arbitrary positive integer; it can easily be checked that [1, 2], for given values of a and b , all of the potential models W_m give the same partition function, and also structural properties can be defined in a way which is independent of m , and actually calculated using any convenient choice.

There are, in addition, a number of rigorous results connecting dimensionality, anisotropy, and existence or absence of an ordering transition [3, 4] for such systems. Thus when $d = 1$, the system is known to disorder at all finite temperatures; when $d = 2$ and $a \neq b$ an ordering transition is known to exist [3], whereas the system disorders at all finite temperatures in the isotropic case $a = b$, but possesses a transition to a low temperature phase with slow decay of correlations and infinite susceptibility (Kosterlitz–Thouless transition [4]); when $d = 3$, even the isotropic model can produce an ordering transition [3]. The nematic counterpart of the Kosterlitz–Thouless transition in two dimensions has also been investigated by renormalization group theory [5] and by simulation [6].

On a bipartite lattice, the interaction potential (and hence the ordered phase) can thus be interpreted in various ways, for example as ferro- or antiferromagnetic ($m = 1$), nematic or antinematic ($m = 2$); we consider the isotropic case on a three dimensional cubic lattice, extensively studied [7–12] in the (ferro)magnetic interpretation, and report here Monte Carlo simulation results for the nematic interpretation; the potential model which we have actually simulated is therefore

$$U = U_{jk} = -\varepsilon \cos(2(\phi_j - \phi_k)). \quad (4)$$

In order to clarify and qualify the relevance of eqn. (4) as an extreme nematogenic model, let us consider a system consisting of three component unit vectors associated with a three dimensional (or, in general, d dimensional lattice) and interacting via the hamiltonian (Lebwohl–Lasher model in an external field)

$$H = -\varepsilon \sum_{(j < k)} P_2(\mathbf{u}_j \cdot \mathbf{u}_k) + G \sum_k P_2(\cos \theta_k), \quad (5)$$

where $\sum_{(j < k)}$ is restricted to nearest neighbouring pairs, and $\{\theta_k, \phi_k\}$ denote the polar angles defining the orientations of the unit vectors; the quantity G has the form $G = -F^2 \Delta\chi$, where F is an electric or magnetic field, and $\Delta\chi$ is the anisotropy of the corresponding polarizability or susceptibility tensor. The system has been extensively studied by mean field theory (see, for example, [13, 14]), and in some cases by simulation [15, 16]; it is predicted to exhibit critical points, both for $G < 0$ and $G > 0$, although for values of the external field which appear to be unmeasurably large. In the limit $G \rightarrow +\infty$, we effectively have $\sin \theta_k = 1, \forall k$, and the right hand side of equation (5) reduces to $(1/4) \sum_{(j < k)} (3U_{jk} - 1)$, i.e. to the pair potential in equation (4), apart from a numerical factor.

2. Computer simulations

Calculations were carried out on a cubic lattice, using periodic boundary conditions, and different sample sizes ($N = n^3, n = 12, 14, 16$). Equilibration runs took

5000 cycles (where one cycle or sweep corresponds to N attempted moves), and production runs took between 10 000 and 25 000; subaverages for calculating statistical errors were calculated over macrosteps consisting of 250 cycles. Calculated quantities include the potential energy, configurational heat capacity, second and fourth rank ordering tensor and associated order parameters (\bar{T}_2 and \bar{T}_4); orientational correlation functions and singlet orientational distribution function were calculated at selected temperatures. We also investigated director fluctuations, as explained later; director pinning has been reported in the literature for some cases [17–19], and significant fluctuations were observed in others [19].

The second and fourth rank order parameters \bar{T}_2 and \bar{T}_4 are defined by [6]

$$\bar{T}_2 = \langle \cos(2\theta) \rangle, \quad \bar{T}_4 = \langle \cos(4\theta) \rangle, \quad (6)$$

where θ is the angle between the individual molecule and the director, and were calculated as discussed in detail elsewhere [6, 20–22]; we recall there that, for each macrostep, we calculated both the second rank tensor

$$Q_{\lambda\mu} = 2\langle u_\lambda u_\mu \rangle - \delta_{\lambda\mu} \quad (7)$$

and its fourth rank counterpart; $Q_{\lambda\mu}$ is then diagonalized to obtain its eigenvalues $\{q_1, q_2\}$, where $q_1 + q_2 = 0$, and eigenvectors $\{\mathbf{v}_1, \mathbf{v}_2\}$. Let now $q_3 = |q_1|$, let $\bar{q}_1, \bar{q}_2, \bar{q}_3$ denote their averages over all macrosteps, and let $\bar{q}_4 = |\bar{q}_1|$; for each macrostep j the eigenvector ω_j associated with the positive eigenvalue defines the director orientation in the laboratory frame. In the ordered region, the orientation of ω_j was found to be stable over a few macrosteps. Owing to director fluctuations, \bar{q}_3 and \bar{q}_4 do not coincide, and we took \bar{q}_3 to define the order parameter \bar{T}_2 ; this definition was found to be consistent with the asymptotic limit of the correlation function $G_2(r)$, and overestimates finite size order in the disordered region, where the director is loosely defined [20–23]. We also defined the angle

$$\psi_j = \arccos(|\omega_j \cdot \omega_{j+1}|), \quad (8)$$

i.e. the angle between the directors of two consecutive macrosteps, and calculated both its average $\bar{\psi}$ and its maximum value ψ_{\max} .

Correlation functions are defined by

$$G_{2L}(r) = \langle \cos(2L(\phi_j - \phi_k)) \rangle \text{ as functions of } r = |\mathbf{x}_j - \mathbf{x}_k|, \quad L = 1, 2 \quad (9)$$

and were calculated at selected temperatures, by analysing one configuration every two sweeps; their plots (not reported here) show a regular and monotonic decay to a limiting value consistent with the corresponding order parameter, i.e.

$$\lim_{r \rightarrow \infty} G_{2L}(r) = \bar{T}_{2L}^2. \quad (10)$$

The singlet orientational distribution function was calculated at $T^* = 2.16$, as reported elsewhere [23]; it is an even function of $\cos(\theta)$, and can be expanded as [20]

$$S(\theta) = (1/\pi) \left(1 + 2 \sum_{k \leq 1} a_{2k} \cos(2k\theta) \right) \quad (11)$$

or

$$S(\theta) = b_0 \exp \left(\sum_{k \geq 1} b_{2k} \cos(2k\theta) \right), \quad (12)$$

where the angle θ can be restricted between 0 and $\pi/2$, and the quantities a_{2k} are even rank order parameters.

3. Results and discussion

Results for the heat capacity are shown in figure 1; those for the order parameters are shown in figure 2, and show a pronounced sample size effect at and above the transition temperature. A number of results are known in the literature for this model, obtained by various techniques, such as the analysis of the high temperature series for the partition function [7, 8], renormalization group [9, 10], and extensive simulations [11, 12]: the system exhibits a second order transition [7, 8, 11, 12] at $T_c^* = 2.203 \pm 0.006$, whose critical exponents [24] have been calculated; for example $\beta = 0.36 \pm 0.01$ and $\nu = 0.67 \pm 0.02$. Using finite size scaling (see, for example, [12]), we have obtained similar values for the critical exponents, and the estimate $T_c^* = 2.215 \pm 0.009$ for the transition temperature. Molecular field theory [25] predicts $T_{c, MF}^* = 3$ and $\beta_{MF} = 1/2$ [25]; molecular field approach can be refined via cluster variational techniques [26–29]; we have used a two site cluster treatment [28, 29], and obtained $T_{c, TS}^* = 2.034$.

For comparison, we also mention that, allowing for the symmetries discussed previously, the present model possesses various counterparts consisting of three component unit vectors, also associated with a simple cubic lattice: the ‘magnetic’ one is the classical Heisenberg model, with a transition temperature $T_c^* = 1.4432 \pm 0.0002$

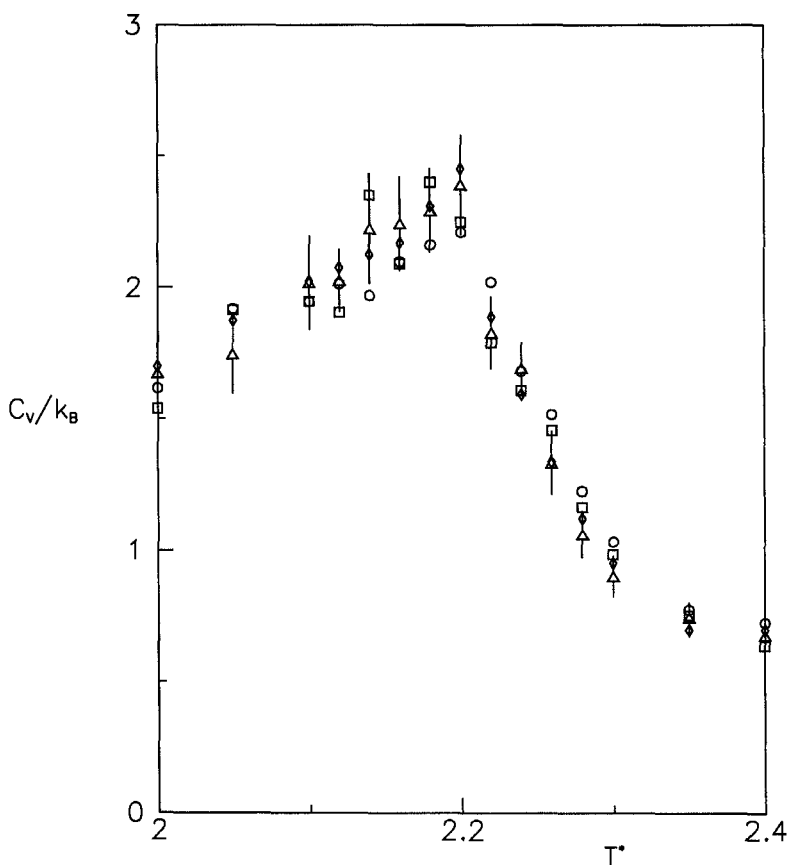


Figure 1. Configurational specific heat: (a) (○): fluctuation quantities, $n=12$; (b) (□): fluctuation quantities, $n=14$; (c) (△): fluctuation quantities with error bars, $n=16$; (d) (◇): estimate obtained via least squares fitting and numerical differentiation of the potential energy.

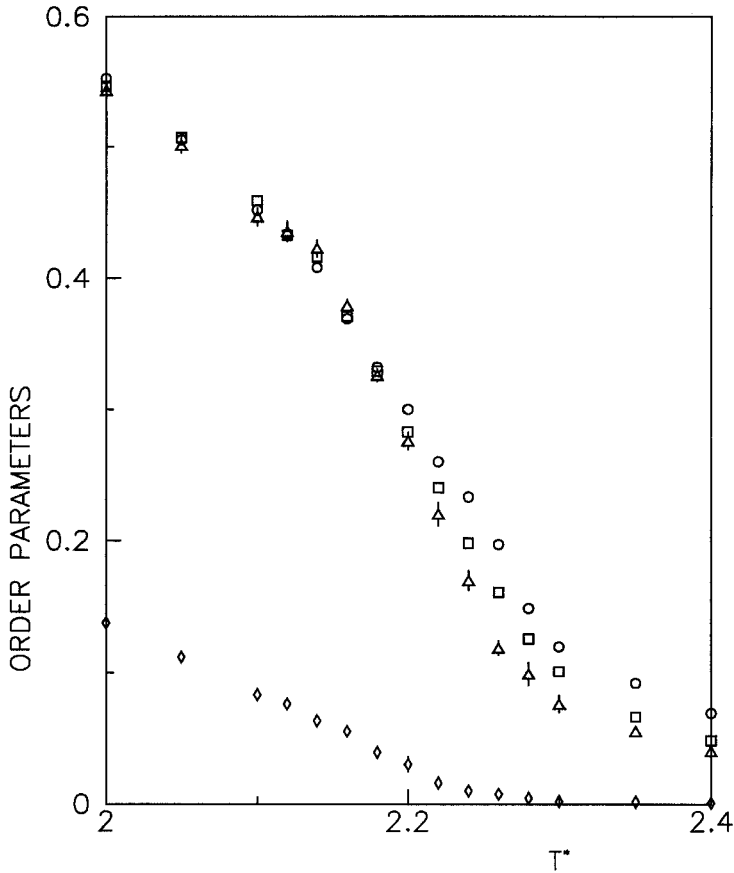


Figure 2. Order parameters: (a) (\circ): \bar{T}_2 , $n=12$; (b) (\square): \bar{T}_2 , $n=14$; (c) (\triangle): \bar{T}_2 , $n=16$; (d) (\diamond): \bar{T}_4 ; the different sample sizes given the same results to within the associated statistical errors.

[30], and the nematic one is the well-known Lebwohl–Lasher model, with $T_c^* = 1.1232 \pm 0.0006$ [22]; a three component antinematic counterpart, defined by the nearest neighbour potential

$$U = \varepsilon P_2(\mathbf{u}_j \cdot \mathbf{u}_k), \quad (13)$$

has also been studied in the literature [31] and its transition temperature is estimated to be $T_c^* = 0.66 \pm 0.04$.

As for the singlet orientational distribution function (see figure 3), a few order parameters were calculated both from the original histogram and by a linear least square fit (see equation (11)); we found

$$a_2 = 0.374 \pm 0.003,$$

$$a_4 = 0.059 \pm 0.004,$$

$$a_6 = 0.005 \pm 0.002,$$

$$a_8 = 0.0005 \pm 0.002.$$

The quantities a_2 and a_4 are in good agreement with the order parameters $\bar{T}_2 = 0.369 \pm 0.005$ and $\bar{T}_4 = 0.055 \pm 0.004$ obtained via the ordering tensors, and with far richer

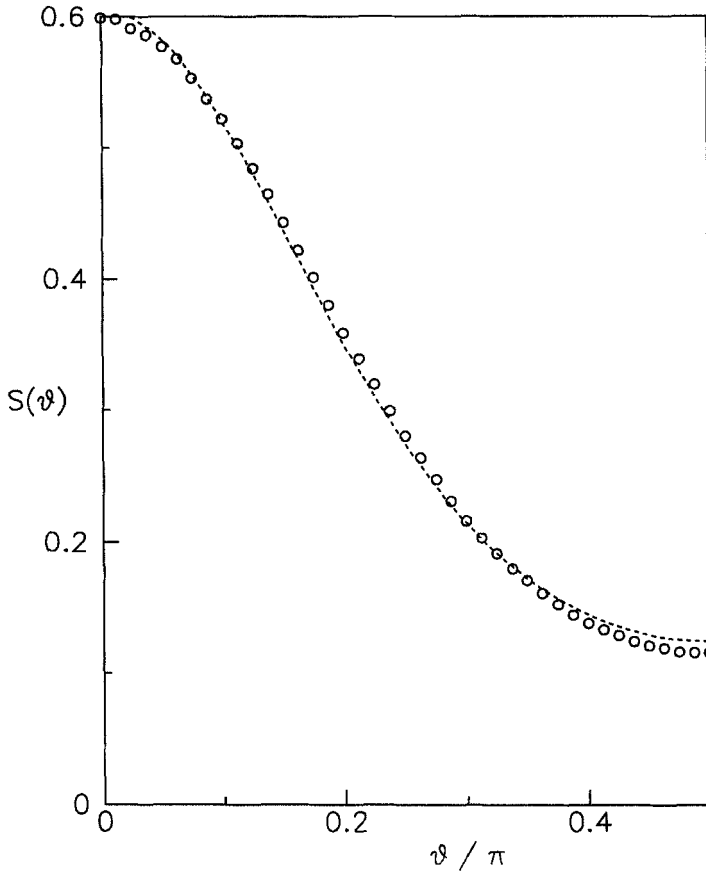


Figure 3. Results for the singlet orientational distribution function at $T^*=2.16$: (a) (○): simulation results; (b) (---): least squares fit obtained from equation (12), by truncating the series at $k=1$.

statistics. We also determined some of the fitting parameters in equation (12) numerically: truncation at $k=1$ gives $b_2=0.793$ and produces a reasonable agreement with the simulation results; inclusion of the next term b_4 improves the agreement and makes calculated and simulation results coincide to within the symbol size. On the other hand, molecular field theory predicts [25] $b_{2k}=0, k>1$ and $b_2=6\bar{T}_2/T^*$, which gives 1.027 in this case; the ratio between the two values of b_2 is 0.772, close to the value $T_c^*/T_{MF}^*=0.734$; comparison shows that, as often, molecular field theory works in a qualitative way.

Results for $\bar{\psi}$ and ψ_{\max} and for the two sample sizes $n=12$ and $n=16$ are reported in figure 4; for each quantity, results for $n=14$ fall in between, and were not reported for the sake of clarity. Both quantities show a rapid increase at the transition temperature, and mostly decrease with increasing sample size; the mean values $\bar{\psi}$ are affected by large fluctuations (of their same order of magnitude), as can be inferred from the fact that ψ_{\max} may well be three times larger than $\bar{\psi}$. In their Monte Carlo study of the Lebwohl-Lasher model, Luckhurst and Simpson [19] found significant director fluctuations when $n=10$ and director pinning when $n=20$; comparison with their results suggests two points. On the one hand, our director fluctuations may be larger because of a smaller number of angular variables being involved in our simulation and on the other

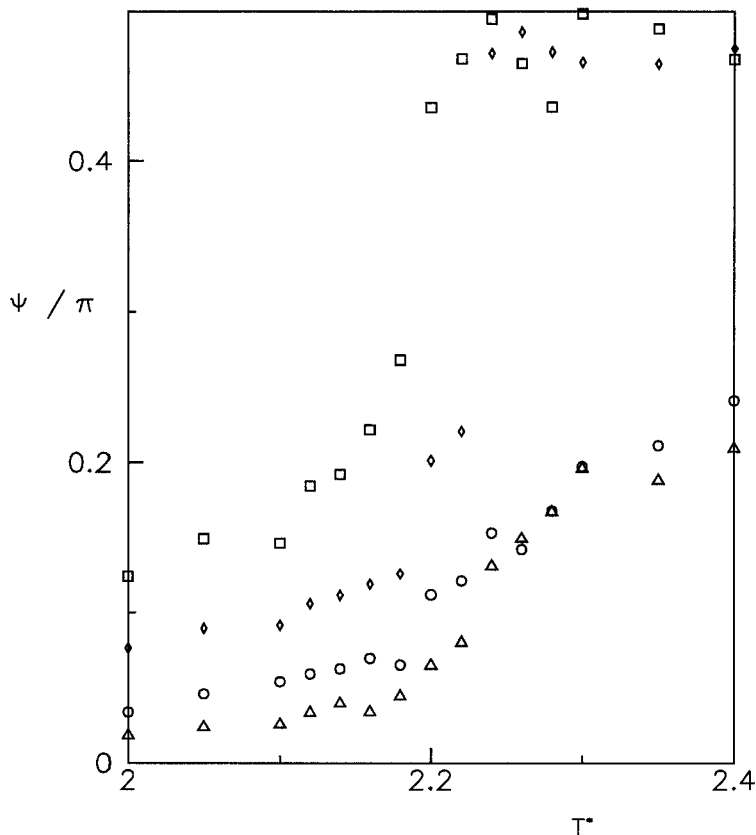


Figure 4. Director fluctuations: (a) (Δ): $\bar{\psi}$, $n=12$; (b) (\circ): $\bar{\psi}$, $n=16$; (c) (\diamond): ψ_{\max} , $n=12$; (d) (\square): ψ_{\max} , $n=16$.

hand, larger director fluctuations are also consistent with the second order character of the disordering transition, as opposed to the weak first order character of the Lebwohl-Lasher model.

The present calculations were carried out on, among other machines, a cluster of VAX computers, belonging to the Sezione di Pavia of Istituto Nazionale di Fisica Nucleare (INFN); computer time on a CRAY machine was allocated by the Italian Consiglio Nazionale delle Ricerche (CNR). The author wishes to thank Professor G. R. Luckhurst (Department of Chemistry, University of Southampton) for helpful discussion and suggestions.

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