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S. Romano[a]
[a] Department of Physics 'A. Volta', The University, and unita' G.N.S.M.-C.N.R./C.I.S.M.-M.P.I., Pavia, Italy

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Monte Carlo simulation of a two dimensional anisotropic plane rotator model

by S. ROMANO

Department of Physics 'A. Volta', The University, and unita' G.N.S.M.-C.N.R./ C.I.S.M.-M.P.I., via A. Bassi 6, I-27100 Pavia, Italy

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We have studied a classical system, consisting of two-component unit vectors (plane rotators) associated with a two dimensional square lattice, and interacting via the nearest neighbour pair potential(s)

$$W_m = c\varepsilon[a\cos(m\phi_j)\cos(m\phi_k) + b\sin(m\phi_j)\sin(m\phi_k)]$$
$$c = \pm 1, \quad \varepsilon > 0, \quad a \geqslant 0, \quad b \geqslant 0.$$

where m is a positive integer and $\{\phi_k\}$ are the angles defining the orientation of the plane rotators in an arbitary reference 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, for given values of a and b, 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 has been proven rigorously to possess a Kosterlitz–Thouless transition when $a = b$, and to possess a low temperature order–disorder transition when $0 \leqslant |b| < a$; when $m = 2$, this entails the existence of nematic- or antinematic- like order, depending on the sign of c. We have chosen $b = 0$, and characterized the system quntitatively by Monte Carlo simulation; calculations were carried out in the nematic representation ($c = -1$, $m = 2$). Simulation results suggest a second order transition taking place at $T_c^* = kT_c/\varepsilon = 1{\cdot}315 \pm 0{\cdot}015$; the molecular field treatment over estimates this value by 50 per cent.

1. Introduction

It is by now well known that isotropic interactions in classical, continuous spin systems associated with a lattice of low dimensionality ($d = 1, 2$) can support orientational order at finite temperature only when sufficiently long ranged [1, 2]; on the other hand, the ordering transition can be brought about by anisotropic nearest neighbour interactions when $d \geqslant 2$ [3]. This paper studies a potential model of the latter kind, known rigorously to possess an ordering transition at finite temperature, and uses numerical simulation to elucidate its physical properties.

We consider a classical system, consisting of n-component unit vectors $\{\mathbf{u}_k\}$, associated with a two dimensional square lattice; let $\mathbf{x}_k$ denote their coordinates, and let V_{jk} be their translationally invariant pair interaction potential, restricted to nearest neighbours. When $n = 2$, the unit vectors lie in a plane (which can be identified with the lattice plane); they are then referred to as plane rotators, and their orientation is uniquely defined by a set of angles $\{\phi_k\}$. We restrict our discussion to anisotropic nearest neighbour potentials of the form

$$V = V_{jk} = c\varepsilon\left[au_{j,1}u_{k,1} + b\sum_{\lambda=2}^{n} u_{j,\lambda}u_{k,\lambda}\right], \tag{1}$$

$$\varepsilon > 0, \quad c = \pm 1, \quad a \geqslant 0, \quad b \geqslant 0; \tag{2}$$

the subscript λ refers to cartesian components, and the larger of the two numbers a and b can be taken as unity. The potential is invariant with respect to the simultaneous inversion of all the spins, but not with respect to their simultaneous rotation by an arbitrary angle. Moreover, in the absence of an external field, the two potential models V and $-V$ possess essentially the same properties (spin-flip symmetry); we are then reduced to consider only ferromagnetic coupling between all components.

When $n = 2$, an additional symmetry property has to be considered [4, 5]: we generalize equation (1) slightly to give

$$W_m = W_{m,jk} = c\varepsilon[a\cos(m\phi_j)\cos(m\phi_k) + b\sin(m\phi_j)\sin(m\phi_k)], \qquad (3)$$

where m is a positive integer. For given values of a and b, all of the potential models W_m possess the same partition function, and the structural properties can be defined in a way independent of m, and so actually calculated using any convenient value of m. A number of rigorous results are known for these models.

(*a*) When $n = 2$, $a = b = 1$, the system disorders at all finite temperatures, but a Kosterlitz–Thouless transition is known to exist [6], involving a low temperature phase with power law decay of correlations and infinite susceptibility; the transition temperature is estimated to be $T_c^* = 0{\cdot}89 \pm 0{\cdot}001$, where $T_c^* = kT/\varepsilon$ [7–9].

(*b*) When $n = 3$ and $0 \leqslant (a/b) < (2/q)\tau$, a Kosterlitz–Thouless transition is also known to exist, involving correlations in the lattice plane [10]; here q is the coordination number and τ is the transition temperature for the corresponding isotropic plane rotator model.

(*c*) When $n = 2, 3$ and $0 \leqslant |b| < a = 1$, the system is known to possess a low temperature transition to an orientationally ordered phase, and the transition temperature is estimated to be $T_c^* = O(1 - b)$ [3, 11–13]; moreover, for $n = 2$ and $m = 2$, the ordered phase can be interpreted as nematic-like ($c = -1$) or antinematic-like ($c = +1$) as well. There has been some debate about nematic-like orientational order in low dimensional systems [14, 15], whose absence has been proved rigorously in some cases [16]; here we can rely on its proven existence for the specified range of parameters. Similar results also hold for the quantum ferromagnetic counter-parts of these models [17].

As a step towards a better understanding of its physical behaviour, we decided to carry out Monte Carlo simulations for an anisotropic plane rotator model; simulation requires a more precise definition of the potential, thus we chose $b = 0$, both in order to have a pronounced effect, and for computational ease. We also chose the nematic interpretation, i.e. $c = -1$, $m = 2$ in equation (3), so that the model actually used in the simulation is

$$W_2 = -\varepsilon\cos(2\phi_j)\cos(2\phi_k). \qquad (4)$$

The common reference direction for defining the angles can be identified with the lattice x axis.

2. Computational aspects

The calculations were carried out on a square sample, consisting of $N = L^2$ particles, and surrounded by a periodic replica of itself; sample size effects were examined by repeating calculations at some temperatures with $L = 10, 20, 30, 40, 50$; the results reported here refer to $L = 50$. In the ordered region, sample size effects seem to saturate for $L \geqslant 30$, whereas spurious order in the disordered region

decreases with increasing L, roughly like $1/L$. Calculations were started from the ground state configuration at the lowest temperature investigated and performed in cascade, i.e. the equilibrated configuration produced at one temperature 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 2000 and 4000 cycles (where one cycle corresponds to N attempted moves), and production runs took between 4000 and 10,000 cycles; subaverages for evaluating statistical errors were calculated over macrosteps consisting of 200 cycles.

Calculated quantities include the potential energy, the configurational specific heat C_v (both as a fluctuation quantity and by least square fitting and numerical differentiation of the energy), the orientational correlation functions and the order parameters. The singlet orientational distribution function (SODF) was also calculated at one temperature in the ordered region ($T^* = 1.25$). Structural quantities can be defined in a way independent of m [4, 5]; for example the magnetic moment per particle and its mean square values are given by

$$\mathbf{M}_1 = \langle F(m)\rangle_m, \quad \bar{M} = \langle\sqrt{[N\mathbf{F}(m).\mathbf{F}(m)]}\rangle_m, \quad M_2 = \langle\mathbf{F}(m).\mathbf{F}(m)\rangle_m, \tag{5}$$

$$\mathbf{F}(m) = (1/N)\sum_{k=1}^{N}[\cos(m\,\phi_k)\mathbf{e}_1 + \sin(m\phi_k)\mathbf{e}_2], \tag{6}$$

where $\mathbf{e}_1$ and $\mathbf{e}_2$ are the orthogonal unit vectors of the square lattice, and $\langle\ldots\rangle_m$ denotes an average with respect to the potential W_m.

We can also define m-independent orientation correlation functions by

$$G_p(r) = \langle\cos[pm(\phi_j - \phi_k)]\rangle_m, \text{ as functions of } r = |\mathbf{x}_j - \mathbf{x}_k|; \quad p = 1, 2, \tag{7}$$

these were calculated at a few selected temperatures, in order to save computer time.

Nematic order parameters, $\bar{T}_2$ and $\bar{T}_4$, can be defined and calculated as discussed in detail elsewhere [18–20], i.e. via the second rank ordering tensor

$$Q_{\lambda\mu} = 2\langle u_\lambda u_\mu\rangle_2 - \delta_{\lambda\mu} \tag{8}$$

and its fourth rank counterpart. Moreover, since $\sin\phi$ is an odd function of its argument, whereas $\cos\phi$ is even, the condition $b = 0$ entails in this case

$$\langle\sin(pm\phi_j)\rangle_m = 0, \quad \forall j \tag{9a}$$

$$\langle\sin(pm\phi_j)\sin(pm\phi_k)\rangle_m = 0, \quad j \neq k, \tag{9b}$$

$$\langle u_\lambda u_\mu\rangle_2 = \delta_{\lambda\mu}\langle u_\lambda^2\rangle_2, \quad \langle u_\lambda u_\mu u_\nu u_\varrho\rangle_2 = \delta_{\lambda\mu}\delta_{\nu\varrho}\langle u_\lambda^2 u_\nu^2\rangle_2, \tag{10a}$$

$$Q_{11} = \bar{T}_2, \bar{T}_{2p} = (1/N)\left\langle\sum_{k=1}^{N}\cos(pm\phi_k)\right\rangle_m; \tag{10b}$$

i.e. the ordering tensors are diagonal, and the director coincides with the lattice x axis; this was verified in the course of simulation, to within the statistical errors.

The singlet orientational distribution function was calculated at $T^* = 1{\cdot}25$, inside the ordered region, over a chain consisting of 10000 cycles, and we analysed a configuration every second cycle, according to the procedure reported elsewhere [19, 21, 22]; such a length was needed in order to achieve reasonable statistics. In the present case the distribution function is an even function of $\cos\vartheta$, where ϑ is the angle formed by the individual molecule with the director; it can be expanded as [19]

$$S(\vartheta) = (1/\pi)\left[1 + 2\sum_{k>0} a_{2k}\cos(2k\vartheta)\right], \tag{11}$$

where the quantities a_{2k} are even rank order parameters; taking into account the underlying a symmetry, ϑ can be restricted between 0 and $\pi/2$.

We recall that the usual procedure for calculating order parameters and the singlet distribution function [18–22] need to compensate for director fluctuations. In the present case, the very anisotropy of the interaction keeps the director pinned in the ordered phase, so that the angle ϑ in equation (11) can be identified with the angle ϑ, defining the particle orientations in the lattice frame; director pinning is also known in other simulation studies (e.g. [23]).

3. Results and comparison with other treatments

Results for the potential energy, the specific heat and the order parameters are plotted in figures 1 and 3, and indicate a disordering transition taking place at scaled temperatures between 1·3 and 1·35. The energy and order parameter results suggest a continuous change across the transition, and specific heat results suggest a weak, possibly logarithmic, singularity; on the whole, this seems to point to a second order [24, 25] phase transition. We have fited the results for the order parameter over a certain range $[T_1^*, T_2^*](T_1^* < T_2^* \leqslant 1{\cdot}3125$, i.e. inside the ordered region), using the functional form [24, 25]

$$\bar{T}_2(T^*) = (T_c^* - T^*)^\beta \tag{12}$$

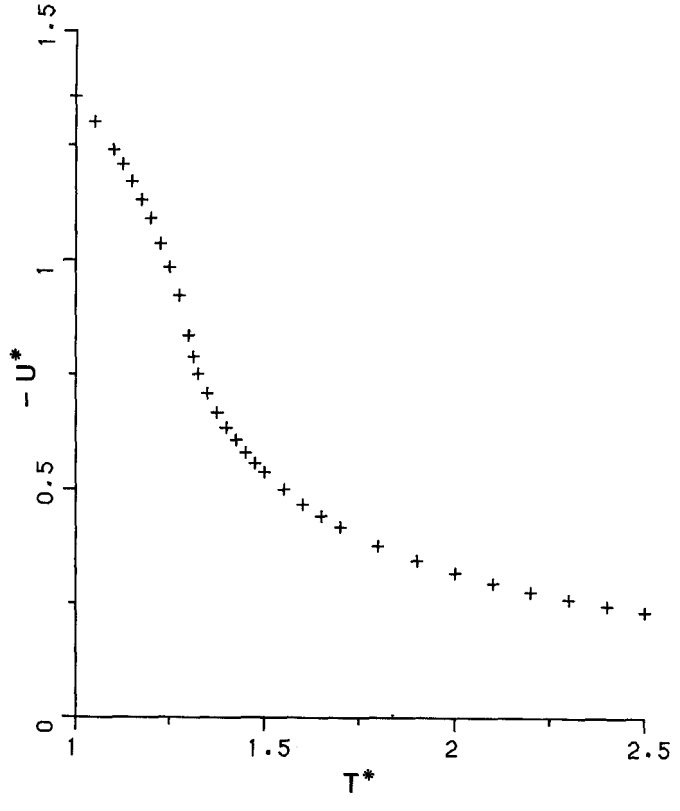

Figure 1. Results for the potential energy; the relative statistical error is usually not greater than 0·5 per cent.

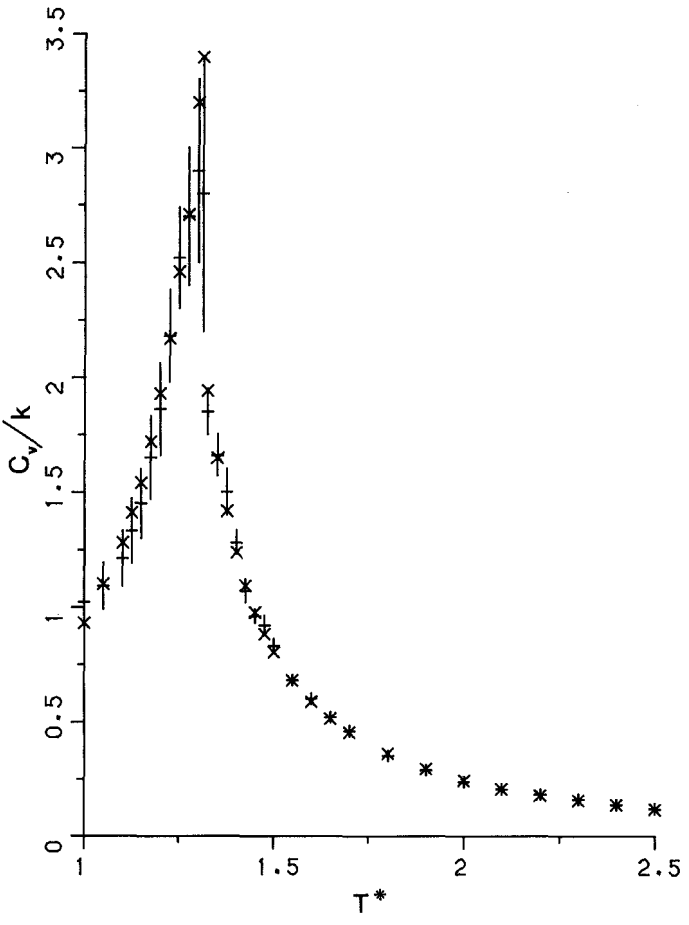

Figure 2. The configurational specific heat: fluctuation quantities with error bars, and results obtained by least-square fitting of the energy.

and determined the two parameters (transition temperature and critical exponent) by means of the general non-linear least square program MINUIT in the CERN library; we also tried different values of T_1^* and T_2^*, and consistently found

$$T_c^* = 1{\cdot}3150 \pm 0{\cdot}0025, \quad \beta = 0{\cdot}183 \pm 0{\cdot}003. \tag{13}$$

However, the numbers quoted (returned by the fitting programme) are not the whole story: comparison with other models where exact results are also known (e.g. [26]) or sample size effects have been investigated more extensively (e.g. [20, 27]), suggests that T_c^* is affected by an uncertainty of the order of a percent, and that the estimate of β is erroneously large. We thus propose $T_c^* = 1{\cdot}315 \pm 0{\cdot}015$; as for critical exponents, the present system is expected to belong to the same universality class as its one component (discrete) counterpart, i.e. the Ising model, for which $T_c^* = 2{\cdot}269$, $\beta = 1/8$, $\eta = 1/4$. The three component counterpart of the present model ($a = 1$, $b = 0$, $n = 3$ in equation (1)) also belongs to the same universality class, and its transition temperature has been estimated to be $T_c^* = 0{\cdot}88 \pm 0{\cdot}01$ [27].

The disordering transition is known to be weakly first order in real nematics and for various short range potential models studies in three dimensions, where the order

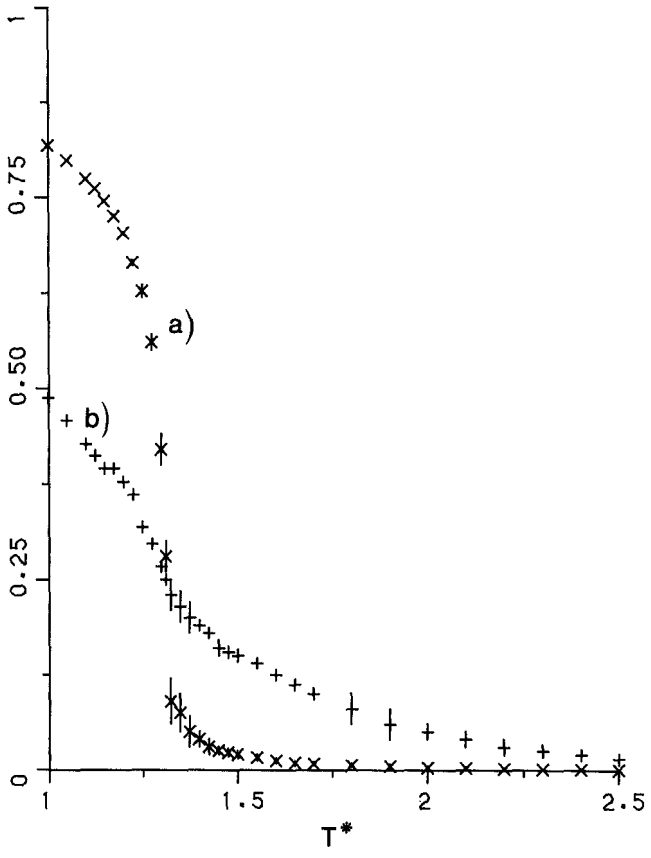

Figure 3. Results for the order parameters (*a*) $\bar{T}_2$; (*b*) $\bar{T}_4$.

parameter at the transition ranges typically between 0·3 and 0·5 (e.g. [20, 23, 28, 29]). The correlation functions $G(r)$ (see figure 4) were found to decrease with distance in an essentially monotonic way, and to converge to their asymptotic values $\bar{T}_{2p}^2$ [19] in the ordered phase. In the ordered region $G_1(r)$ is well fitted by the functional form

$$G_1(r) = c_1 + c_2/(c_3 + r^q). \tag{14}$$

In the disordered region, G_1 should tend to zero as r tends to infinity; owing to finite sample size and periodicity, we found for $G_1(r)$ a long distance limit of the order of 0·005. In order to compensate for the esidual order, we have fitted $G_1(r)$ to the functional form [7, 8]

$$G_1(r) = c_1 + h(r) + h(L - r); \tag{15a}$$

$$h(r) = c_2 \exp(-sr)/(c_3 + r^q); \quad 0 < r < L/2. \tag{15b}$$

$h(r)$ has a rather general and flexible functional form, consistent with known or expected asymptotic behaviour of the correlation function (i.e. exponential decay, inverse power law or the product of the two [24, 25]). Some fitting parameters are reported in the table, and inclusion of the correction term $h(L - r)$ did not change appreciably the quality of the fit for $T^* > 1{\cdot}35$. If we try to fit $G_1(r)$ in the ordered region by the sum of $h(r)$ and a constant term, then the best-fit value of the parameter s is found to be zero to within a small error.

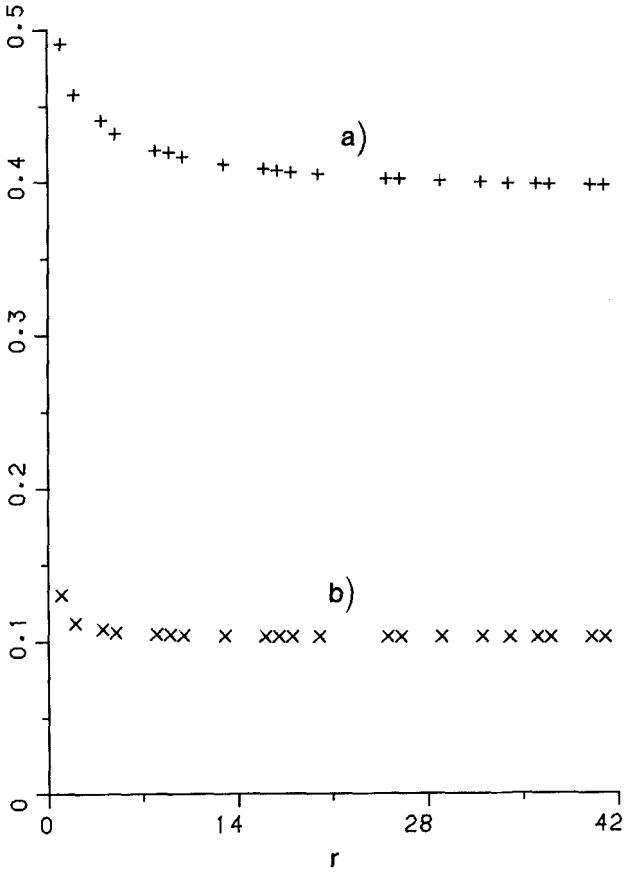

Figure 4. Plots of the orientational correlation functions at the temperature $T^* = 1{\cdot}25$: (*a*) $G_1(r)$; (*b*) $G_2(r)$; the correlation functions $G(R)$ are defined in the text.

Fitting parameters for the correlation function G_1 (see equations (14) and (15)), as a function of temperature.

T^*	q	s
1·250	1·35	—
1·275	1·08	—
1·300	0·82	—
1·3125	0·54	—
1·325	0·40	0·052
1·350	0·62	0·079
1·375	0·68	0·083
1·400	0·76	0·148
	(±0·03)	(±0·004)

A simple molecular field approximation [28, 29] can be developed, leading to the one particle potential of mean torque

$$\tilde{V}(\phi) = -4\bar{T}_{2,\mathrm{MF}} \cos(2\phi), \tag{16}$$

where $\bar{T}_{2,\mathrm{MF}}$ is determined by the usual self-consistency condition

$$\bar{T}_{2,\mathrm{MF}} = \mathrm{I}_1(\varrho)/\mathrm{I}_0(\varrho), \quad \varrho = 4\bar{T}_{2,\mathrm{MF}}/T^* \tag{17}$$

and I_k are modified Bessel functions of order k. Upon solving the equation numerically, $\bar{T}_{2,\mathrm{MF}}$ is found to decrease continuously to zero at the temperature $T^*_{c,\mathrm{MF}} = 2$, and the transition is found to be second order [30, 31]; the molecular field approximation gives the following critical exponents [24, 25]

$$\alpha = 0, \quad \beta = 1/2. \tag{18}$$

The transition temperature is here overestimated by 50 per cent, in contrast to the reasonable success of the molecular field approach for nearest-neighbour nematogenic models in three dimensions [20, 23, 28, 29]. The molecular field approach works reasonably well also for some isotropic long range models of low dimensionality ($d = 1, 2$), where it overestimates the transition temperature by 20 per cent at worst [5, 32], and its critical exponents are confirmed by renormalization group results [33, 34].

At the transition temperature, the correlation function G_1 is predicted to possess the asymptotic power law behaviour [24, 25]

$$G_1(r) \propto r^{-(d-2+\eta)}. \tag{19}$$

Our simulation results cannot claim to allow an accurate determination of the critical quantities, which requires larger sample sizes (and greater computational resources); a crude estimate based on the results in the table gives $\eta = 0{\cdot}50 \pm 0{\cdot}05$, which is too large by a factor two.

As for the singlet orientational distribution function (figure 5), the coefficients a_{2k} in equation (11) were directly calculated from a 201 bin histogram [21, 22], which was smoothed by regrouping its bins and reducing their number to 41; as a double-check, the order parameters were recalculated from the smoothed histogram via a linear least-square fit. We obtained a rather good fit by truncating the expansion at $k = 6$, and found a variance of 0·000033 and the values:

$$a_2 = 0{\cdot}624 \pm 0{\cdot}002, \quad a_4 = 0{\cdot}319 \pm 0{\cdot}002, \quad a_6 = 0{\cdot}111 \pm 0{\cdot}002,$$

$$a_8 = 0{\cdot}035 \pm 0{\cdot}002, \quad a_{10} = 0{\cdot}009 \pm 0{\cdot}002, \quad a_{12} = 0{\cdot}002 \pm 0{\cdot}002.$$

Truncation at $k = 4$ gave a variance of 0·0006, and the same values for the coefficients a_2 to a_8; the coefficients a_2 and a_4 agree with the values of $\bar{T}_2$ and $\bar{T}_4$, obtained as averages over the whole Monte Carlo chain, i.e. $0{\cdot}627 \pm 0{\cdot}008$ and $0{\cdot}319 \pm 0{\cdot}001$. The molecular field treatment of nematic models predicts for $S(\vartheta)$ an expression of the form [30, 31]

$$S(\vartheta) = \exp\left[b_0 + \sum_{k>0} b_{2k} \cos(2k\vartheta)\right], \tag{20}$$

where the coefficients b_{2k} are also predicted to depend on the order parameters; for the present model this means $b = 0$, $k > 1$. Truncation of the series in equation (20) at $k = 2$ gave a variance of 0·002, and inclusion of higher order terms up to $k = 4$ reduced it to 0·00005. This contrasts with other simulated short range nematic potential models in three dimensions and with experimental data on real ones [35–37], where a good fit was obtained by truncating the series in equation (20) at $k = 1$. Comparison with other known results indicates that the combination of low dimensionality, anisotropy and short range character of the interaction makes this potential model rather different from the molecular field limit.

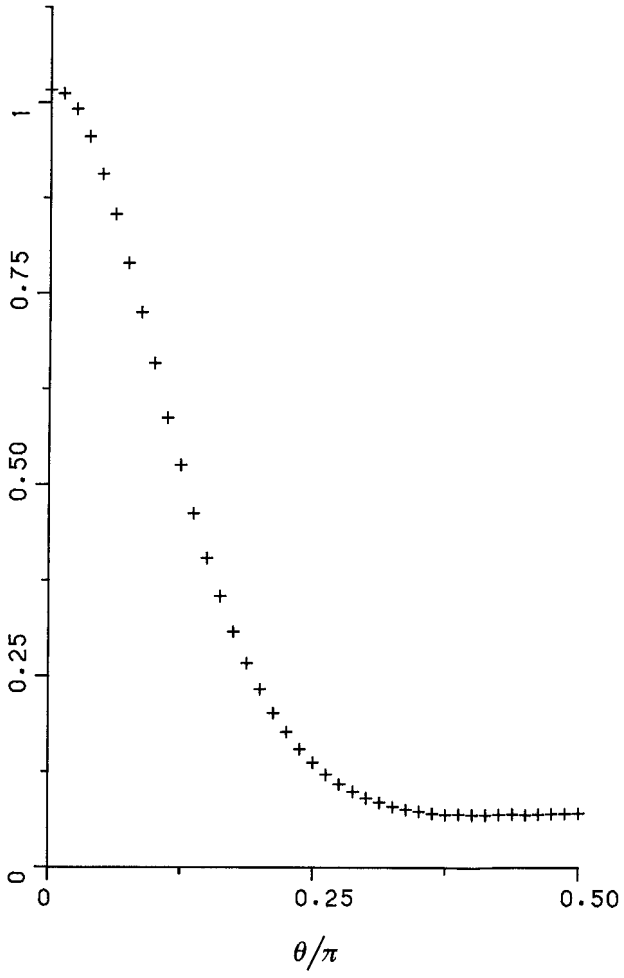

Figure 5. The plot of the singlet orientational distribution function determined at $T^* = 1{\cdot}25$.

The present calculations were carried out on, among other machines, a VAX 8350 computer, 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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