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One dimensional classical spin models with long range anisotropic interaction. An extreme nematogenic lattice model

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One dimensional classical spin models with long range anisotropic interaction

An extreme nematogenic lattice model

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We consider a classical system, consisting of n-component unit vectors (classical spins, $n=2, 3$), asssociated with a one dimensional lattice $\{\mathbf{u}_k | k \in Z\}$, and interacting via a translationally invariant pair potential of the long range, ferromagnetic, and anisotropic form

$$W_{jk} = -\varepsilon |j-k|^{-p} \left[a(u_{j,1}u_{k,1}) + b \sum_{\lambda=2}^{n} (u_{j,\lambda}u_{k,\lambda}) \right],$$

where $\varepsilon > 0$ is a positive quantity setting energy and temperature scales (i.e. $T^* = kT/\varepsilon$), $a \geqslant 0$. $b \geqslant 0$, $p > 1$ and $u_{k,\lambda}$ denotes the cartesian components of the unit vector $\mathbf{u}_k$. Available rigorous results entail the existence of an ordering transition at a finite temperature for $1 < p < 2$, and for the borderline cases $p = 2$, $b = 0$ (thus $a = 1$), studied here by Monte Carlo simulation. Moreover, the case $n = 2$ can be interpreted both as a ferromagnet and as an extreme case of a nematogenic lattice model, and was investigated accordingly, also by calculating the singlet orientational distribution function at one temperature in the ordered region. Simulation results showed a broad, qualitative similarity between the two models. The estimated transition temperatures are $T_C^* = 1{\cdot}04 + 0{\cdot}02$ ($n=2$) and $T_C^* = 0{\cdot}735 \pm 0{\cdot}015$ ($n=3$); we conjecture them to be of second order, although a Thouless effect (as in the Ising counterpart) cannot be completely ruled out. The molecular field approximation overestimates the transition temperature by about 50 per cent.

1. Introduction

Over the past 20 years, the study of spin systems associated with a low dimensional lattice and interacting via long range potentials has attracted a significant amount of theoretical work, and the present paper continues along this line. It uses rigorous results implying the existence of an ordering transition and simulation to characterize the physical properties. We consider a classical system, consisting of n-component unit vectors (classical spins, $n=2, 3$), associated with a one dimensional lattice $\{\mathbf{u}_k | k \in Z\}$, and interacting via a translationally invariant pair potential of the long range, ferromagnetic, and, in general, anisotropic form

$$W_{jk} = -\varepsilon |j-k|^{-p} \left[a(u_{j,1}u_{k,1}) + b \sum_{\lambda=2}^{n} (u_{j,\lambda}u_{k,\lambda}) \right], \tag{1}$$

where $\varepsilon > 0$ is a positive quantity setting the energy and temperature scales (i.e. $T^* = kT/\varepsilon$), $a \geqslant 0$, $b \geqslant 0$, $p > 1$ and $u_{k,\lambda}$ denote the cartesian components of the unit vector $\mathbf{u}_k$ (i.e. $u_{k,1}$ is the x component, etc.); the larger of the two numbers a and b can be taken as unity. The condition $p > 1$ is needed in order to avoid a ground state with an

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infinite energy per spin. When $a=b$, the interaction is isotropic, i.e. it only depends on the mutual orientation.

A number of theoretical results are now known concerning the existence or absence of a finite temperature transition to a ferromagnetically ordered phase [1–4]. It has been proved that the system disorders at all finite temperatures when $p>2$, and that the ordering transition exists when $1<p<2$ [2–4]; the border line case $p=2$ has also been extensively studied.

1.1. *Ising model* ($n=1$)

The ordering transition also exists for $p=2$ [5, 6], and the critical exponents have been proved to be mean field-like for $1<p\leqslant 3/2$ as well as for more general single spin distributions [6–8]. Estimates of the transition temperatures are reported in the literature, with an uncertainty of the order of one per cent

$$T_C^*(n=1, p=3/2)=4{\cdot}33 \quad [9, 10],$$
$$T_C^*(n=1, p=2)=1{\cdot}52 \quad [11, 12].$$

1.2. *Continuous spins* ($n=2, 3$)

Let their orientations in an arbitrary reference frame be defined by the usual angles (φ_k) or (ϑ_k, φ_k); when $n=2$, the interaction potential can be rewritten in a slightly more general way by

$$V_m = W_{jk,m} = -\varepsilon|j-k|^{-p}[a\cos(m\varphi_j)\cos(m\varphi_k) + b\sin(m\varphi_j)\sin(m\varphi_k)], \tag{2}$$

where m is an arbitrary positive integer. We can check that, for any given values of p, a and b, the partition function is independent of m, and structural quantities (e.g. orientational correlation functions) can be defined in a way independent of m, and actually calculated using any convenient value of it. The choice $m=1$ defines a ferromagnetic model, whereas $m=2$ provides a rather extreme lattice model of a nematic liquid crystal. In the isotropic case $a=b$, an ordering transition exists for $1<p<2$ [2, 4], and available correlation inequalities [13–16] show that this also happens for $n=3$, $a=0$.

When $p\geqslant 2$, the system disorders at all finite temperatures [17–19]; when $p=2$, it may possess a transition to a low temperature phase with infinite susceptibility [20]. If this is true, then correlation inequalities [13–16] show that it also holds for the case $n=3, a=0$, which is anisotropic in spin space but continuously degenerate with respect to the angle φ. When $p=2$, the same rigorous inequalities [13–16] imply the existence of an ordering transition for $n=2$, $a>b\geqslant 0$ and for $n=3$, $b=0$.

About the interplay between anisotropy and dimensionality, we point out that, in two dimensions, the nearest neighbour counterparts of present anisotropic models can produce an ordering transition at finite temperature, whereas a long range behaviour of the potential is needed for the isotropic models, i.e. $2<p<4$ [1, 4]. Some estimates of the transition temperatures for isotropic continuous spin models are reported in the literature, with an uncertainty of the order of 1 per cent:

$$T_C^*(n=2, p=3/2, a=b)=2{\cdot}16 \quad [21],$$
$$T_C^*(n=3, p=3/2, a=b)=1{\cdot}48 \quad [22].$$

The transition properties of the isotropic models have also been investigated by other techniques [23, 24], including renormalization group (for example [25–27]), high temperature series expansion [11], simulation (for example [12, 21, 22]), and spherical model treatment, which predicts the existence of an ordering transition for $1<p<2$ [28].

Apart from the rigorous results mentioned here, very little is known about the anisotropic models, whose properties we now try to elucidate by simulation. This, in turn, requires a more precise definition of the potential model, and so we chose $p=2$, $n=2$ or 3 and $b=0$, both for computational simplicity and in order to obtain a more pronounced effect (the temperature of the disordering transition can be expected to decrease to zero as b tends to a). The potential models which we have actually simulated are thus

$$W_{jk}=-\varepsilon|j-k|^{-2}\cos(\varphi_j)\cos(\varphi_k), \quad n=2 \tag{3}$$

and

$$W_{jk}=-\varepsilon|j-k|^{-2}\cos(\vartheta_j)\cos(\vartheta_k), \quad n=3. \tag{4}$$

The common reference direction for defining the angles φ_k or ϑ_k, respectively, can be identified with the lattice axis. For $n=2$, we have carried out most calculations using the ferromagnetic interpretation (see equation (2)).

The ground state energy, in both cases [29], is

$$U_0^*=U_0/\varepsilon=-\zeta(2)=-\sum_{k=1}^{\infty}k^{-2}=-\pi^2/6=-1{\cdot}645. \tag{5}$$

Concerning the extreme character of the nematogenic model defined by $n=2$, we recall that there has been some debate about nematic-like orientational order in one or two dimensional systems [30, 31]. In some cases its absence has been proved rigorously, [1, 32], whereas we can rely here on its proved existence, although at the cost of severe mathematical constraints on the form of the potential.

2. Computational aspects

Calculations were carried out using periodic boundary conditions, and the energy of a configuration was summed in closed form by means of the identity [33]

$$\left(\frac{\pi}{\sin\pi x}\right)^2=\sum_{L\in Z}(x+L)^{-2}, x\notin Z \tag{6}$$

Two sample sizes, $N=1000$ and $N=2000$ were used; calculations were performed in cascade, i.e. the equilibrated configuration obtained at one temperature was used to start both the production run at the same temperature and the equilibration run at the next higher temperature. The starting configuration for simulation with the larger sample was obtained by doubling an equilibrated configuration of the smaller one. Equilibration runs took between 2000 and 5000 cycles (where one cycle corresponds to N attempted moves), and production runs took between 5000 and 10 000 cycles; subaverages for evaluating the statistical errors were calculated over macrosteps consisting of 250 cycles.

Calculated quantities include the potential energy, the configurational heat capacity (evaluated both as a fluctuation quantity and by least-square fitting and

numerical differentiation of the potential energy), and various structural ones; the magnetic moment per particle and its mean square value are given by

$$\mathbf{M}=(1/N)\langle\mathbf{F}\rangle, \bar{M}=(1/N)\langle\sqrt{(\mathbf{F}\cdot\mathbf{F})}\rangle, M_2=(1/N)^2\langle\mathbf{F}\cdot\mathbf{F}\rangle \tag{7}$$

$$\mathbf{F}=\sum_{k=1}^{N}\mathbf{u}_k. \tag{8}$$

Taking into account that

$$\int_0^{2\pi}\sin\varphi\cos\varphi\,d\varphi=0, \quad \int_0^{2\pi}\begin{Bmatrix}\sin\varphi\\ \cos\varphi\end{Bmatrix}d\varphi=0, \tag{9}$$

the specific form of the potential entails that only one component of $\mathbf{M}$ (hereafter called M_1) is different from zero; in the ordered region, M_1 coincides with $\bar{M}$ to within the statistical errors, and becomes much smaller (roughly speaking, less than one half in magnitude) in the disordered region. The orientational correlation functions are defined by

$$G_L(r)\begin{cases}=\langle P_L(\mathbf{u}_j\cdot\mathbf{u}_k)\rangle, & n=3\\ & \text{as functions of } r=|j-k|;\\ =\langle\cos(Lm(\varphi_j-\varphi_k))\rangle_m, & n=2\end{cases} \tag{10}$$

where P_L are Legendre polynomials, and $\langle\ldots\rangle$ denotes an average with respect to the potential V_m. Because of the symmetry of the potential, they reduce to

$$G_L(r)\begin{cases}=\langle P_L(\cos\vartheta_j)P_L(\cos\vartheta_k)\rangle, & n=3,\\ =\langle\cos(Lm\vartheta_j)\cos(Lm\vartheta_k)\rangle_m, & n=2.\end{cases} \tag{11}$$

Calculations were carried out at a few temperatures, for $L=1,2$.

As we have pointed out before, when $n=2$, the choice $m=2$ defines a nematogenic (lattice) model, whose order parameters $\bar{T}_2$ and $\bar{T}_4$ can be defined and calculated as discussed in detail elsewhere [34–36], i.e. via the second rank ordering tensor

$$Q_{\lambda\mu}=2\langle u_\lambda u_\mu\rangle_2-\delta_{\lambda\mu} \tag{12}$$

and its fourth rank counterpart. Moreover, the underlying symmetry of the potential requires that

$$\langle u_\lambda u_\mu\rangle_2=\delta_{\lambda\mu}\langle u_\lambda^2\rangle_2, \quad \langle u_\lambda u_\mu u_\nu u_\rho\rangle_2=\delta_{\lambda\mu}\delta_{\nu\rho}\langle u_\lambda^2 u_\nu^2\rangle_2, \tag{13}$$

i.e. the ordering tensors are diagonal, the director coincides with the lattice x axis, and the relevant nematic order parameters reduce to the m-independent quantities

$$\bar{T}_{2L}=(1/N)\left\langle\sum_{k=1}^{N}\cos(Lm\varphi_j)\right\rangle_m. \tag{14}$$

These, in turn, can be calculated using the ferromagnetic interpretation ($m=1$ as in equation (2)), so that $\bar{T}_2$ is just M_1; this was also checked and verified numerically by carrying out an independent simulation at $T^*=1$, now using the nematic interpretation ($m=2$ as in equation (2)), i.e. the potential

$$V_2=W_{jk,2}=-\varepsilon|j-k|^{-2}\cos(2\varphi_j)\cos(2\varphi_k), \quad n=2. \tag{15}$$

This additional simulation was also used to calculate the singlet orientational distribution function, over a chain consisting of 10000 cycles, and analysing a

configuration every second cycle, according to the procedure reported elsewhere [34, 37]. In the present case, this distribution function is an even function of $\cos\tilde{\varphi}$, where $\tilde{\varphi}$ is the angle made by the individual molecule with the director, and can be formally expanded as [37]

$$S(\tilde{\varphi})=(1/\pi)\left[1+2\sum_{k>0}a_{2k}\cos(2k\tilde{\varphi})\right], \tag{16}$$

where the coefficients a_{2k} are even rank order parameters: taking into account the underlying symmetry, $\tilde{\varphi}$ can be restricted between 0 and $\pi/2$. We recall that the usual procedure for calculating the order parameters and the distribution function [34–37] needs 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 $\tilde{\varphi}$ in equation (16) can be identified with the angle φ defining the particle orientations in the lattice frame. Director pinning is also known in other simulation studies (for example [38, 39]), carried out with anisotropic potential models.

3. Results

The results for the potential energy (figures 1 and 2) were not affected by the increase in the sample size, to within statistical errors of the order of 0·25 per cent; they suggest a continuous change across the transition.

The configurational specific heat is plotted in figures 3 and 4; results for the fluctuation quantities obtained with the two sample sizes agree to within statistical errors of the order of 10 per cent, and show a peak, and possibly a singularity, at the transition. Order parameter results are plotted in figures 5 and 6, and exhibit a pronounced sample size effect above the transition temperature; the significant amount of finite size order is also reflected by the slow decay of the correlation functions (not shown here). We estimate the transition temperatures for the two models to be

$$T_C^*(n=2, p=2, b=0)=1{\cdot}04\pm0{\cdot}02,$$

and

$$T_C^*(n=3, p=2, b=0)=0{\cdot}735\pm0{\cdot}015.$$

As for the singlet orientational distribution function (see figure 7), the coefficients a_{2k} in equation (16) were directly calculated from a 201 bin histogram [37], 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 very good fit by truncating the expansion at $k=6$, and found a variance of 0·000059 and the following values

$$a_2=0{\cdot}603\pm0{\cdot}004, \quad a_4=0{\cdot}343\pm0{\cdot}004,$$
$$a_6=0{\cdot}114\pm0{\cdot}003, \quad a_8=0{\cdot}039\pm0{\cdot}003,$$
$$a_{10}=0{\cdot}009\pm0{\cdot}003, \quad a_{12}=0{\cdot}002\pm0{\cdot}004.$$

Truncation at $k=4$ gave a variance of 0·00019, and the same values for the coefficients a_2–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. $0{\cdot}597\pm0{\cdot}008$ and $0{\cdot}342\pm0{\cdot}003$.

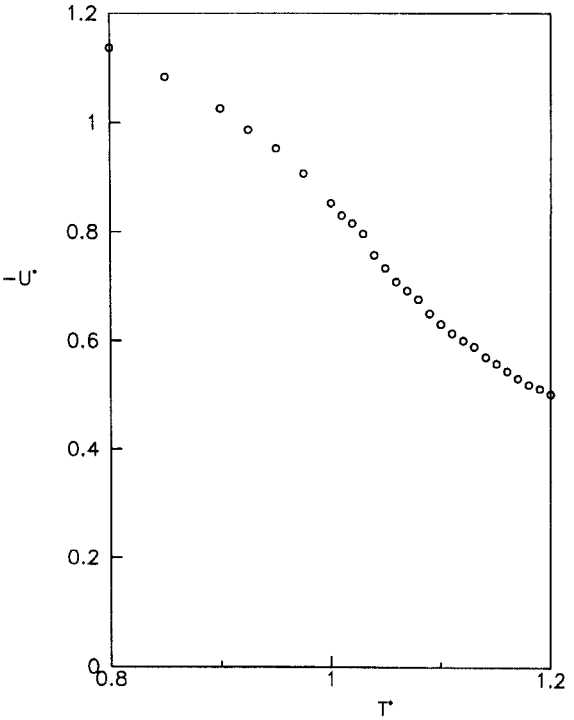

Figure 1. Results for the potential energy, $n=2$.

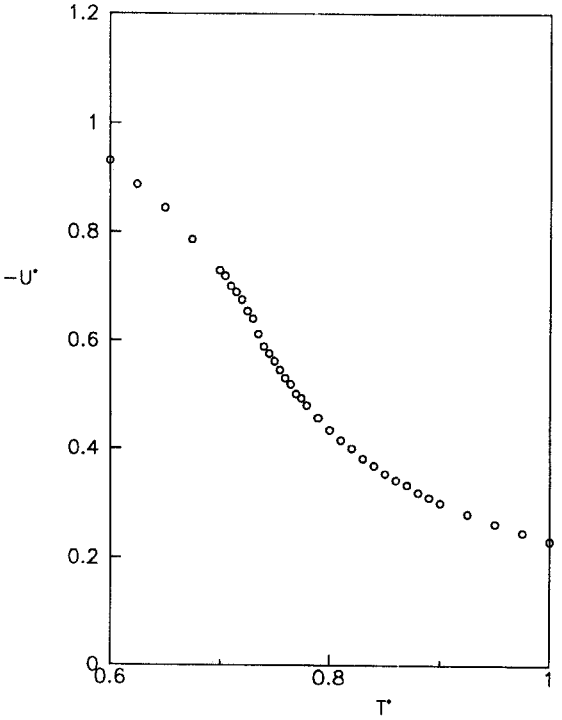

Figure 2. Results for the potential energy, $n=3$.

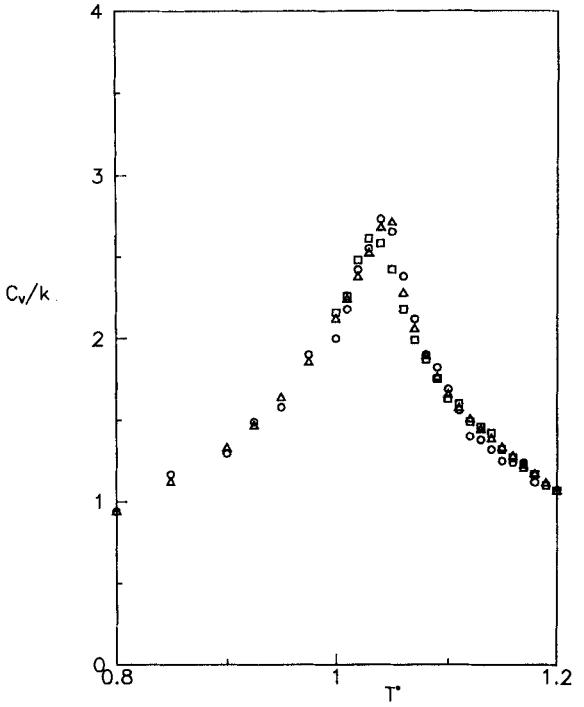

Figure 3. Configurational heat capacity, $n=2$: (*a*) (circles), fluctuation quantities, $N=1000$; (*b*) (squares), fluctuation quantities, $N=200$; (*c*) (triangles), results obtained by a least square fit and numerical differentiation of the potential energy. The fluctuation quantities are affected by statistical errors of the order of 10 per cent.

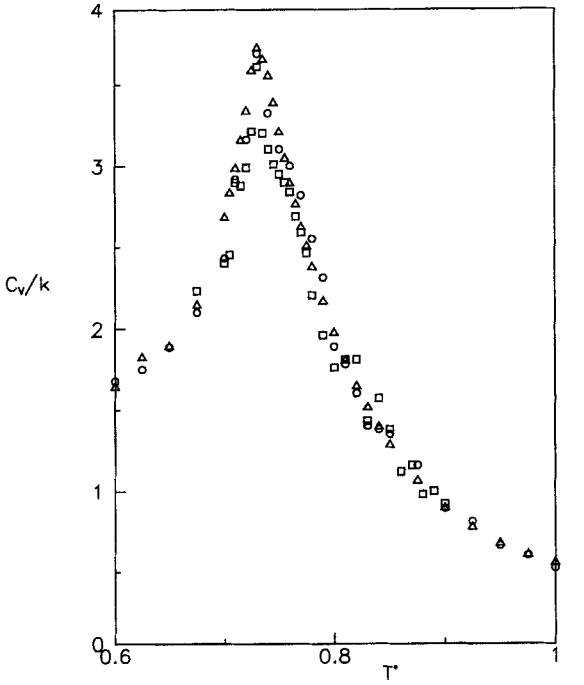

Figure 4. Configurational heat capacity, $n=3$: (*a*) (circles), fluctuation quantities, $N=1000$; (*b*) (squares), fluctuation quantities, $N=2000$; (*c*) (triangles), results obtained by a least square fit and numerical differentiation of the potential energy. The fluctuation quantities are affected by statistical errors of the order of 10 per cent.

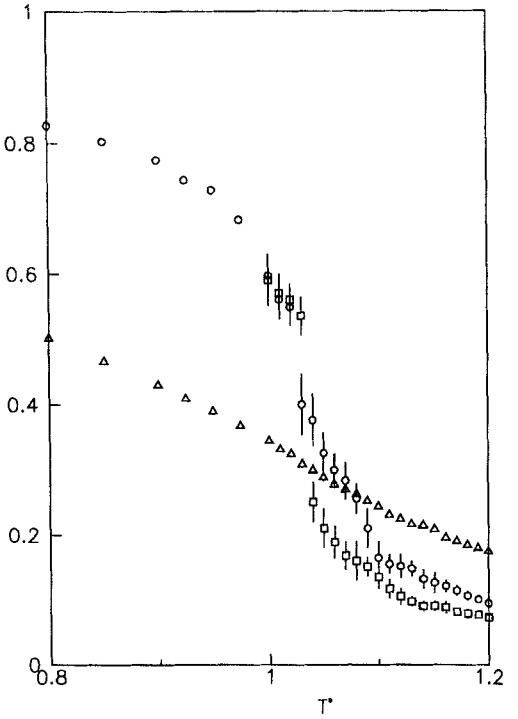

Figure 5. Order parameters, $n=2$: (*a*) (circles), $\bar{M}$, $N=1000$; (*b*) (squares), $\bar{M}$, $N=2000$; (*c*) (triangles), $\bar{T}_4$; the two sample sizes give the same results to within the associated statistical errors.

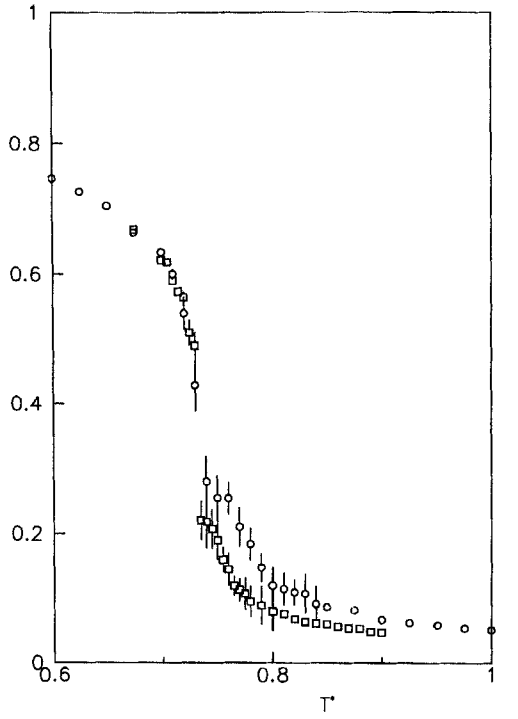

Figure 6. Order parameters, $n=3$: (*a*) (circles), $\bar{M}$, $N=1000$; (b) (squares), $\bar{M}$, $N=2000$.

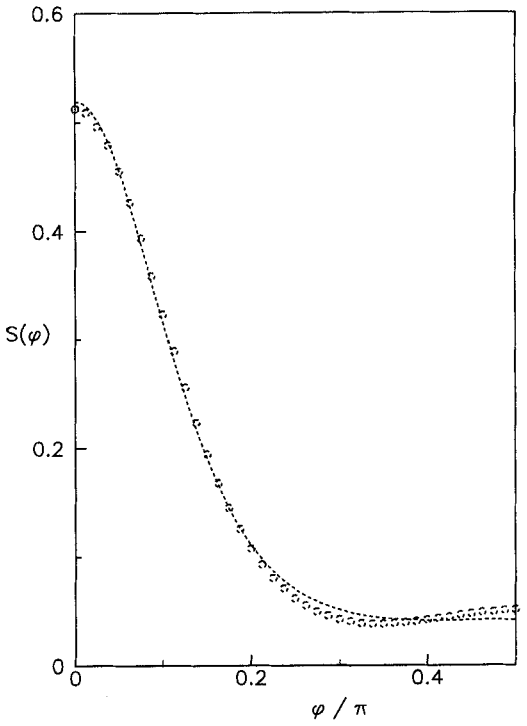

Figure 7. Plot of the singlet orientational distribution function at the T^* of 1, for $n=2$; (*a*) (circles): simulation results; (*b*) (dashed line): least-square fit obtained from equation (17), by truncating the series at $k=2$.

4. Comparisons

The Ising counterpart of the present model exhibits a Thouless effect, i.e. a transition where the magnetization drops discontinuously to zero, whereas the energy and possibly the specific heat change continuously [5, 8, 12, 27]. The simulation results suggest that the specific heat reaches its maximum at a somewhat higher temperature [12]. We conjecture that the transitions are second order, although a Thouless effect cannot be completely ruled out. The disordering transition is known to be weakly first order in real nematics and for various realistic short range nematogenic potential models studied in three dimensions, where the order parameter at the transition ranges is typically between 0·3 and 0·5 (for example [36, 39–41]).

A simple molecular field approximation [42–44] can be developed, which predicts in both cases second order transitions at the temperatures

$$T_C^*(n=2, p=2, b=0) = |U_0^*| = 1{\cdot}645$$

and

$$T_C^*(n=3, p=2, b=0) = (2/3)|U_0^*| = 1{\cdot}096.$$

The ratios between the transition temperature estimated by simulation and the molecular field result are 0·63 ($n=2$) and 0·67 ($n=3$), respectively, and show that the theory performs slightly better for $n=3$. The transition temperature is here overestimated by 50 per cent, in contrast to the reasonable success of the same approach for nearest neighbour nematogenic models in three dimensions [36, 38, 39, 40, 45]. 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 [21, 22, 46, 47] and its estimates for the critical exponents are confirmed by renormalization group results [25, 26]. The molecular field treatment of nematic models predicts for $S(\varphi)$ an expression of the form [40, 41]

$$S(\varphi)=\exp\left[b_0+\sum_{k>0} b_{2k}\cos(2k\varphi)\right], \tag{17}$$

where the coefficients b_{2k} are also predicted to depend on the order parameters; for the present model this means $b_{2k}=0, k>1$. Truncation of the series in equation (17) at $k=2$ gave a variance of 0·0015, and a reasonable overall agreement (see figure 7); inclusion of higher order terms up to $k=4$ reduced the variance to 0·00052 and gave a good overall agreement. The plots obtained by truncating the two series in equations (16) and (17) at $k=4$ were found to coincide with the original results, to the resolution of the figure. This contrasts with other simulated short range nematic potential models in three dimensions, and with experimental data on real ones [48–50], where a good fit was obtained by truncating the series in equation (21) at $k=1$.

The molecular field treatment can be refined by using various cluster-variational techniques (for example [24, 51–53]), 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 [53], and later applied to nematics (for example [54, 55]). For example, a two site cluster treatment [53–55] can be developed for $n=2$, and predicts a transition with finite discontinuities for energy, heat capacity and order parameters, taking place at $T_C^*=1{\cdot}093$; the discrepancy is thus reduced to less than 10 per cent.

The present calculations were carried out on, among other machines, a VAX 8350 computer, belonging to the Sezione di Pavia of the 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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