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Computer simulation study of a one dimensional plane rotator system with long-range interactions

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We consider a classical system of particles, consisting of two-dimensional unit vectors associated with a one-dimensional lattice $\{\mathbf{u}_k | k \in Z\}$ and interacting via translationally invariant pair potential(s)

$$W_m = -\epsilon r^{-3/2} T_m(\mathbf{u}_j, \mathbf{u}_k), \quad r = |j - k|, \quad \epsilon > 0;$$

here m is a positive integer and T_m is a Tchebyshev polynomial of the first kind

$$T_m(\mathbf{u}_j \cdot \mathbf{u}_k) = \cos[m(\varphi_j - \varphi_k)],$$

where $\{\varphi_k\}$ are the angles defining the orientations of the plane rotators in an arbitrary reference frame. For the case $m = 1$, Fröhlich *et al.* have proved rigorously the existence of a ferromagnetically ordered phase at low but finite temperature; moreover, all the potential models W_m give the same partition function, and several mean values can be defined in an m -independent way. For example, when $m = 2$, this entails the existence of nematic-like order. The system was characterized quantitatively by Monte Carlo simulation, and calculations were performed in the nematic representation ($m = 2$); simulation results suggest a second-order transition at $T_c^* (\equiv kT_c/\epsilon) = 2.16 \pm 0.01$. Comparison with molecular field and spherical model treatments is also reported: the former, but not the latter, agrees reasonably well with the simulation results.

1. Introduction

We consider a classical system of particles, consisting of n -component unit vectors $\{\mathbf{u}_k\}$, associated with a d -dimensional lattice Z^d ; let \mathbf{x}_k denote their coordinates, and let V_{jk} be their translationally invariant pair interaction potential. When $n = 2$, the unit vectors lie in a plane (in the lattice plane when $d = n = 2$); they are then referred to as plane rotators, and their orientation in an arbitrary laboratory frame is uniquely defined by a set of angles $\{\varphi_k\}$. In addition to a few exactly soluble models [1, 2], over the last twenty years, various rigorous results have been obtained, concerning the existence or the absence of an ordered phase at low but finite temperature, depending on d, n , and the functional form of the potential [3, 4]. We restrict our discussion to isotropic potential models, i.e. functional forms left unchanged by applying to all the unit vectors any linear (orthogonal) transformation of the group $O(n)$:

$$V_{jk} = f(r_{jk})\Psi(\tau_{jk}), \tag{1}$$

where

$$\mathbf{r} = \mathbf{r}_{jk} = \mathbf{x}_j - \mathbf{x}_k, \quad r = |\mathbf{r}|, \quad \tau = \tau_{jk} = \mathbf{u}_j \cdot \mathbf{u}_k. \tag{2}$$

For example, when f has a finite range, an ordered phase may survive for $d = 2$, $n = 1$, but it cannot for $d = 1$ and arbitrary n , nor for $d = 2$, $n \geq 2$ [5–10]. Such theorems do not rule out a Kosterlitz–Thouless transition in two dimensions, whose existence has also been proved rigorously in some cases [11]. Under appropriate conditions, Romerio [12] has proved the absence of orientational order for a two-dimensional liquid of plane rotators, i.e. for potential models of the form in equation (2), but where the coordinates $\{\mathbf{x}_k\}$ are allowed to vary continuously.

It was also pointed out [13] that the vanishing of order in the thermodynamic limit need not exclude its existence for a finite but macroscopically large sample: for example, it is sometimes possible to prove [13] that the relevant quantity (order parameter or transition temperature) vanishes in the thermodynamic limit like $(1/\ln N)$, where N is the number of particles in the system.

For comparison, we also mention that, when $d = n = 3$, nearest-neighbour isotropic potential models such as [4]

$$V_{jk} = -\varepsilon\tau_{jk}, \quad \varepsilon > 0 \quad (3)$$

or [14]

$$V_{jk} = -\varepsilon P_2(\tau_{jk}) \quad (4)$$

are known to produce overall orientational order; here $P_2(\tau)$ is the second Legendre polynomial. On the other hand, it is by now well known that a long-range potential can stabilize an ordered phase when $d \leq 2$; to be more specific, we shall consider the ferromagnetic models

$$V_{jk} = -\varepsilon r_{jk}^{-d-\sigma} \tau_{jk}, \quad d = 1, 2, \quad \sigma > 0, \quad (5)$$

whose behaviour has been extensively investigated as a function of d , n , and σ . When $d \leq 2$ and $n \leq 2$, a ferromagnetic phase is known to exist only in the cases

$$d = 1, \quad n = 1, \quad 0 < \sigma \leq d, \quad [15–17],$$

$$d = 1, \quad n = 2, \quad 0 < \sigma < d, \quad [16, 18, 19],$$

$$d = 2, \quad n = 2, \quad 0 < \sigma < d, \quad [16, 20].$$

These powerful results also imply the existence of a disordering transition; on the other hand, they do not provide quantitative estimates for, say, the transition temperature.

The behaviour of critical exponents in the $d - n - \sigma$ space has been extensively investigated by renormalization group techniques [21–29], and various regions and boundaries have been investigated; the systems' thermodynamic properties were calculated explicitly by the spherical model [30] treatment, which is known to be their exact limit when n tends to infinity [30, 31]; rigorous bounds on the correlation function have also been obtained for the disordered phases [32, 33]. In contrast, simulation results for such systems are rather scarce in the literature [34–35] and the corresponding antiferromagnetic long-range models have been studied far less extensively [36–40], in contrast to the wealth of results available for their short-range counterparts.

From now on, we shall restrict our attention to $d = 1$, $n = 2$ (plane rotators on a linear lattice, so that $x_j = j \in \mathbb{Z}$); we also point out an important symmetry property of plane rotators. We define

$$I_1 = \int_0^{2\pi} \Delta[\cos(t), \sin(t)] dt, \quad (6)$$

where Δ is an arbitrary integrable function, and

$$I_m = \int_0^{2\pi} \Delta[\cos(mt), \sin(mt)] dt, \quad \forall m \in \mathbb{Z} - \{0\}. \quad (7)$$

It can easily be proved that

$$I_m = I_1. \quad (8)$$

Moreover, on the basis of the trigonometric identity

$$\sum_{k=1}^m \exp(2\pi ik/m) = 0, \quad m \geq 2, \quad (9)$$

it is easy to check that

$$\int_0^{2\pi} \left\{ \begin{array}{l} \cos \\ \sin \end{array} \right\} (\Lambda t) \Delta[\cos(mt), \sin(mt)] dt = 0, \quad (10)$$

where Λ is an integer, but not a multiple of m ; on the other hand, when Λ is a multiple of m , say $\Lambda = Lm$, equation (7), is obtained again so that the value of the integral depends on L but not on m .

Let us consider the potential models

$$W_m = f(r)T_m(\tau), \quad m \in \mathbb{Z}, \quad m \geq 1, \quad (11)$$

where T_m are Tchebyshev polynomials of the first kind [41]

$$\begin{aligned} T_m(\tau) &= \cos[\arccos(m\tau)] \\ &= \cos[m(\varphi_j - \varphi_k)]. \end{aligned} \quad (12)$$

Equations (8) and (10) imply that all the potential models W_m have the same partition function and that several mean values can be defined in an m -independent way, as we shall see later. As a step towards a better understanding of its physical behaviour, we decided to carry out a Monte Carlo simulation for a potential model defined by $d = 1, n = 2, 0 < \sigma < 1; \sigma = 0$ produces a ground state with an infinite energy per particle, whereas for $\sigma = 1$ the system disorders at all finite temperatures in the thermodynamic limit. Simulation requires a more precise definition of the potential, thus it seemed to be both simple and reasonable to choose the midpoint $\sigma = 1/2$, i.e.

$$W_m = -\epsilon r^{-3/2} T_m(\tau); \quad (13)$$

the case $m = 1$ produces a ferromagnetically ordered phase, and $m = 2$ defines a lattice model of a nematic liquid crystal. Thus the rigorous results obtained by Fröhlich *et al.* [16] ensure the existence of an ordered phase at low temperatures, and numerical simulation helps characterize it quantitatively. There has been some debate about nematic-like orientational order in low-dimensional systems [42–43], and in some cases its absence has been proved rigorously [7–10, 12]; here we can rely on the proved existence of a transition to an ordered phase [16]. Most theorems concerning the absence of orientational order are based on isotropic pair potentials (cf. equation (1)) and need not hold for more general functional forms [12, 43].

The system's ground state corresponds to the degenerate configuration

$$\varphi_k = \bar{\varphi} + 2\pi l_k/m, \quad l_k = 0, 1, 2, \dots, m - 1, \quad (14)$$

where $\bar{\varphi}$ is an arbitrary constant reflecting the continuous $O(n)$ degeneracy, and the value m induces an additional discrete one. The ground-state energy, in units of $\varepsilon/\text{particle}$, is

$$U_0^* = - \sum_{j=1}^{\infty} j^{-3/2} = -\zeta(3/2) = -2.612, \tag{15}$$

where the function ζ is defined by [41]

$$\zeta(s) = \sum_{k=1}^{\infty} k^{-s}. \tag{16}$$

2. Computational aspects

The calculations were performed using periodic boundary conditions and the Ewald-Kornfeld algorithm for lattice summations [44-47]. We consider a periodically repeated sample, consisting of N particles, with integer coordinates $\{x_j = j\}$ and fractional ones $y_j = x_j/N$, in an arbitrary configuration $\Omega = \{\varphi_k\}$. The relevant formulae for the potential energy of the configuration, based on Tosi's review paper [46], are

$$U(\Omega)/\varepsilon = -(N^{-3/2}/\Gamma(3/4))(D_1 + D_2 + D_3 + D_4), \tag{17}$$

where

$$D_1 = -(2/3)N\omega^{3/2}, \tag{18}$$

$$D_2 = 2\sqrt{(\pi\omega)\mathbf{F}(m) \cdot \mathbf{F}(m)}; \tag{19}$$

$$\mathbf{F}(m) = \sum_{k=1}^N [\cos(m\varphi_k)\mathbf{e}_1 + \sin(m\varphi_k)\mathbf{e}_2], \tag{20}$$

$$D_3 = (1/2) \sum_{j,k} T_m(\mathbf{u}_j \cdot \mathbf{u}_k) \sum_1' |y_j - y_k + 1|^{-3/2} \cdot \Gamma(3/4, \omega^2 |y_j - y_k + 1|^2), \tag{21}$$

$$D_4 = \pi \sum_{h>0} \lambda h \Gamma(-1/4, (\pi h/\omega)^2) \cdot [C_1^2(h) + C_2^2(h) + C_3^2(h) + C_4^2(h)], \tag{22}$$

$$C_{1,2}(h) = \sum_{k=1}^N \sin(2\pi h y_k) \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} (m\varphi_k), \tag{23}$$

$$C_{3,4}(h) = \sum_{k=1}^N \cos(2\pi h y_k) \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} (m\varphi_k), \tag{24}$$

and

$$\Gamma(3/4) = 1.2254167024. \tag{25}$$

Here \mathbf{e}_1 and \mathbf{e}_2 are two arbitrary orthogonal unit vectors and ω is a real positive number which only affects the rates of convergence of the two series (in opposite senses); the series in D_3 ranges over the direct lattice and excludes the case $1 = 0$ when $j = k$; the series in D_4 ranges over the reciprocal lattice excluding $h = 0$. The incomplete gamma function is defined by

$$\Gamma(z, p) = \int_p^{+\infty} t^{z-1} \exp(-t) dt, \tag{26}$$

and the recurrence property [41, 46]

$$\Gamma(z + 1, p) = z\Gamma(z, p) + p^z \exp(-p) \quad (27)$$

can be used to reduce the functions with negative z to functions with positive z .

We chose ω to be 6.75 and truncated the series in D_2 at $h \leq 20$; the other series was truncated according to the usual nearest-image prescription; calculations were performed mostly with $m = 2$, in the nematic representation. As a compromise between available computational resources and desired accuracy, we chose $N = 1024$ particles. At the lowest temperature investigated, calculations were started from the ground-state configuration (cf. equation (14)); dimensionless reduced temperatures and potential energies are given by

$$T^* = kT/\varepsilon, \quad U^* = \langle W \rangle / (N\varepsilon), \quad (28)$$

where $\langle W \rangle$ is the mean sample energy and U^* is the mean energy per particle.

The calculations were performed in increasing temperature order, 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 8000; sub-averages for evaluating statistical errors were calculated over macrosteps consisting of 200 cycles. Calculated quantities include energy, configurational specific heat C_v (both as a fluctuation quantity and by least-square fitting and numerical differentiation of the energy), Kirkwood g -factors, orientational correlation functions and order parameters. The singlet orientational distribution function was calculated at one temperature in the ordered region (at $T^* = 2$).

On the basis of equations (8) and (10), several quantities can be defined in an m -independent way; for example, the magnetic moment per particle and its mean square value are given by

$$\mathbf{M}_1 = (1/N)\langle \mathbf{F}(m) \rangle_m; \quad M_2 = (1/N^2)\langle \mathbf{F}(m) \cdot \mathbf{F}(m) \rangle_m, \quad (29)$$

where $\langle \dots \rangle_m$ denotes an average with respect to the potential W_m . We also define m -independent Kirkwood g -factors [48] and orientational correlation functions by

$$g_{2L} = \{2/[N^*(N-1)]\} \left\langle \sum_{j < k} T_{Lm}(\mathbf{u}_j \cdot \mathbf{u}_k) \right\rangle_m, \quad L = 1, 2 \quad (30)$$

and

$$G_L(r) = \langle T_{Lm}(u_j \cdot u_k) \rangle_m, \quad \text{as functions of } r = |j - k|, \\ L = 1, 2, 3, 4; \quad (31)$$

here g_2 essentially coincides with M_2 ; orientational correlation functions were calculated at a few selected temperatures, both below and above the transition, in order to save computer time.

In keeping with nematics, we define the order parameters by the mean values [49-51]

$$\bar{T}_{2L} = (1/N) \left\langle \sum_{k=1}^N T_{2L}(\mathbf{u}_k \cdot \mathbf{v}) \right\rangle_2, \quad L = 1, 2, \quad (32)$$

where the unit vector \mathbf{v} defines the director. Since its orientation is not, in general, known in advance and can change in the course of simulation, we had to follow a

more elaborate procedure in order to compensate for director fluctuations (similar difficulties arise for M_1 in the magnetic case). We have calculated for each macrostep [49–51] both the traceless second-rank ordering tensor

$$Q_{\lambda\mu} = 2\langle u_\lambda u_\mu \rangle - \delta_{\lambda\mu}, \tag{33}$$

and its fourth-rank equivalent

$$B_{\lambda\mu\nu\rho} = [48\langle u_\lambda u_\mu u_\nu u_\rho \rangle - 8(\delta_{\nu\rho}\langle u_\lambda u_\mu \rangle + \delta_{\mu\rho}\langle u_\lambda u_\nu \rangle + \delta_{\mu\nu}\langle u_\lambda u_\rho \rangle + \delta_{\lambda\rho}\langle u_\mu u_\nu \rangle + \delta_{\lambda\nu}\langle u_\mu u_\rho \rangle + \delta_{\lambda\mu}\langle u_\nu u_\rho \rangle) + 2(\delta_{\lambda\mu}\delta_{\nu\rho} + \delta_{\lambda\nu}\delta_{\mu\rho} + \delta_{\lambda\rho}\delta_{\mu\nu})]/6. \tag{34}$$

$Q_{\lambda\mu}$ is then diagonalized to obtain its eigenvalues $\{q_1, q_2\}$ where $q_1 + q_2 = 0$, and eigenvectors $\{v_1, v_2\}$. The eigenvector associated with the positive eigenvalue gives the director orientation in the laboratory frame. Additional checks indicate it to be stable over the macrostep length used here [49]. (In equations (33) and (34), $\langle . . . \rangle$ means $\langle . . . \rangle_2$.) Let now $q_3 = |q_1|$ and let \bar{q}_1, \bar{q}_2 and \bar{q}_3 indicate their averages over all macrosteps, and let $\bar{q}_4 = |\bar{q}_1|$; owing to director fluctuations over several macrosteps, \bar{q}_3 and \bar{q}_4 do not coincide, although they do so at low temperatures, and agree qualitatively in the ordered phase; we take \bar{q}_3 to define the order parameter \bar{T}_2 for the ordered phase [49–51].

In the disordered region, the director is loosely defined [51], and the order parameter should be zero apart from sample size effects; here \bar{q}_3 can be expected to overestimate the amount of orientational order, and \bar{q}_4 to underestimate it; we also calculated and report the quantity

$$\bar{q}_5 = (\bar{q}_3 + \bar{q}_4)/2. \tag{35}$$

In principle the disordering temperature has to be known and then we should switch from one definition to the other; this piece of information is supplied by the thermodynamic properties. For each macrostep we reorder the eigenvalues to give $\{q'_1, q'_2 | q'_2 > 0\}$; the correspondingly reordered eigenvectors $\{v'_1, v'_2\}$ define the column vectors of an orthogonal matrix **A** such that

$$\sum_{j=1}^2 \sum_{k=1}^2 A_{\lambda j} A_{\mu k} Q_{jk} = q'_\lambda \delta_{\lambda\mu}, \tag{36}$$

which, in turn induces an orthogonal transformation of **B**

$$B'_{\lambda\mu\nu\rho} = \sum_{i=1}^2 \sum_{j=1}^2 \sum_{k=1}^2 \sum_{l=1}^2 A_{\lambda i} A_{\mu j} A_{\nu k} A_{\rho l} B_{ijkl}. \tag{37}$$

We define [51]

$$\bar{T}_4 = \bar{B}'_{2222}, \tag{38}$$

where the bar denotes an average over all macrosteps. As for the singlet orientational distribution function, after equilibration we generated 10·24 million moves at $T^* = 2$ and analysed every 2048th configuration as described later; such a length was necessary in order to achieve reasonable statistics. In the present case the distribution function is an even function of ϑ , where ϑ is the angle formed by the individual molecule with the director. This can be expanded as [50]

$$S(\vartheta) = (1/\pi) \left[1 + 2 \sum_{k>0} a_{2k} \cos(2k\vartheta) \right], \tag{39}$$

where the quantities a_{2k} are even rank order parameters, and ϑ can be restricted between 0 and π . The whole Monte Carlo chain was sub-divided into macrosteps, and configurations to be analysed were dumped on a disc file; the ordering tensor was averaged and diagonalized, and the eigenvector \mathbf{v} associated with its positive eigenvalue defined the director. The configurations to be analysed were retrieved, and for each particle the quantity $\gamma = \arcsin(|\mathbf{v} \cdot \mathbf{u}_i|)$ was calculated and converted to an integer counter for a 201-bin histogram.

3. Results and comparison with other treatments

The results for the potential energy, the specific heat, the order parameters and the Kirkwood g -factors are plotted in figures 1 to 4, and clearly indicate a disordering transition taking place at temperatures between 2.15 and 2.2. The energy and order parameter results suggest a continuous change across the transition, and the specific heat suggests a weak discontinuity; we propose therefore a second-order transition at $T_c^* = 2.16 \pm 0.01$. The transition is known to be weakly first-order in real nematics and for various short-range potential models studied in three dimensions, where the order parameter at the transition typically ranges between 0.3 and 0.5 [51 (a), 52–61]. Among them, the Lebwohl–Lasher lattice model (cf. equation (4)) has been extensively simulated, and its transition temperature is estimated to be 1.1232 ± 0.0006 for a sample consisting of 27,000 particles [51 (a)]; simulation estimates obtained with smaller sample sizes may differ by up to 2 per cent [51 (a), 54 (c)]. We also notice a broad

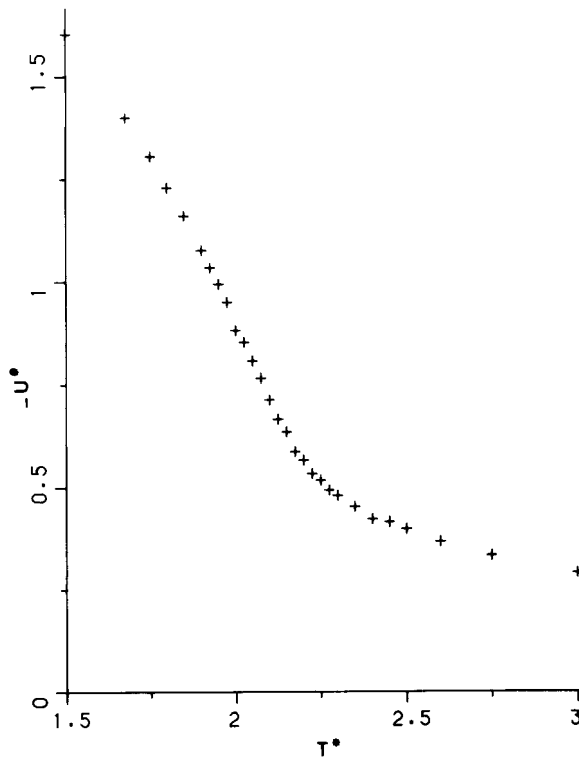


Figure 1. Results for the potential energy; the relative statistical error is usually not greater than 0.5 per cent.

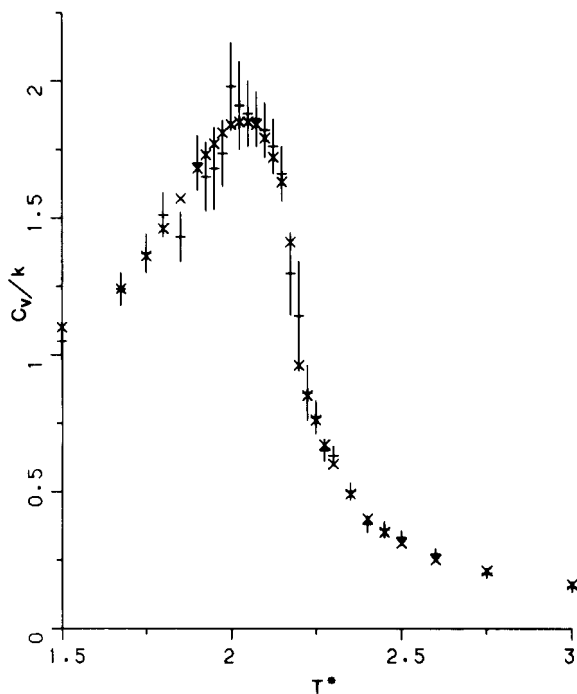


Figure 2. The configurational specific heat: fluctuation quantities with error bars, and results obtained by least-square fitting of the energy.

qualitative similarity with a simulated two-dimensional potential model defined by $d = 2$, $n = 2$, $\sigma = 1$ [62], where $T_c^* = 3.96 \pm 0.02$. For another comparison, we consider the two one-dimensional lattice models with nearest-neighbour interactions defined by equation (4) ($n = 3$) and by its T_2 counterpart ($n = 2$) respectively. They have been solved exactly [7], and found to disorder at all finite temperatures; simulation results [63] agree rather well with the exact ones, and only mimic orientational disorder when the sample size exceeds 1000.

All the orientational correlation functions (cf. figure 5) were found to decrease with distance in an essentially monotonic way, and higher-order ones quickly decay to zero, already in the ordered phase. We found $|G_3(r)| \leq 0.01$ and $|G_4(r)| \leq 0.003$ at all distances for $T^* = 2$, and $|G_2(r)| \leq 0.01$ at all distances for $T^* = 2.25$. In the ordered region, the long-distance limits of G_1 and G_2 agree with the corresponding order parameters, according to [49–50]

$$\bar{T}_{2L}^2 = \lim_{r \rightarrow \infty} G_L(r), \quad L = 1, 2; \quad (40)$$

in this region $G_1(r)$ is well fitted by the functional form

$$G_1(r) = c_1 + c_2/(c_3 + r^p). \quad (41)$$

On the basis of equation (40), the quantities \bar{T}_{2L} (calculated in the nematic representation via the ordering tensors) can be taken as m -independent order parameters. In the disordered region, G_1 should tend to zero as r tends to infinity; owing to finite sample size, periodicity and long-rangedness of the potential, we found for G_1 a long-distance limit of the order of 0.0025. In order to compensate for the residual order, we fitted

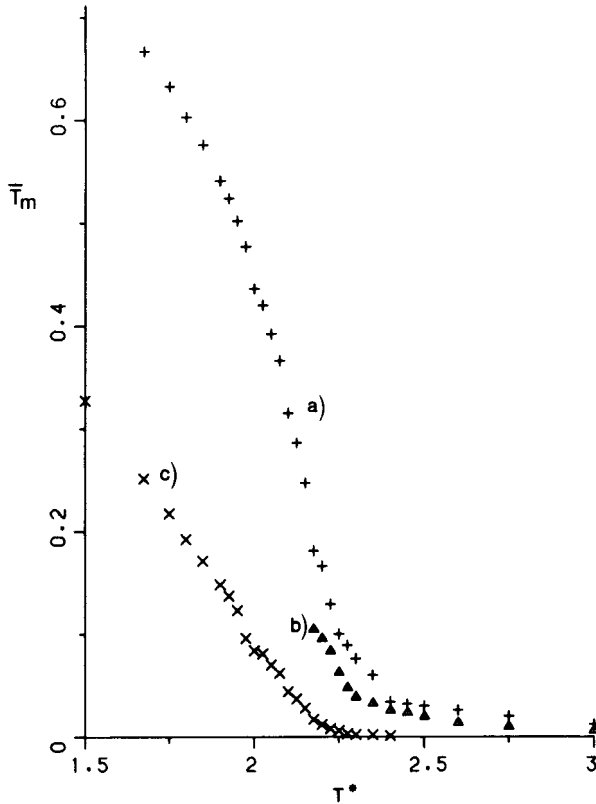


Figure 3. The results for the order parameters (a) \bar{T}_2 as calculated via \bar{q}_3 ; (b) \bar{T}_2 as calculated via \bar{q}_5 ; (c) \bar{T}_4 ; the quantities \bar{q}_3 and \bar{q}_5 are defined in the text.

G_1 by the function form [64–65]

$$\left. \begin{aligned} G_1(r) &= c_1 + h(r) + h(N - r); \\ h(r) &= c_2 \exp(-sr)/(c_3 + r^p); \quad 0 < r < N/2. \end{aligned} \right\} \quad (42)$$

$h(r)$ has a rather general and flexible function form, consistent with known or expected behaviour of the correlation function [31–33, 66]. The fitting parameters were determined using the general non-linear least-square program MINUIT in the CERN library, and some of them are reported in the table; inclusion of the term $h(N - r)$ did not appreciably change the quality of the fit for $T^* \geq 2.5$.

A simple molecular field approximation [48, 67–69] can be developed starting from equation (13) for the pair potential and expressing it in terms of the angles φ_j and φ_k for the two particles. The potential ($m = 1$) is then averaged over the orientation of the second particle according to the prescription

$$\langle \sin \varphi_k \rangle = 0 \quad \text{and} \quad \langle \cos \varphi_k \rangle = \bar{P}_{1, \text{MF}}; \quad (43)$$

summation over the interparticle vectors allowed by the lattice gives the one-particle pseudopotential as

$$\tilde{W}(\varphi) = -2 |U_0^*| \bar{P}_{1, \text{MF}} \cos \varphi,$$

with

$$|U_0^*| = 2.612. \quad (44)$$

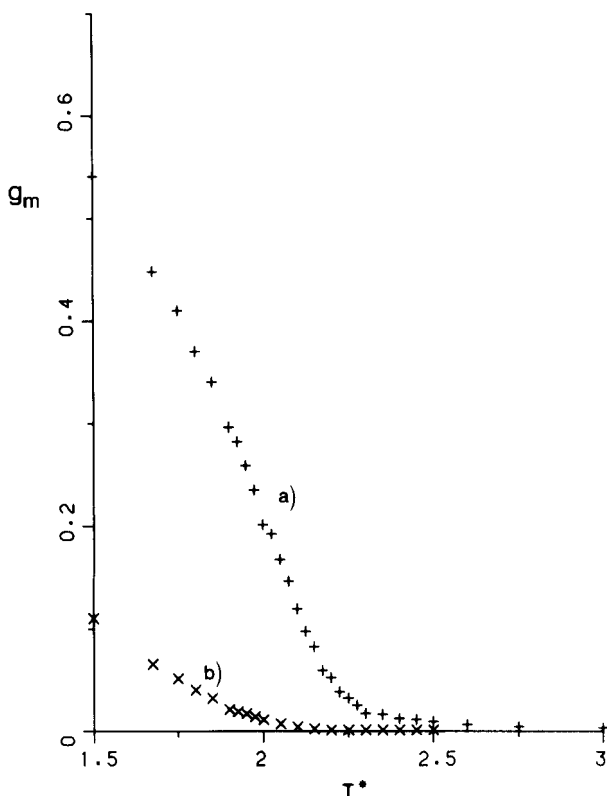


Figure 4. The results for the Kirkwood g -factors: (a) g_2 ; (b) g_4 as a function of temperature.

Fitting parameters in equations (41) and (42) as a function of temperature.

T^*	p	s
1.50	0.66	—
1.75	0.62	—
2.00	0.64 (± 0.04)	—
2.25	0.56	0.009
2.50	0.69	0.005
2.75	0.84	0.007
3.00	0.91 (± 0.06)	0.011 (± 0.003)

Here $\bar{P}_{1,MF}$ is determined by the usual self-consistency condition

$$\bar{P}_{1,MF} = \frac{\int_0^{2\pi} \cos(\varphi) \exp(-\tilde{W}/T^*) d\varphi}{\int_0^{2\pi} \exp(-\tilde{W}/T^*) d\varphi}$$

$$= I_1(\varrho)/I_0(\varrho),$$

with

$$\varrho = 2|U_0^*|\bar{P}_{1,MF}/T^*, \quad (45)$$

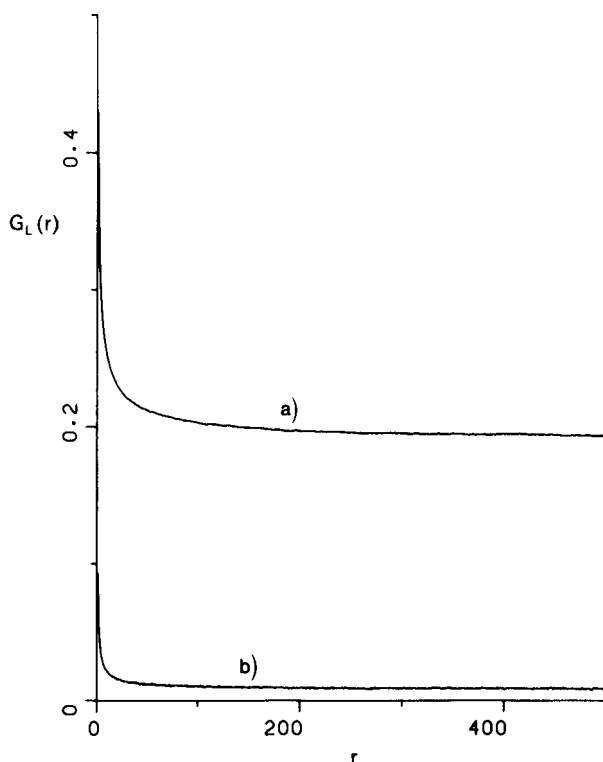


Figure 5. Plots of the orientational correlation functions at the temperature T^* of 2. (a) $G_1(r)$; (b) $G_2(r)$; the correlation functions $G_L(R)$ are defined in the text.

where I_1 are modified Bessel functions of order 1. Upon solving equation (45) numerically, $\bar{P}_{1,MF}$ is found to decrease continuously to zero at the temperature $T_{c,MF}^* = |U_0^*|$, and the transition is found to be second order [67–69]. The transition temperature is overestimated by 20 per cent at worst; a similar success of the molecular field approximation has been found for various simulated short-ranged nematogenic models in three dimensions [52–61]. Critical exponents, with the meaning of symbols as defined by Fisher and Stanley [31, 66], have been calculated by various treatments, and are reported here for the sake of completeness. The molecular field approximation gives

$$\alpha = 0, \quad \beta = 1/2. \quad (46)$$

In the spherical model treatment [30] substitution of the stronger condition

$$\mathbf{u}_k \cdot \mathbf{u}_k = 1, \quad k = 1, 2, \dots, N, \quad (47)$$

with the weaker one

$$\sum_{k=1}^N \mathbf{u}_k \cdot \mathbf{u}_k = N \quad (48)$$

enables the thermodynamics to be solved explicitly. On the basis of Joyce's results [30(b)], the transition temperature is found to be

$$\begin{aligned} \Theta_S &= T_{c,SM}^* = 2 \cdot 0.7959 \cdot |U_0^*|, \\ &= 4.158; \end{aligned} \quad (49)$$

the specific heat has the constant value

$$C_v = 0.5k, \quad T^* \leq \Theta_s, \quad (50)$$

and changes continuously, but with a discontinuous slope, at the transition temperature. The order parameter (mean magnetic moment per spin) is given by

$$M = \sqrt{[1 - (T^*/\Theta_s)]}, \quad T^* \leq \Theta_s. \quad (51)$$

Here the agreement between the spherical model and the simulation results is rather bad, in contrast with the reasonable success of the molecular field predictions. The critical properties calculated by the spherical model treatment [30] are

$$\alpha = 0, \quad \beta = 1/2, \quad \nu = 2, \quad \eta = 1.5, \quad \gamma = 1 \quad (52)$$

$$\left. \begin{aligned} \xi(T) &\propto (1/t)^2 |\ln t|^2, & \chi(T) &\propto (1/t) |\ln t|, \\ t &= (T^* - T_c^*)/T_c^*, & t &> 0 \end{aligned} \right\} \quad (53)$$

$$M(t = 0, H) \propto H^{1/3} |\ln H| \quad (\text{critical isotherm}). \quad (54)$$

Critical exponents for a general (d, n, σ) potential model have been obtained by several authors via renormalization group techniques [21–29]; the results for $d = 1, \sigma = 1/2$ and arbitrary n are [28, 29]

$$\nu = 2, \quad \eta = 1.5, \quad \gamma = 1, \quad \forall n \quad (55)$$

$$\alpha = 0 \text{ up to order } 1/n \quad (56)$$

and

$$\left. \begin{aligned} \xi(T) &\propto (1/t)^2 |\ln t|^{2n'}, & \chi(T) &\propto (1/t) |\ln t|^{n'}, \\ n' &= (n + 2)/(n + 8), \end{aligned} \right\} \quad (57)$$

in agreement with the spherical model in the limit $n \rightarrow \infty$. At the transition temperature, the correlation function G_1 possesses the asymptotic power law behaviour [31–33, 66]

$$G_1(r) \propto r^{-(d-2+\eta)} \quad (58)$$

and both spherical model and renormalisation group treatments give $\eta = 1.5$. Our simulation results cannot claim to allow an accurate determination of the critical quantities, which requires larger sample sizes (and greater computational resources). Yet it should be noted that a crude conjecture based on the results in the table gives $s = 0, p = 0.6 \pm 0.05$ at the transition, i.e. $\eta = 1.6 \pm 0.05$.

As for the distribution function (cf. figure 6), the coefficients a_{2k} in equation (39) were calculated directly from the histogram, 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 squares fit. We obtained rather good agreement by truncating the expansion at $k = 4$, and found a variance of 0.000027 with the values

$$a_2 = 0.412 \pm 0.002,$$

$$a_4 = 0.071 \pm 0.002,$$

$$a_6 = 0.008 \pm 0.002,$$

$$a_8 = 0.001 \pm 0.002.$$

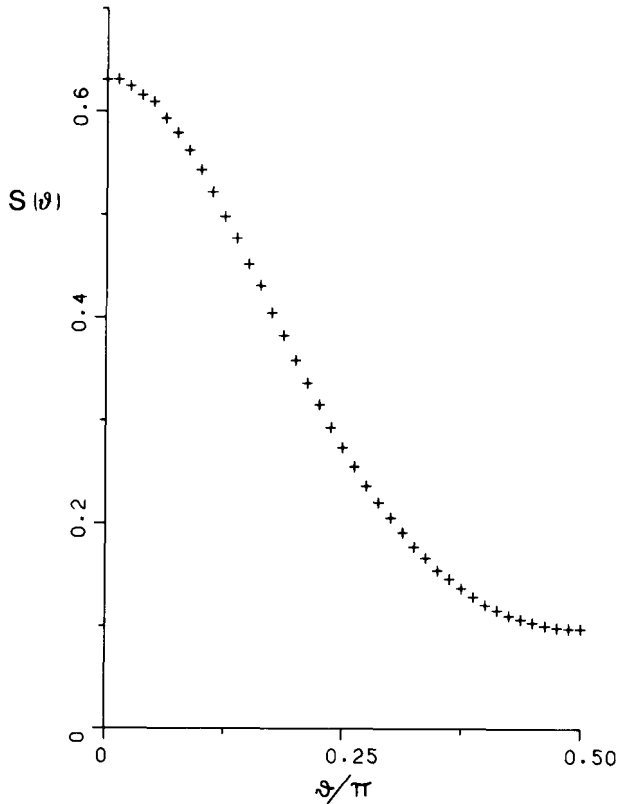


Figure 6. A plot of the singlet orientational distribution function at $T^* = 2$.

Inclusion of higher-order terms up to $k = 6$ led to coefficients a_{2k} ($k > 4$) smaller than 0.0005 in magnitude and did not appreciably improve the fit. The values a_2 and a_4 agree very well with the corresponding values $\bar{P}_2 = 0.413 \pm 0.003$ and $\bar{P}_4 = 0.072 \pm 0.003$, as obtained via the ordering tensors and a far better statistics. The molecular field treatment predicts for $S(\vartheta)$ an expression of the form [50, 69]

$$S(\vartheta) = \exp \left[b_0 + \sum_{k>0} b_{2k} \cos(2k\vartheta) \right], \quad (59)$$

where the coefficients b_{2k} are also predicted to depend on the order parameters; truncation of the series in equation (59) at $k \leq 2$ gave a variance of 0.00011, and inclusion of higher-order terms up to b_8 reduced it to 0.000027. This contrasts with other simulated short-range potential models in three dimensions, and with experimental data on real nematics [70–72], where a good fit was obtained by truncating the series in equation (59) at $k = 1$. The simulation results point to the conclusion that the long-range character of the potential produces an overall mean-field-like behaviour of the system.

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