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Monte Carlo simulation of a one dimensional classical Heisenberg model with long range interactions

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We have studied a classical system, consisting of three dimensional unit vectors associated with a one dimensional lattice $\{\mathbf{u}_k | k \in Z\}$ and interacting via the translationally invariant pair potential

$$V_{jk} = -\varepsilon r^{-3/2} \mathbf{u}_j \cdot \mathbf{u}_k, \quad r = |j - k|, \quad \varepsilon > 0.$$

This potential model has been proven rigorously to possess a ferromagnetically ordered phase at low but finite temperature. We also consider the pair interaction defined by

$$V'_{jk} = (-1)^{j+k} V_{jk},$$

the two potential models have the same partition function, and essentially the same structural properties, thus V' possesses a low-temperature transition to an antiferromagnetically ordered phase. In turn, V' can be regarded as an extreme case of a nematogenic lattice model, whose structural properties can still be evaluated under V. The system was characterized quantitatively by Monte Carlo simulation, whose results are compatible with a second order transition at $T_c^*(=kT_c/\varepsilon)$ of $1{\cdot}48 \pm 0{\cdot}02$. Comparison with molecular field and spherical model treatments is also reported; the former, but not the latter, agrees reasonably with the simulation results.

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. The present paper continues this tradition, considering a potential model known rigorously to possess an ordering transition at finite temperature, and using numerical simulation to elucidate its physical properties. We consider a classical system, consisting of n component unit vectors $\{\mathbf{u}_k\}$, associated with a d dimensional lattice, Z^d; $\mathbf{x}_k$ denote their coordinates, and V_{jk} is 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 $\{\varphi_k\}$. 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

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

It is worth recalling two important symmetry properties of these potential models:

(*a*) Plane rotators: we rewrite the potential (equation (1)) in the slightly more general form

$$W_m = f(r)\Psi[T_m(\tau)], \tag{3}$$

where m is an arbitrary positive integer, and T_m are Tchebyshev polynomials of the first kind [1]:

$$\begin{aligned} T_m(\tau) &= \cos\,[\arccos\,(m\tau)] \\ &= \cos\,[m(\varphi_j - \varphi_k)]. \end{aligned} \tag{4}$$

For given functional forms of f and Ψ, all of the potentials W_m have the same partition function, and their structural properties can be defined in a manner independent of m.

(*b*) Spin-flip in bipartite lattices: for any $\mathbf{x}_j = \{j_\lambda | \lambda = 1, 2, \ldots, d\}$, we define

$$q_j = \prod_{\lambda=1}^{d} (-1)^{j_\lambda}, \tag{5}$$

the lattice consists of two interpenetrating sublattices, and each lattice node j belongs to either of them, according to the sign of q_j, and is surrounded by nearest neighbours belonging to the other sublattice, then second nearest neighbours belonging to its own, and so on. We consider the two potential models

$$V_{jk} = f(r)\Delta(\tau), \quad V'_{jk} = q_j q_k V_{jk}, \tag{6}$$

where Δ is an arbitrary odd function of its argument.

V and V' give the same partition function, and their structural properties (e.g. correlation functions and ordering tensors) can be related via the simple transformation

$$\langle (u_{j\mu}u_{kv})^L \rangle' = (q_j q_k)^L \langle (u_{j\mu}u_{kv})^L \rangle, \tag{7}$$

where L is an arbitrary integer, μ and v refer to cartesian components, and $\langle \cdots \rangle$ and $\langle \cdots \rangle'$ denote averages with respect to V and V', respectively.

In addition to a few exactly soluble models [2, 3], various rigorous results have been obtained, concerning the existence or absence of an ordered phase at low but finite temperature, depending on d, n, and the functional form of the potential. 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 $d = 2$, $n \geqslant 2$ [2, 4]. When $d = 2$ and $n = 2$, such theorems do not rule out a transition to a low-temperature phase with an inverse-power decay of correlations and infinite susceptibility, i.e. a Kosterlitz–Thouless transition, whose existence has also been proven rigorously in some cases [5]. For comparison, we also mention that, when $d = n = 3$, nearest-neighbour isotropic potential models such as the classical Heisenberg model [4]

$$V_{jk} = -\varepsilon\tau_{jk}, \quad \varepsilon > 0 \tag{8}$$

or the Lebwohl–Lasher lattice model [6]

$$V_{jk} = -\varepsilon P_2(\tau_{jk}) \tag{9}$$

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

ferromagnetic potential

$$V_{jk} = -F(r_{jk})\tau_{jk}, \quad F(r) = +|f(r)| \tag{10}$$

can stabilize an ordered phase when $d \leqslant 2$, and spin-flip symmetry entails the existence of the corresponding antiferromagnetic transition (so that V and V' can unambiguously be referred to as ferro and antiferromagnetic representations, respectively). Moreover, these results imply the existence of nematic-like order for plane rotators when $m = 2$, i.e. orientational order but no net magnetization.

We specialize our discussion to the functional forms

$$F(r) = r^{-d-\sigma}, \quad d = 1, 2, \quad \sigma > 0, \tag{11}$$

whose behaviour has been extensively investigated as a function of d, n, and σ. When $d \leqslant 2$ and $n \leqslant 3$, a ferromagnetic phase is known to exist only in the following cases [7–13]

$$d = 1, \quad n = 1, \quad 0 < \sigma \leqslant d,$$

$$d = 1, \quad n = 2 \quad 3, \; 0 < \sigma < d,$$

$$d = 2, \quad n = 2, \quad 3, \; 0 < \sigma < d.$$

These powerful theorems also entail the existence of a disordering transition; on the other hand, they do not provide quantitative estimates for, say, the transition temperature or order parameters.

The behaviour of critical exponents in the $d - n - \sigma$ space has often been investigated by renormalization group techniques (see, e.g., [14, 15]). The system's thermodynamics was calculated explicitly by the spherical model [16] treatment, which is known to be their exact limit when n tends to infinity [16, 17]; rigorous bounds on the correlation functions have also been obtained for the disordered phases [18, 19]. Simulation results for such systems are still rather scarce in the literature (e.g. [20–22]). The corresponding antiferromagnetic long range models defined by the plus sign in equation (10) have been studied far less extensively (e.g. [23]), and no such existence theorems are known for them. This is in marked contrast to the wealth of results available in the literature for their short range counterparts. From now on, we restrict our attention to $n = 3$ (the classical Heisenberg model), $d = 1$, so that $x_j = j \in Z$. As a step towards a better understanding of its physical behaviour, we decided to carry out Monte Carlo simulations for a potential model defined by $d = 1$, $n = 3$, $0 < \sigma < 1$. When σ vanishes the ground state has an infinite energy per particle, and order at all finite temperatures, whereas for $\sigma = 1$ the system disorders in the thermodynamic limit at all finite temperatures. Simulation requires a more precise definition of the potential (i.e. of σ), thus it seemed to be both simple and reasonable to choose the midpoint $\sigma = 1/2$, i.e.

$$V_{jk} = -\varepsilon r^{-3/2}\tau, \tag{12}$$

thus extending previous numerical work on its Ising [24, 25] and plane-rotator [22] counterparts.

The rigorous results obtained by Fröhlich *et al.* [8] ensure the existence of an ordered phase at low temperature and numerical simulation helps characterize it quantitatively. The ground state energy, in units ε/particle, is

$$U_0^* = -\sum_{j=1}^{\infty} j^{-3/2} = -\zeta(3/2) = -2{\cdot}612, \tag{13}$$

where the function ζ is defined by [1]

$$\zeta(s) = \sum_{k=1}^{\infty} k^{-s}. \tag{14}$$

2. Computational aspects

The calculations were performed using periodic boundary conditions and the Ewald–Kornfeld algorithm for summing the long range interaction [26–28]. 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 orientational configuration $\Omega = \{\mathbf{u}_k\}$. The relevant formulae for the potential energy of the configuration, based on Tosi's review [28], are

$$U(\Omega)/\varepsilon = -(N^{-3/2}/\Gamma(3/4))(D_1 + D_2 + D_3 + D_4), \tag{15}$$

where

$$D_1 = -(2/3)N\omega^{3/2}, \tag{16}$$

$$D_2 = 2\sqrt{(\pi\omega)}\mathbf{m}\cdot\mathbf{m}, \quad \mathbf{m} = \sum_{k=1}^{N} \mathbf{u}_k, \tag{17}$$

$$D_3 = (1/2)\sum_{j,k}(\mathbf{u}_j\cdot\mathbf{u}_k)\sum_{1}{}' |y_j - y_k + 1|^{-3/2}\Gamma(3/4, \omega^2|y_j - y_k + 1|^2), \tag{18}$$

$$D_4 = \pi\sum_{h>0}\sqrt{h}\Gamma(-1/4, (\pi h/\omega)^2)[C_x^2(h) + C_y^2(h) + C_z^2(h) + S_x^2(h) + S_y^2(h) + S_z^2(h)], \tag{19}$$

$$C_\lambda(h) = \sum_{k=1}^{N} \cos(2\pi h y_k)u_{k\lambda}, \tag{20a}$$

$$S_\lambda(h) = \sum_{k=1}^{N} \sin(2\pi h y_k)u_{k\lambda}, \tag{20b}$$

$$\lambda = x, y, z. \tag{20c}$$

$$\Gamma(3/4) = 1.\ 22541\ 67024. \tag{21}$$

Here ω is a real positive number which only affects the rates of convergence of the two series (in opposite senses) and is usually chosen accordingly [28]; the series in D_3 ranges over the direct lattice and excludes the case $l = 0$ when $j = k$; the series in D_4 ranges over the reciprocal lattice excluding $h = 0$. The incomplete gamma function is defined by

$$\Gamma(z, p) = \int_p^{+\infty} t^{z-1}\exp(-t)\,dt \tag{22}$$

and the recurrence property [1, 28]

$$\Gamma(z + 1, p) = z\Gamma(z, p) + p^z\exp(-p) \tag{23}$$

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 $h \leqslant 10$; the other series was truncated according to the usual nearest image prescription. Calculations were carried out using the ferromagnetic potential. As a compromise between available computational resources and desired accuracy, we used 1000 particles. At the lowest temperature investigated, calculations were started from the ground state configuration; dimensionless reduced temperatures and potential energies are given by

$$T^* = kT/\varepsilon, \quad U^* = \langle V \rangle/(N\varepsilon), \tag{24}$$

where $\langle V \rangle$ is the mean sample energy and U^* is the mean energy per particle. 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 10000 cycles. Subaverages for evaluating statistical errors were calculated over macrosteps consisting of 200 cycles.

Calculated quantities include energy, configurational specific heat C_v (obtained both as a fluctuational quantity and by least-square fitting and numerical differentiation of the energy), orientational correlation functions and order parameters. The orientational correlation functions are defined by

$$G_L(r) = \langle P_L(\mathbf{u}_j \cdot \mathbf{u}_k) \rangle, \quad \text{as functions of } r = |j - k|, \quad L = 1, 2. \tag{25}$$

The magnetic order parameter is defined by

$$M = (1/N)\langle \sqrt{(\mathbf{m} \cdot \mathbf{m})} \rangle = (1/N)\langle \sqrt{(\mathbf{m}' \cdot \mathbf{m}')} \rangle', \quad \mathbf{m}' = \sum_{k=1}^{N} q_k \mathbf{u}_k, \tag{26}$$

where the spin-flip symmetry has been taken into account. The antiferromagnetic representation possesses overall orientational order but no net magnetic moment, and can be regarded as exhibiting secondary nematic behaviour, or as an extreme case of a nematogen, and investigated accordingly (the antiferromagnetic representation has a finite sublattice magnetization, whereas a nematic lattice model does not). We see from equation (7) that its nematic ordering tensors and singlet orientational distribution function can be evaluated directly in the ferromagnetic representation, used here for actual calculations. Nematic ordering tensors and associated order parameters $\bar{P}_2$ and $\bar{P}_4$ were defined and calculated as discussed in detail elsewhere [29–31]. The singlet orientational distribution function was calculated at $T^* = 1{\cdot}0$, over a chain consisting of 10 000 cycles, and we analysed every second cycle, according to the procedure reported elsewhere [30, 32]; such a length was needed in order to achieve reasonable statistics. In the present case the distribution function is an even function of cos ϑ, where ϑ is the angle formed by an individual molecule with the director. It can be expanded as [30]

$$S(\vartheta) = (1/2)\left[1 + \sum_{k>0} (4k + 1) a_{2k} P_{2k}(\cos \vartheta)\right], \tag{27}$$

where the quantities a_{2k} are even rank order parameters; because of the symmetry, ϑ can be restricted between 0 and $\pi/2$ [30, 32].

3. Results and comparison with other treatments

Results for the potential energy, specific heat and order parameters are plotted in figures 1 to 3, and indicate a disordering transition taking place at temperatures

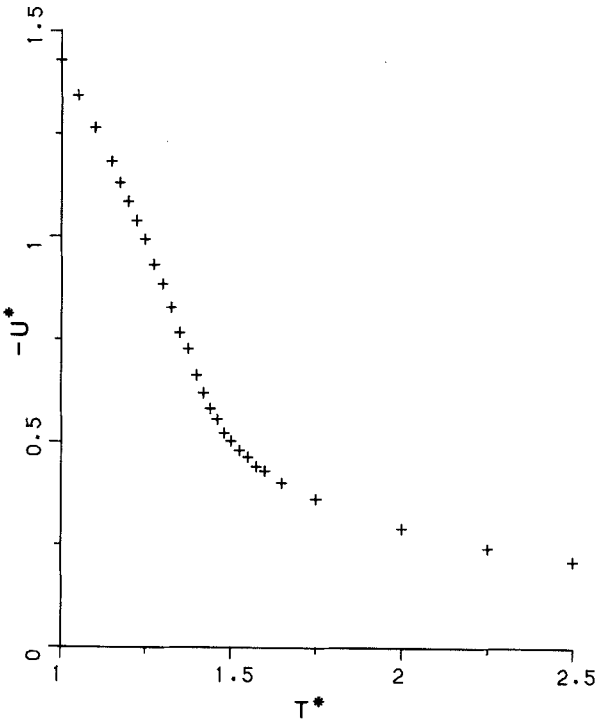

Figure 1. Results for the potential energy; the relative statistical error is usually not greater than 0·5%.

between 1·4 and 1·5. The energy and order parameter results suggest a continuous change across the transition, and the specific heat results are compatible with a weak discontinuity. On the whole, this seems to rule out a first order transition, and to suggest a second or possibly higher order one. The specific heat peaks before the transition, and these results show a broad qualitative similarity with the simulated plane rotator counterpart of the present model [22].

The results for $\bar{P}_4$ (not reported here) are rather small, even in the ordered region: for example, at $T^* = 1{\cdot}0$, we found $\bar{P}_2 = 0{\cdot}317 \pm 0{\cdot}001$ and $\bar{P}_4 = 0{\cdot}030 \pm 0{\cdot}0005$; this is likely to be a reflection of the secondary nematic character of our model. We fitted the results for the (magnetic) order parameter over a certain range $[T_1^*, T_2^*]$ ($T_2^* < 1{\cdot}50$, i.e. inside the ordered region) using the functional form [17]

$$M(T^*) = (T_c^* - T^*)^\beta \tag{28}$$

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

$$T_c^* = 1{\cdot}48 \pm 0{\cdot}02, \quad \beta = 0{\cdot}50 \pm 0{\cdot}01. \tag{29}$$

The value of T_c^* was recalculated and confirmed by fitting $M(T^*)$ as a quadratic or cubic polynomial in $\sqrt{(T_c^* - T^*)}$.

Critical temperature estimates for the Ising [24, 25] and plane rotator [22] counterparts of our potential model are shown in table 1. For comparison we also mention the nearest neighbour models on a simple cubic lattice defined by equations (8) and

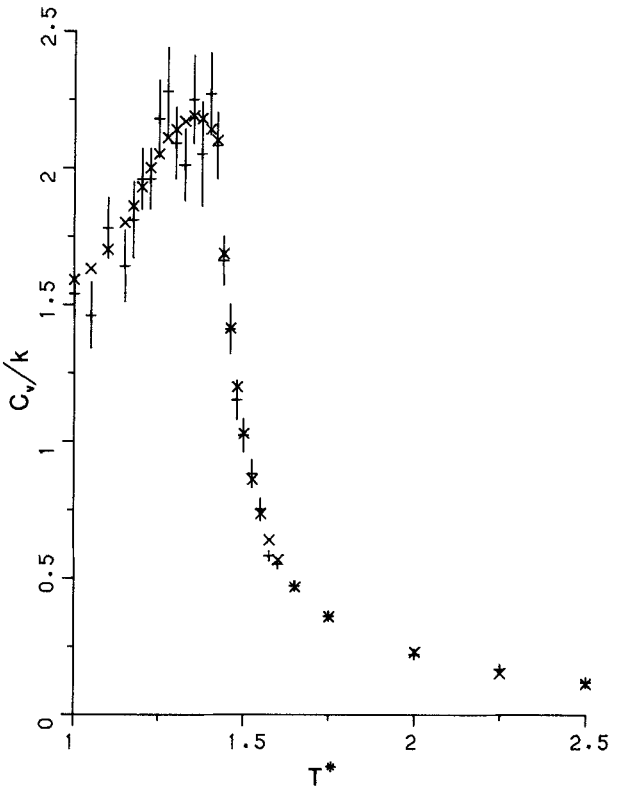

Figure 2. Configurational specific heat: fluctuation quantitities with error bars, and results obtained by least-square fitting of the energy.

Table 1. Critical temperatures calculated for the present potential model and for its Ising [24, 25] and plane-rotator [22] counterparts, by using exact numerical methods (series analysis in [24, 25]; simulation in [22] and in the present work) and the molecular field approximation. The estimated uncertainty on T_c^* is of the same order ($\approx 1\%$) in all three cases, and the spherical model result is 4·158 [16].

n	T_c^*	$T_{c,MF}^*$
1	4·33	5·224
2	2·16	2·612
3	1·48	1·742

(9) respectively. They have been studied extensively, and their estimated transition temperatures are 2·89 ± 0·02 for the classical Heisenberg model [33] and 1·1232 ± 0·0006 for the Lebwohl–Lasher model [31]; their one dimensional counterparts have been solved exactly, and found to disorder at all finite temperatures [2, 34].

The disordering 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 [29, 30]. The orientational correlation functions (see figure 4) were found to decrease with distance in an essentially monotonic way. In the ordered region $G_1(r)$ is well fitted by the functional form

$$G_1(r) = c_1 + c_2/(c_3 + r^p). \tag{30}$$

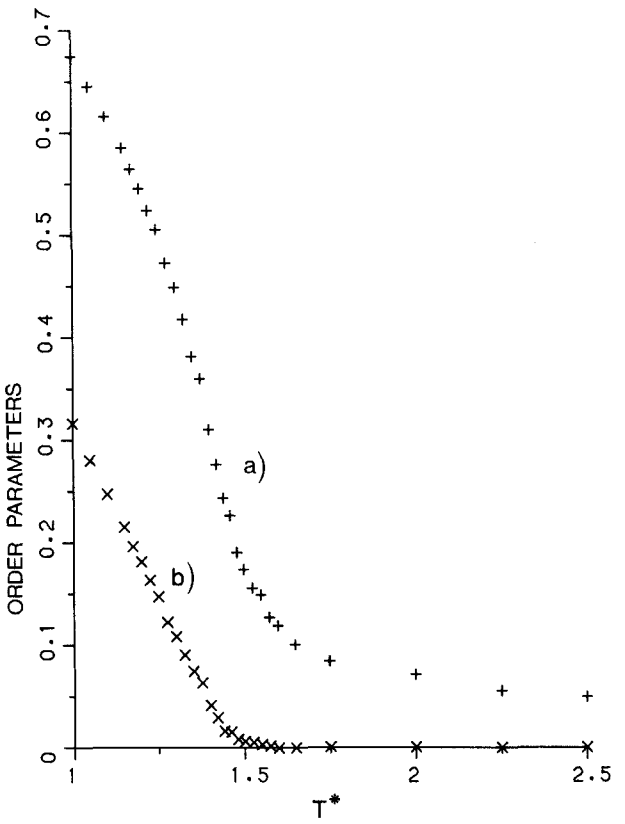

Figure 3. Results for the order parameters: (*a*) M; (*b*) $\bar{P}_2$; the results for $\bar{P}_2$ in the ordered region show a linear dependence on temperature.

In the disordered region, G_1 should tend to zero as r tends to infinity; owing to the finite sample size, periodicity and long ranged nature of the potential, we found for G_1 a long distance limit of the order of 0·0025. In order to compensate for this residual order, we have fitted G_1 by the functional form [35, 36]

$$G_1(r) = c_1 + h(r) + h(N - r); \quad h(r) = c_2 \exp(-sr)/(c_3 + r^p); \quad 0 < r < N/2. \tag{31}$$

$h(r)$ has a rather general and flexible functional form, consistent with known or expected behaviour of the correlation function [17–19, 37]; some fitting parameters are reported in table 2 and inclusion of the term $h(N - r)$ did not appreciably change the quality of the fit for $T^* \geqslant 1{\cdot}65$.

A simple molecular field approximation [17, 38, 39] can be developed for the magnetic system, leading to the single particle pseudopotential

$$\tilde{V}(\vartheta) = -2|U_0^*|P_{1,\mathrm{MF}} \cos \vartheta, \tag{32}$$

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

$$\bar{P}_{1,\mathrm{MF}} = L(\varrho), \quad L(\varrho) = \mathrm{cotgh}\,(\varrho) - 1/\varrho, \quad \varrho = 2|U_0^*|\bar{P}_{1,\mathrm{MF}}/T^*. \tag{33}$$

Upon solving equation (33) numerically, $\bar{P}_{1,\mathrm{MF}}$ is found to decrease continuously to zero at the temperature $\theta_M = T^*_{c,\mathrm{MF}} = (2/3)|U_0^*|$, and the transition is found to be

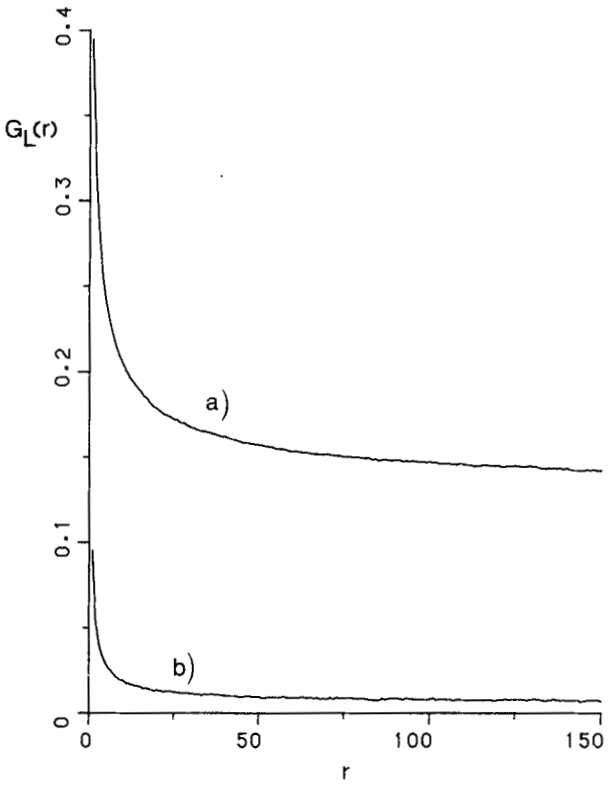

Figure 4. Plots of orientational correlation functions at the temperature $T^* = 1{\cdot}35$: (*a*) $G_1(r)$; (*b*) $G_2(r)$; the correlation functions $G_L(R)$ are defined in the text.

Table 2. Fitting parameters for the correlation function G_1 (see equations (30) and (31)), as function of temperature.

T^*	p	s
1·350	0·59	—
1·375	0·66	—
1·400	0·63	—
1·420	0·63	—
1·440	0·60	—
1·460	0·62	—
1·480	0·66	—
	(±0·02)	
1·500	0·69	0·0012
1·525	0·67	0·0015
1·550	0·71	0·0030
1·575	0·74	0·0016
1·600	0·74	0·0086
1·650	0·88	0·0060
1·750	0·83	0·0070
2·000	1·03	0·0070
	(±0·03)	(±0·001)

second order [38, 39]. The transition temperature is over estimated by some 20 per cent; a similar success of the molecular field approximation is known for both Ising and plane-rotator counterparts of the present model (see table 1). In addition to $\bar{P}_{1,\mathrm{MF}}$, we can define the quantity

$$\bar{P}_{2,\mathrm{MF}} = \frac{\int_0^\pi P_2(\cos\vartheta)\exp(-\tilde{V}/T^*)\sin\vartheta\, d\vartheta}{\int_0^\pi \exp(-\tilde{V}/T^*)\sin\vartheta\, d\vartheta},$$
$$= 1 - T^*/\theta_{\mathrm{M}}; \tag{34}$$

as order parameter this is also in good qualitative agreement with the simulation results (see figure 3).

Critical exponents, have been calculated by various treatments, and are reported here for completeness sake, with the symbols as defined by Fisher and Stanley [17, 37]. The molecular field approximation gives:

$$\alpha = 0, \quad \beta = 1/2. \tag{35}$$

In the spherical model treatment [16], substitution of the stronger condition

$$\mathbf{u}_k \cdot \mathbf{u}_k = 1, \quad k = 1, 2, \ldots, N, \tag{36}$$

with the weaker one

$$\sum_{k=1}^{N} \mathbf{u}_k \cdot \mathbf{u}_k = N \tag{37}$$

enables us to solve for the thermodynamics explicitly. On the basis of Joyce's results [16], the transition temperature is found to be

$$\theta_{\mathrm{S}} = T^*_{\mathrm{c,SM}} = 1{\cdot}5918|U_0^*| = 4{\cdot}158 \tag{38}$$

and the specific heat has the constant value

$$C_{\mathrm{v}} = 0{\cdot}5k, \quad T^* \leqslant \theta_{\mathrm{S}}, \tag{39}$$

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

$$M = \sqrt{[1 - T^*/\theta_{\mathrm{S}})]}, \quad T^* \leqslant \theta_{\mathrm{S}}. \tag{40}$$

As for the transition temperature, the agreement between the spherical model and the simulation results is rather poor, in contrast with the reasonable success of the molecular field treatment.

The critical properties calculated by the spherical model treatment [16] are

$$\alpha = 0, \quad \beta = 1/2, \quad \nu = 2, \quad \eta = 1{\cdot}5, \quad \gamma = 1 \tag{41}$$

$$\xi(T) \propto (1/t)^2|\ln t|^2, \quad \chi(T) \propto (1/t)|\ln t|, \quad t = (T^* - T_{\mathrm{c}}^*)/T_{\mathrm{c}}^*, \quad t > 0 \tag{42}$$

$$M(t = 0, H) \propto H^{1/3}|\ln H| \text{(critical isotherm)}. \tag{43}$$

Critical exponents for a general (d, n, σ) potential model have been obtained by several authors via renormalization group techniques; the results for $d = 1, \sigma = 1/2$ and arbitrary n are [14, 15]

$$\nu = 2, \quad \eta = 1{\cdot}5, \quad \gamma = 1, \quad \forall n \tag{44}$$

$$\alpha = 0 \text{ up to order } 1/n \tag{45}$$

and

$$\xi(T) \propto (1/t)^2 |\ln t|^{2n'}, \quad \chi(T) \propto (1/t)|\ln t|^{n'}, \quad n' = (n+2)/(n+8), \tag{46}$$

in agreement with the spherical model in the limit $n \to \infty$. Combining the renormalization group results and the scaling relation [17, 37]

$$\alpha + 2\beta + \gamma = 2, \tag{47}$$

we also obtain

$$\beta = 1/2 \tag{48}$$

up to order $1/n$. At the transition temperature, the correlation function G is predicted to possess the asymptotic power-law behaviour [17, 37]

$$G_1(r) \propto r^{-(d-2+\eta)} \tag{49}$$

and both spherical model and renormalization group treatments give $\eta = 1{\cdot}5$. 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 table 1 gives $s = 0$, $p = 0{\cdot}66 \pm 0{\cdot}02$ at the transition, or $\eta = 1{\cdot}66 \pm 0{\cdot}02$, i.e. a very rough approximation to the renormalization group result, whereas we find a reasonable estimate for β.

As for the singlet orientational distribution function (see figure 5), the coefficients a_{2k} in equation (27) were calculated directly from a 201-bin histogram [32], 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 $k = 5$, and found a variance of 0·0004 and the following values

$$\begin{aligned} a_2 &= 0{\cdot}316 \pm 0{\cdot}001, \\ a_4 &= 0{\cdot}029 \pm 0{\cdot}001, \\ a_6 &= 0{\cdot}0002 \pm 0{\cdot}0004, \\ a_8 &= -0{\cdot}001 \pm 0{\cdot}0004, \\ a_{10} &= -0{\cdot}0008 \pm 0{\cdot}0003. \end{aligned}$$

Truncation at $k = 2$ gave a variance of 0·0009, and the same values for a_2 and a_4, in good agreement with those obtained via the ordering tensors and a far better statistics, i.e. $\bar{P}_2 = 0{\cdot}317 \pm 0{\cdot}001$ and $\bar{P}_4 = 0{\cdot}030 \pm 0{\cdot}0005$. The molecular field treatment of nematic models predicts for $S(\vartheta)$ an expression of the form [30, 39]

$$S(\vartheta) = \exp\left[b_0 + \sum_{k>0} b_{2k} P_{2k}(\cos\vartheta)\right], \tag{50}$$

where the coefficients b_{2k} are also predicted to depend on the order parameters; truncation of the series in equation (50) at $k \leqslant 2$ gave a variance of 0·004, and inclusion of higher-order terms up to b_8 reduced it to 0·0004. This contrasts with other simulated short-range nematic potential models in three dimensions, and with experimental data on real ones [40–42], where a good fit was obtained by truncating the series in equation (50) at $k = 1$. The simulation results point to the conclusion

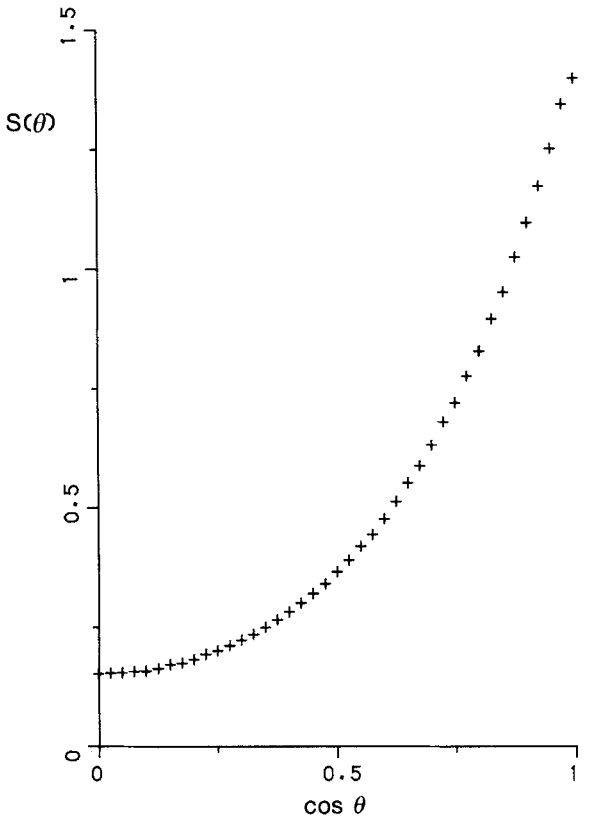

Figure 5. Plot of the singlet orientational distribution function at $T^* = 1$.

that the long range character of the potential produces an overall molecular field-like behaviour of the system.

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 Richerche (CNR). The author wishes to thank Professor G. R. Luckhurst (Department of Chemistry, University of Southampton) for helpful discussion and suggestions.

References

[1] Abramowitz, M., and Stegun, I. A. (editors), 1964, *Handbook of Mathematical Functions* (Dover).
[2] Domb, C., and Green, M. S. (editors), 1972, *Phase Transitions and Critical Phenomena*, Vol. 1 (Academic Press).
[3] Baxter, R. J., 1982, *Exactly Solved Models in Statistical Mechanics* (Academic Press).
[4] Sinai, Ya. G., 1982, *Theory of Phase Transitions; Rigorous Results* (Pergamon Press).
[5] Fröhlich, J., and Spencer, T., 1981, *Commun. Math. Phys.*, **81**, 527.
[6] Angelescu, N., and Zagrebnov, V. A., 1982, *J. Phys.* A, **15**, L 639.
[7] Dyson, F. J., 1969, *Commun. Math. Phys.*, **12**, 91; 1969, **12**, 212; 1971, *Ibid.*, **21**, 269.
[8] Fröhlich, J., Israel, R., Lieb, E. H., and Simon, B., 1978, *Commun. Math. Phys.*, **62**, 1.
[9] Fröhlich, J., and Spencer, T., 1982, *Commun. Math. Phys.*, **84**, 87.

[10] ROGERS, J. B., and THOMPSON, C. J., 1981, *J. statist. Phys.*, **25**, 669.
[11] SIMON, B., 1981, *J. statist. Phys.*, **26**, 307.
[12] SIMON, B., and SOKAL, A. D., 1981, *J. statist. Phys.*, **25**, 679.
[13] KUNZ, H., and PFISTER, C. E., 1976, *Commun. Math. Phys.*, **46**, 245.
[14] SUZUKI, M., 1972, *Physics Lett.* A, **42**, 5.
[15] FISHER, M. E., MA, S., and NICKEL, B. G., 1972, *Phys. Rev. Lett.*, **29**, 917.
[16] JOYCE, G. S., 1972, *Phase Transitions and Critical Phenomena*, Vol. 2, edited by C. Domb and M. S. Green (Academic Press), Chap. 10.
[17] STANLEY, H. E., 1971, *Introduction to Phase Transitions and Critical Phenomena* (Oxford University Press).
[18] ITO, K. R., 1982, *J. statist. Phys.*, **29**, 747.
[19] MESSAGER, A., MIRACLE-SOLE, S., and RUIZ, J., 1984, *Ann. Inst. Henri Poincare-Phys. Theor.*, **40**, 85.
[20] ROMANO, S., 1987, *Nuovo Cim.* B, **100**, 447.
[21] DAGOTTO, E., and MOREO, A., 1988, *Phys. Rev.* B, **37**, 7873.
[22] ROMANO, S., 1988, *Liq. Crystals*, **3**, 1215.
[23 *a*] BAK, P., and BRUINSMA, R., 1982, *Phys. Rev. Lett.*, **49**, 249.
[23 *b*] BRUINSMA, R., and BAK, P., 1983, *Phys. Rev.* B, **27**, 5824.
[24] NAGLE, J. F., and BONNER, J. C., 1970, *J. Phys.* C, **3**, 352.
[25] UZELAC, K., and GLUMAC, Z., 1988, *J. Phys.* A, **21**, L421.
[26] EWALD, P. P., 1921, *Annln Phys.*, **64**, 253.
[27] KORNFELD, H., 1924, *Z. Phys.*, **22**, 27.
[28] TOSI, M. P., 1964, *Solid State Phys.*, **16**, 1.
[29] ZANNONI, C., 1979, *The Molecular Physics of Liquid Crystals*, edited by G. R. Luckhurst and G. W. Gray (Academic Press), Chap. 9.
[30] ZANNONI, C., Chap. 3 in [29].
[31] FABBRI, U., and ZANNONI, C., 1986, *Molec. Phys.*, **58**, 763.
[32] ROMANO, S., 1986, *Europhys. Lett.*, **2**, 431.
[33] RUSHBROOKE, G. S., BARKER, G. A., and WOOD, P. J., 1972, *Phase Transitions and Critical Phenomena*, Vol. 2, edited by C. Domb and M. S. Green (Academic Press), Chap. 5.
[34 *a*] VUILLERMOT, P. A., and ROMERIO, M. V., 1973, *J. Phys.* C, **6**, 2922.
[34 *b*] KOHRING, G., and SHROCK, R. E., 1987, *Nucl. Phys.* B, **285**, 504.
[35] TOBOCHNICK, J., and CHESTER, G. V., 1979, *Phys. Rev.* B, **20**, 3761.
[36] FUCITO, F., 1983, *Physics Lett.*, A, **94**, 99.
[37] FISHER, M. E., 1967, *Rep. Prog. Phys.*, **30**, 615.
[38] DOMB, C., and BROUT, R., 1965, *Magnetism: A Treatise on Modern Theory and Materials*, edited by G. T. Rado and H. Suhl (Academic Press).
[39] LUCKHURST, G. R., Chap. 4 in [29].
[40] SIMPSON, P., 1982, Ph.D. Thesis, University of Southampton.
[41] HASHIM, R., 1984, Ph.D. Thesis, University of Southampton.
[42] LEADBETTER, A. J., and NORRIS, E. K., 1979, *Molec. Phys.*, **38**, 669.