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Monte Carlo simulation of disordered one dimensional systems with long range antiferromagnetic interactions

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We consider a classical system, consisting of m-component unit vectors ($m = 2$ and 3), associated with a one dimensional lattice $\{\boldsymbol{u}_k | k \in Z\}$ and interacting via translationally and rotationally invariant pair potentials of the form

$$V = V_{jk} = c\varepsilon|j - k|^{-p}(\boldsymbol{u}_j \cdot \boldsymbol{u}_k), \quad c = \pm 1, \quad \varepsilon > 0, \quad p > 1.$$

The system has been proven rigorously to possess an orientationally ordered phase stable at low but finite temperature when $c = -1$, $1 < p < 2$, and to disorder at all finite temperatures for $c = \pm 1$ and $p \geqslant 2$. This theorem also holds for the corresponding spherical model, whereas, in the Ising model, the ordered phase survives for $1 < p \leqslant 2$. We report here Monte Carlo simulation results for the antiferromagnetic models defined by $c = +1$, $p = 2$, $m = 2$ and 3. Comparison with their exactly soluble nearest neighbour counterparts shows that the long range antiferromagnetic interaction significantly weakens finite range correlations; this effect is more pronounced for $m = 3$ than for 2.

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 along this line, studying potential models known rigorously to disorder at all finite temperatures, and using simulation techniques to elucidate their physical properties.

We consider a classical system, consisting of m-component unit vectors (classical spins) associated with a one dimensional lattice $\{\boldsymbol{u}_k | k \in Z\}$ and interacting via a translationally and rotationally invariant (i.e. O(m) invariant) pair potential of the general form

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

$$r = r_{jk} = |j - k|, \quad \tau = \tau_{jk} = \boldsymbol{u}_j \cdot \boldsymbol{u}_k. \tag{1 b}$$

We restrict our discussion to $m = 2$ and 3 (i.e. plane rotators and classical Heisenberg model), so that the orientation of the spins in an arbitrary laboratory frame can be defined by the usual polar angles $\{\varphi\}(m = 2)$ or $\{\vartheta, \varphi\}(m = 3)$. When $m = 2$, $\tau_{jk} = \cos(\varphi_j - \varphi_k)$, and equation (1) can be generalized slightly to give

$$W_L = V_{jk,L} = f(r_{jk})\Psi[\cos(L(\varphi_j - \varphi_k))], \tag{2}$$

where L is an arbitrary positive integer. For assigned functional forms of f and Ψ, all the potential models W_L have the same partition function, and their structural properties can be defined in a way independent of L.

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In the thermodynamic limit, no orientationally ordered phase can survive at finite temperature if the function f has a finite range [1]. However, it has been pointed out [2] 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 [2] 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; spontaneous (or residual) ordering of a finite sample is also found simulations, at sufficiently low temperature, even with nearest-neighbour potential models [3–6].

On the other hand, it is also well-known that a sufficiently long ranged potential can produce a transition to a truly ordered phase, stable at low but finite temperature [1]. To be more specific, we shall consider the inverse-power models

$$V_{jk} = c\varepsilon r_{jk}^{-p}\tau_{jk}, \quad c = \pm 1, \quad p > 1, \quad \varepsilon > 0 \tag{3}$$

where c defines the ferromagnetic or antiferromagnetic character of the interaction. Their behaviour has been extensively investigated, especially in the ferromagnetic case $c = -1$. The ordered phase survives at finite temperature provided

$$c = -1, \quad 1 < p < 2,$$

whereas the system disorders at all finite temperatures when

$$c = \pm 1, \quad p \geqslant 2$$

[7–11]. In equation (3), the conditions $p = 1, c = -1$, would produce a system with infinite ground state energy, and order at all temperatures.

Similar results also hold for the spherical model [12]; in the corresponding Ising model, where the broken symmetry is discrete rather than continuous, the ordered phase survives for $1 < p \leqslant 2$ [13, 14]; rigorous bounds have also been established for the correlation functions in the disordered phases [15, 16]. Simulation results for such systems are still comparatively scarce in the literature (e.g. [17–19]). The corresponding antiferromagnetic long range models have been studied far less extensively (e.g. [20–24]), and no such theorems entailing the existence of an ordering transition at finite temperature are known for them, nor are there numerical estimates of their physical properties. This is in marked contrast to the wealth of results available in the literature for their short range counterparts.

We report here Monte Carlo calculations for the antiferromagnetic potential models defined by $p = 2, m = 2$ and 3, and aim at studying the effect of a long range interaction on finite range order, in comparison with their nearest neighbour counterparts, for which exact solutions are known [25–27]. Nearest neighbour ferro- and antiferromagnetic models are related by spin-flip symmetry, and possess essentially the same properties in the absence of external fields. The system's ground state corresponds to a staggered configuration (i.e. with spins pointing alternatively up and down), which can be defined by

$$\left.\begin{aligned} \varphi_k &= (1 + (-1)^k)\pi/2, \quad m = 2 \\ \vartheta_k &= (1 + (-1)^k)\pi/2, \quad m = 3 \end{aligned}\right\} \tag{4}$$

and whose energy, in units ε per particle, is in both cases [28]

$$U_0^* = \sum_{j=1}^{\infty} (-1)^j j^{-2} = -\eta(2) = -\pi^2/12 = -0{\cdot}8225. \tag{5}$$

The named theorems have been proven for (ferro)magnetic interactions, i.e. $\Psi(\tau) = \tau$ in equation (1), and are supplemented by other theoretical treatments (e.g. renormalization group), whereas no such results are known for $m = 3, \Psi(\tau) = P_2(\tau)$, which is of more direct interest in the theory of nematics. On the other hand, owing to the symmetry properties of plane rotators (equation (2)), magnetic results for them automatically imply a nematic counterpart [17, 18], so that, for example, the plane rotator ground state in equation (4) can also be regarded as an antinematic one, consisting of two interpenetrating sublattices with mutually orthogonal directors.

2. Computational aspects

Calculations were performed using periodic boundary conditions, so that the energy of a configuration was summed in closed form by means of the identity [29]

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

As a compromise between available computational resources and desired accuracy, we have 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

$$T^* = kT/\varepsilon, \quad U^* = \langle V \rangle/(N\varepsilon), \tag{7}$$

where $\langle V \rangle$ is the mean sample energy and U^* is the mean energy per particle. Calculations were performed in order of increasing temperature, 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 potential energy, configurational specific heat C_v (both as a fluctuation quantity and by least-square fitting and numerical differentiation of the energy), magnetic moments and orientational correlation functions. Magnetic moment and staggered magnetic moment are defined by

$$\mathbf{M} = (1/N) \left\langle \sum_{k=1}^{N} \boldsymbol{u}_k \right\rangle, \mathbf{M}' = (1/N) \left\langle \sum_{k=1}^{N} (-1)^k \boldsymbol{u}_k \right\rangle, \tag{8}$$

$\mathbf{M}$ monitors ferromagnetic order, whereas $\mathbf{M}'$ accounts for the antiferromagnetic order. The orientational correlation functions are defined by

$$G_L(r) = \begin{cases} = \langle P_L(\mathbf{u}_j \cdot \mathbf{u}_k) \rangle, \quad m = 3, \\ \qquad \text{as functions of } r = |j - k| \\ = \langle T_L(\mathbf{u}_j \cdot \mathbf{u}_k) \rangle = \langle \cos[L(\varphi_j - \varphi_k)] \rangle, \quad m = 2 \end{cases} \tag{9}$$

where T_L and P_L denote Tchebyshev and Legendre polynomials, respectively. Calculations were carried out for $L = 1$ and 2, and the correlation functions were computed at a few selected temperatures (in order to save computer time), once every second cycle. For graphical convenience, we have defined and plotted the more smoothly varying function

$$E_1(r) = (-1)^r G_1(r). \tag{10}$$

The corresponding m-component nearest neighbour models defined by [25–27]

$$W = c\tau \tag{11}$$

have been solved exactly for arbitrary m; we report here some formulae, and use them for comparison with our simulation results. The partition function for an assembly of N spins is

$$Q_N(T) = [\Gamma(m/2)(a/2)^{1-m/2} I_{m/2-1}(a)]^{N-1}; \quad a = -c/T^*. \tag{12}$$

Potential energy and specific heat per particle are given by

$$U^* = c f_m^{(a)}, \quad f_m^{(a)} = I_{m/2}(a)/I_{m/2-1}(a), \tag{13}$$

$$C_v/k_B = a^2\{1 - f_m(a)[(m-1)/a + f_m(a)]\}. \tag{14}$$

The specific heat tends to the limit $(m-1)/2$ as T^* tends to zero, and has an asymptotic inverse square behaviour as T^* goes to infinity; for $m = 1$ and 2, C_v exhibits a maximum at finite temperature, which becomes a broad flat region for $m = 3$, and disappears altogether for $m > 3$; for $m = 2$, we have $T^*_{\max} = 0{\cdot}4306$, $C_v(T_{\max}) = 0{\cdot}67992\,k$. The orientational correlation functions $G_1(r)$ decay exponentially with distance according to

$$G_1(r) = [f_m(a)]^r, \tag{15}$$

because of the nearest neighbour character of the interaction, $G_1(1)$ coincides in magnitude with the energy; we also give formulae for higher-order correlation functions when $m = 2$ and 3:

$$G_L(r) = \begin{cases} = [I_L(a)/I_0(a)]^r, & m = 2 \\ = \left\{\int_{-1}^{+1} P_L(t)\exp(at)\,dt \Big/ \int_{-1}^{+1} \exp(at)dt\right\}^r, & m = 3. \end{cases} \tag{16}$$

Here I_k are modified Bessel functions of order k [28]; taking into account the symmetry properties of the functions I_L and P_L, we can again recognize that the sign of c is immaterial, i.e. that, for given m, ferromagnetic and antiferromagnetic nearest neighbour models have essentially the same properties.

3. Results

Results for the potential energy are plotted in figure 1, together with the analytical results for the nearest neighbour models; as the temperature increases, our energy results tend to their nearest neighbour counterparts from below, and show an overall qualitative similarity with them. In order to make this point more precise, let $\varrho = \varrho(m, T^*)$ denote the ratio between the energy of a long range model and the energy of its nearest neighbour counterpart, both being considered at the same reduced temperature T^*. At very low temperatures ϱ is essentially the ratio of the ground state energies, i.e. $\eta(2)$ (see equation (5)), then it decreases with temperature down to 0·75, and again increases with temperature, being closer to one for $m = 3$ than for $m = 2$. The specific heat results reported here (see figure 2) were obtained by least-square fitting and numerical differentiation of the energy; the corresponding fluctuation quantities agree with them to within their statistical uncertainty (up to 10 per cent). Figure 2 shows both similarities and differences between the potential models considered here: on the one hand, the zero temperature limits of the specific

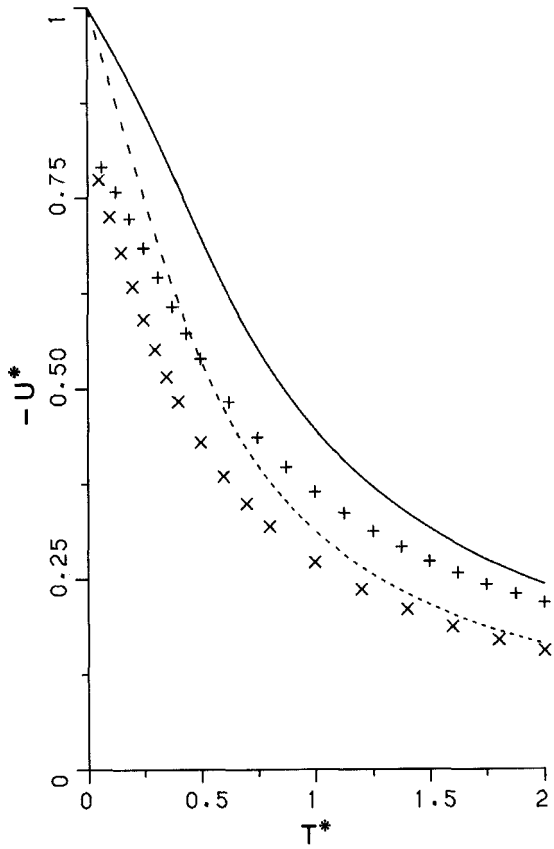

Figure 1. Results for the potential energy: +: present model, $m = 2$; X: present model, $m = 3$; continuous curve: nearest neighbour model, $m = 2$; dashed line: nearest neighbour model, $m = 3$. The relative statistical error is usually smaller than 0·25 per cent.

heat for long range systems agree with their nearest neighbour counterparts, and the curve for $m = 2$ exhibits a peak at $T^* = 0{\cdot}25$, somewhat lower than its nearest neighbour counterpart; on the other hand, the specific heat of the three-component long range model depends linearly on temperature for $T^* \leqslant 0{\cdot}15$, whereas its nearest neighbour counterpart exhibits a constant value in the same temperature range.

As for the residual order, we have found all of the components of **M** to be smaller than 0·005 in magnitude, as they should since the interaction is antiferromagnetic; for $T^* \geqslant 0{\cdot}2$, all components of M were smaller than 0·01 in magnitude; at lower temperature, the component with the largest magnitude may range up to 0·15; on the whole, the residual order remains tolerable. Our system possesses no long range order, and its orientational correlation functions show some short range order, quickly decaying with temperature; there is no unique quantitative definition of this property, so we have decided to report both the values of the correlation functions at nearest neighbour separation (see figures 3 and 4), and the fit of the overall behaviour of $E_1(r)$ with appropriate functional forms. $G_2(r)$ quickly decays to zero, even at the lowest temperature investigated (see figure 5), whereas we found $|G_1(r)| \leqslant 0{\cdot}001$ for $m = 2$, $T^* \geqslant 1$, $r \geqslant 5$; for $m = 3$, this happens at $T^* \geqslant 0{\cdot}6$. The results for $E_1(1)$ (see figure 3) can be analysed by defining the appropriate ratio ϱ, which turns out to be

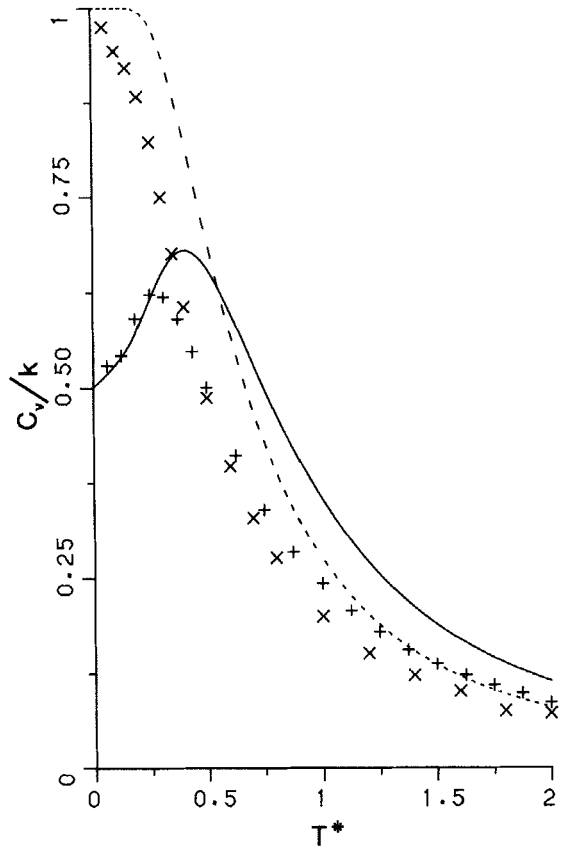

Figure 2. Configurational specific heat. +: present model, $m = 2$; X: present model, $m = 3$; continuous curve: nearest neighbour model, $m = 2$; dashed line: nearest neighbour model, $m = 3$. The relative statistical error is usually smaller than 0·25 per cent.

one at zero temperature, to decrease with temperature down to 0·85, and again to increase with increasing temperature, being closer to one for $m = 3$ than for $m = 2$: among the reported properties, this shows the greatest similarity between long range and nearest neighbour models. A similar analysis can be applied to $G_2(1)$ (see figure 4), and the ratio ϱ shows the same qualitative behaviour, but here its minimum can be as low as 0·65.

It has also been proven [15, 16] that, for some inverse power potential models including the present ones,

$$|G_1(r)| \leqslant Ar^{-b}, \quad A > 0, b > 0 \tag{17}$$

at sufficiently high temperature. At sufficiently low temperatures, we have fitted $E_1(r)$ using the functional form

$$\left.\begin{aligned} E_1(r) &= c_1 + h(r), \\ h(r) &= c_2 \exp(-sr)/(c_3 + r^q). \end{aligned}\right\} \tag{18}$$

Here c_1 compensates for the residual order, and the function h is consistent with the rigorous correlation inequality (see equation (17)). The fitting parameters were

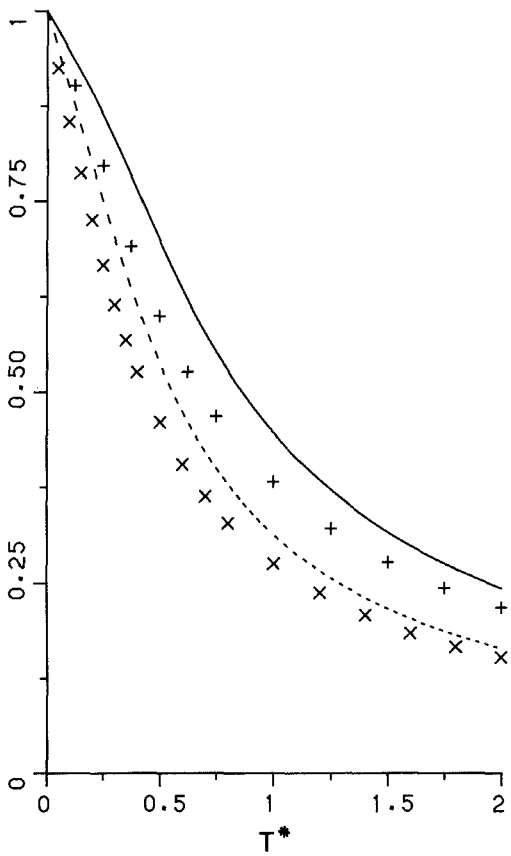

Figure 3. Results for $E_1(1)$ versus temperature. +: present model, $m = 2$; X: present model, $m = 3$; continuous curve: nearest neighbour model, $m = 2$; dashed line: nearest neighbour model, $m = 3$. The relative statistical error is usually smaller than 0·25 per cent.

determined using the general non-linear least-square program MINUIT in the CERN library; some of them are reported in the tables. At the lowest temperature investigated, the power exponent q was found to be essentially zero, i.e. the decay was purely exponential. To comment on the meaning of tables 1 and 2, we consider the ratio

$$[G_1(r)]_{LR}/[G_1(r)]_{nn} \leqslant \exp[-(s - s_{nn})r], \tag{19}$$

which is close to one at nearest-neighbour separation (see figure 3), and may typically drop by a factor ten as r increases to fifteen.

To conclude, we have studied two antiferromagnetic models interaction via long range potentials and known rigorously to disorder at all finite temperatures. Simulation results for thermodynamic properties show broad qualitative similarities between the models and with their nearest neighbour counterparts, whereas simulation results for the structural properties show greater qualitative differences, and point to the conclusion that the very long range nature of the antiferromagnetic interaction significantly weakens finite range correlations in comparison with the nearest neighbour counterparts; this effect is more pronounced for $m = 3$ than for 2. For another comparison, we mention the ferromagnetic counterparts of the present

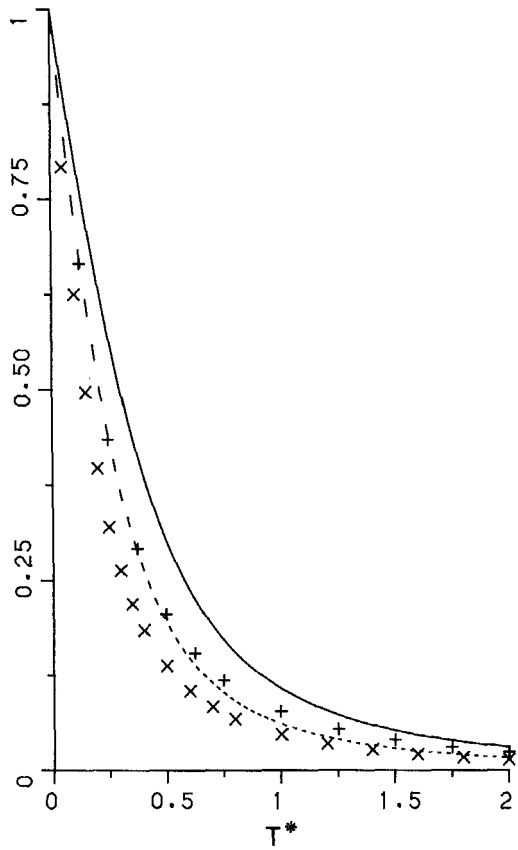

Figure 4. Results for $G_2(1)$ versus temperature. +: present model, $m = 2$; X: present model, $m = 3$; continuous curve: nearest neighbour model, $m = 2$; dashed line: nearest neighbour model, $m = 3$. The relative statistical error is usually smaller than 0·25 per cent.

Table 1. Fitting parameters in equation (18), for various temperatures, for the two component model; s_{nn} refers to the nearest neighbour model, whose E_1 decays exponentially [equation (15)]. At $T^* = 0{\cdot}125$, q is zero to within $\pm 0{\cdot}0005$.

T^*	q	s	s_{nn}
0·125	0·00	0·138	0·067
0·250	0·10	0·264	0·147
0·375	0·13	0·439	0·246
0·500	0·25	0·574	0·360
0·625	0·64	0·677	0·478
0·750	1·24	0·650	0·594
1·000	1·30	1·047	0·807
	($\pm$0·03)	($\pm$0·006)	

models ($p = 2$, $c = -1$ in equation (3)), where finite range correlations are significantly strengthened, possibly to the extent of producing a transition to a low temperature phase with inverse power decay of correlations and infinite susceptibility [30, 31]. Neither the existence nor the absence of an ordering transition at finite temperature have been proven for the antiferromagnetic models defined by

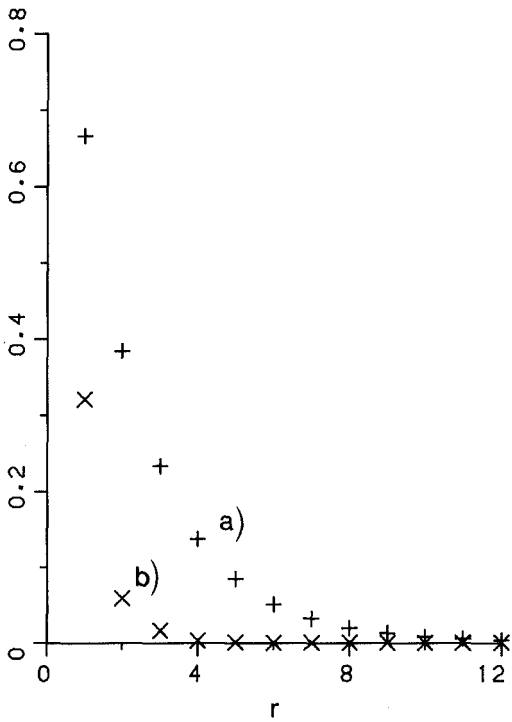

Figure 5. Plots of the orientational correlation functions for the three component model, at the temperature T^* of 0·25. (*a*) $E_1(r)$; (*b*) $G_2(r)$; the results for its nearest neighbour counterpart are $E_1(r) = (0{\cdot}751)^r$; $G_2(r) = (0{\cdot}437)^r$; the correlation functions $G_L(r)$ are defined in the text.

Table 2. Fitting parameters in equation (18), for various temperatures, for the three component model; s_{nn} refers to the nearest neighbour model, whose E_1 decays exponentially [equation (15)]. At $T^* \leqslant 0{\cdot}100$, q is zero to within $\pm$ 0·0005.

T^*	q	s	s_{nn}
0·050	0·000	0·112	0·051
0·100	0·000	0·203	0·105
0·150	0·020	0·291	0·163
0·200	0·030	0·410	0·223
	($\pm$0·005)	($\pm$0·005)	
0·250	0·12	0·49	0·287
0·300	0·21	0·52	0·353
0·350	0·48	0·60	0·421
0·400	0·60	0·63	0·488
0·500	0·67	0·64	0·622
	($\pm$0·03)	($\pm$0·03)	

$1 < p < 2$ in equation (3); our preliminary simulation results for $p = 3/2$ suggest disorder at all finite temperatures.

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

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