Two-dimensional-lattice spin models with long-range antiferromagnetic interactions

S. Romano*
A. Volta.Department of Physics, University of Pavia, via A. Bassi 6, I-27100 Pavia, Italy
(Received 26 December 1990; revised manuscript received 2 April 1991)

We consider a classical system, consisting of m-component unit vectors ($m=2,3$), associated with a two-dimensional lattice $\{\mathbf{u}_k | k\in\mathbb{Z}^2\}$ and interacting via translationally and rotationally invariant antiferromagnetic pair potentials of the long-range form $W=W_{jk}=\varepsilon|\mathbf{x}_j-\mathbf{x}_k|^{-p}\mathbf{u}_j\cdot\mathbf{u}_k$, $p>2$, where ε is a positive quantity, setting energy and temperature scales (i.e., $T^*=k_BT/\varepsilon$), and $\mathbf{x}_k$ are the coordinates of the lattice sites. A spin-wave approach predicts orientational disorder (in the thermodynamic limit) at all finite temperatures and for all $p>2$; this agrees with available rigorous results for $p\geq 4$, whereas no such theorems are known in the literature when $2<p<4$. We also report here Monte Carlo simulation results for the model defined by $m=2$, $p=3$; calculations were carried out between $T^*=0.1$ and $T^*=1$, and sample-size effects were investigated at the lowest temperature examined. Energy and specific-heat results showed a rather smooth behavior, and no sample-size effect; on the other hand, we found a significant amount of finite-size order, and its pronounced decrease with increasing sample size. In the absence of more stringent rigorous results, we conjecture that the present potential models are disordered at all finite temperatures, for all $p>2$.

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, using numerical simulation and spin-wave arguments in the absence of more stringent rigorous results.

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

$$W=W_{jk}=\Psi(r)\mathbf{u}_j\cdot\mathbf{u}_k\ ,\quad \mathbf{r}=\mathbf{r}_{jk}=\mathbf{x}_j-\mathbf{x}_x\ ,\quad r=|\mathbf{r}|\ , \tag{1}$$

where $\mathbf{x}_k$ are the coordinates of the lattice sites.

We restrict our discussion to $d=1,2$ and to $m=2,3$ (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 $\{\varphi_k\}$ ($m=2$) or $\{\vartheta_k,\vartheta_k\}$ ($m=3$); in the following, let Λ denote $\mathbb{Z}^d$.

In the thermodynamic limit, no orientationally ordered phase can survive at finite temperature if the function Ψ 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, Imry has studied an Ising-Kac ferromagnetic model in one dimension,[2] whose spontaneous magnetization vanishes in the thermodynamic limit as $1/\ln N$, where N is the number of particles in the system. Spontaneous (or "residual") ordering of a finite sample is also found in simulations, at sufficiently low temperature, even with nearest-neighbor potential models (see, e.g., the careful study in Ref. 3).

On the other hand, it is also well known that a sufficiently long-ranged (LR) potential can produce a true ordering transition, taking place at some low but finite temperature.[1] To be more specific, we shall consider the inverse-power models

$$W_{jk}=c\varepsilon r^{-p}\mathbf{u}_j\cdot\mathbf{u}_k,\quad c=\pm 1,\quad p>d\ . \tag{2}$$

Here ε is a positive quantity setting energy and temperature scales (i.e., $T^*=k_BT/\varepsilon$, $U^*=\langle W\rangle/N\varepsilon$), c defines the ferromagnetic (FM) or antiferromagnetic (AF) character of the interaction, and the restriction $p>d$ avoids configurations with an infinite energy per particle; their behavior has been extensively investigated, especially in the FM case. It has been proved that the system disorders at all finite temperature when $p\geq 2d$, irrespective of the sign of c, and that the ferromagnetic model possesses an ordering transition at finite temperature, provided that $d<p<2d$.[4-9] For $d=2$ and $p\geq 2d$, available theoretical results entail that the FM planar-rotator models ($m=2$) possess a transition to a low-temperature phase with infinite susceptibility (see, e.g., Refs. 10–12). This is also likely to happen when $d=1$, $p=2$.[13] The FM models have also been investigated by other techniques, including spherical model,[14-16] renormalization group,[17,18] and simulation.[19-21]

In contrast to their FM counterparts, long-range AF models defined by $d<p<2d$ have been studied far less extensively, and no such theorems entailing existence (or absence) of an ordering transition at finite temperature are known in the literature. However, some clues are available; for example, the infinite-range (mean-field) model defined by $p=0$ in Eq. (2) [i.e., by $\Psi(r)$ being a positive constant in Eq. (1)], is known to produce ground-state frustration and disorder at all finite temperatures.[22] In our previous paper,[23] we presented simulation results and spin-wave arguments for $d=1$, suggesting orientational disorder (in the thermodynamical limit) at all finite temperatures, and for all $p>1$. In the following

paragraph, we present a spin-wave argument for $d=2$, which gives a similar result. We also study a model of this kind by computer simulation; this, in turn, requires a complete definition of the interaction potential. Monte Carlo calculations are thus reported here for $d=2$, $m=2$, $c=+1$, $p=3$ (the midpoint of the interesting interval).

SPIN-WAVE THEORY

We first consider the quantities

$$S=S_p(\mathbf{q})=\sum_{\mathbf{h}\in\Lambda}{}' h^{-p}\exp(i\mathbf{h}\cdot\mathbf{q})=\sum_{\mathbf{h}\in\Lambda}{}' h^{-p}\cos(\mathbf{h}\cdot\mathbf{q}) , \quad (3)$$

where the prime excludes the null vector; series of this kind have been studied by various authors, and can be evaluated by techniques based on the ϑ-function transformation and generalizing the Ewald method.[24–29] The general result can be cast in terms of incomplete γ functions;[30] when $\mathbf{q}$ is the null vector, or the vector $\mathbf{R}$ with components (π,π), the expression factorizes into a product of one-dimensional series.[30,31–33]

Here, we then apply spin-wave theory as developed in Ziman's book,[34] explicitly allowing for long-range interactions, and specialize the formulas to an inverse-power law; this treatment correctly predicts orientational disorder at all finite temperatures when $p\geq 4$, thus the discussion can be restricted to the range $2<p<4$.

In the FM case, the dispersion relation is [34]

$$\omega_{\mathrm{FM}}(\mathbf{q})\propto G(\mathbf{q})=\sum_{\mathbf{h}\in\Lambda}{}' h^{-p}[1-\cos(\mathbf{h}\cdot\mathbf{q})] . \quad (4)$$

After applying the named treatment[24–29] and simplifying the notation, the following limiting form is obtained as $\mathbf{q}$ tends to zero:

$$G(\mathbf{q})\cong g_0(p)q^{p-2} . \quad (5)$$

The quantity

$$I_{\mathrm{FM}}=\sum_{\mathrm{BZ}} 1/G(\mathbf{q})\approx\int d\mathbf{q}/G(\mathbf{q}) \quad (6)$$

converges for $2<p<4$, and diverges for $p\geq 4$, thus suggesting the existence of an ordering transition at finite temperature,[34] in agreement with known rigorous results;[1,4,5] the sum in Eq. (6) ranges over the first Brillouin zone (BZ). In the AF case, the dispersion law is[34]

$$\omega^2_{\mathrm{AF}}(\mathbf{q})\propto[A(\mathbf{q})^2-B(\mathbf{q})^2] , \quad (7)$$

$$A(\mathbf{q})=\sum_{\mathbf{h}\in\Lambda}{}' h^{-p}\{-\sigma(\mathbf{h})+\tfrac{1}{2}[1+\sigma(\mathbf{h})]\cos(\mathbf{h}\cdot\mathbf{q})\} , \quad (8)$$

$$B(\mathbf{q})=\tfrac{1}{2}\sum_{\mathbf{h}\in\Lambda}{}' h^{-p}[1-\sigma(\mathbf{h})]\cos(\mathbf{h}\cdot\mathbf{q}) , \quad (9)$$

where $\sigma(\mathbf{h})=\exp(i\mathbf{h}\cdot\mathbf{R})$. After carrying out the appropriate substitutions[24–29] and simplifying the notation, we obtain, to lowest order as $\mathbf{q}$ tends to zero,

$$\begin{aligned} A(\mathbf{q})&\cong D(p)+a_1(p)q^{p-2}+a_2(p)q^2 ,\\ B(\mathbf{q})&\cong D(p)+a_1(p)q^{p-2}-a_2(p)q^2 . \end{aligned} \quad (10)$$

Now the quantity

$$I_{\mathrm{AF}}=\sum_{\mathrm{BZ}} A(\mathbf{q})/[A^2(\mathbf{q})-B^2(\mathbf{q})] \approx\int d\mathbf{q}\, A(\mathbf{q})/[A^2(\mathbf{q})-B^2(\mathbf{q})] \quad (11)$$

diverges for all $p>2$, and this predicts orientational disorder at all finite temperatures.[34]

COMPUTATIONAL ASPECTS AND RESULTS

Calculations were carried out using periodic boundary conditions and the Ewald-Kornfeld algorithm for lattice summations, as outlined in Tosi's review paper;[35] they were started from the ground-state configuration at the lowest temperature, and performed in order of increasing temperature. Both equilibrium and production runs took 6250 cycles (where one cycle corresponds to N attempted moves), and subaverages for evaluating statistical errors were calculated over macrosteps consisting of 250 cycles. Several sample sizes ($N=L^2$, $L=20$, 30, 40, 50, 60, 70, and 80) were examined at the lowest temperature investigated, $T^*=0.1$; calculations were also carried out over a wide temperature range, from $T^*=0.1$ to 1, mostly using one sample size, $L=50$. Calculated quantities include potential energy, configurational specific heat (both as a fluctuation quantity and by least-squares fit and numerical differentiation of the potential energy), magnetic moments, and nematic second-rank ordering tensor with associated order parameter,[36–39] which monitor orientational order independently of sublattice magnetization. The correlation function was also calculated at a few temperatures by analyzing one configuration every second cycle. Magnetic moment, staggered magnetic moment, and their mean-square values are defined by

$$\begin{aligned} &\mathbf{M}_1=(1/N)\langle\mathbf{F}\rangle,\quad M_2=(1/N)\langle\sqrt{\mathbf{F}\cdot\mathbf{F}}\rangle ,\\ &\mathbf{M}_3=(1/N)\langle\mathbf{F}'\rangle,\quad M_4=(1/N)\langle\sqrt{\mathbf{F}'\cdot\mathbf{F}'}\rangle , \end{aligned} \quad (12)$$

where

$$\mathbf{F}=\sum_{k=1}^{N}\mathbf{u}_k,\quad \mathbf{F}'\sum_{k=1}^{N}\sigma(\mathbf{x}_k)\mathbf{u}_k , \quad (13)$$

and $\sigma(\mathbf{x}_k)=\exp(i\mathbf{R}\cdot\mathbf{x}_k)$.

We also define M_5 as the component of $\mathbf{M}_3$ with the larger magnitude (see Table I); both $\mathbf{M}_1$ and $\mathbf{M}_2$ were

TABLE I. Simulation results obtained at $T^*=0.1$ and with different sample sizes $N=L^2$. The results for potential energy and configurational specific heat are $U^*=-1.2720\pm0.000\,04$, $C_V/k_B=0.51\pm0.02$, independent of sample size to within the statistical errors; M_5 denotes the component of $\mathbf{M}_3$ with the larger magnitude.

L	M_4	M_5	$\bar{P}_2$
20	0.944	0.805	0.788
30	0.932	0.925	0.751
40	0.929	0.830	0.743
50	0.919	0.908	0.712
60	0.906	0.895	0.654
70	0.900	0.796	0.662
80	0.880	0.712	0.596
	($\pm$0.004)	($\pm$0.008)	($\pm$0.006)

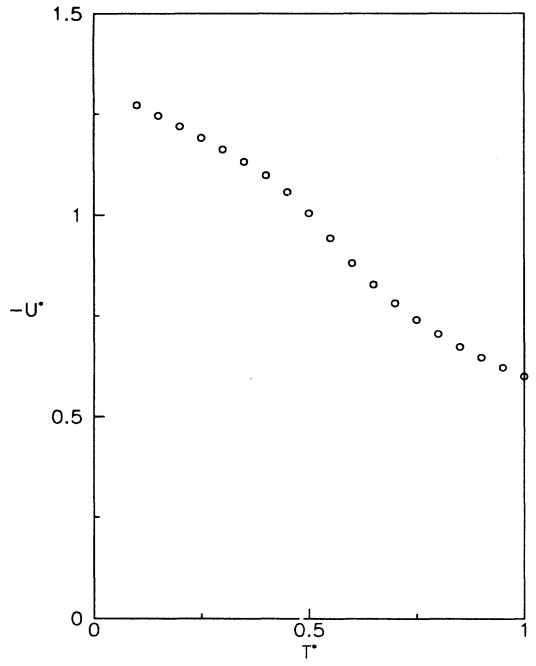

FIG. 1. Results for the relative potential energy; the relative statistical error is not greater than 0.4%.

found to be essentially zero, as they should. The second-rank nematic ordering tensor is defined by

$$Q_{\mu\nu}=2\langle u_\mu u_\nu\rangle-\delta_{\mu\nu}\ , \tag{14}$$

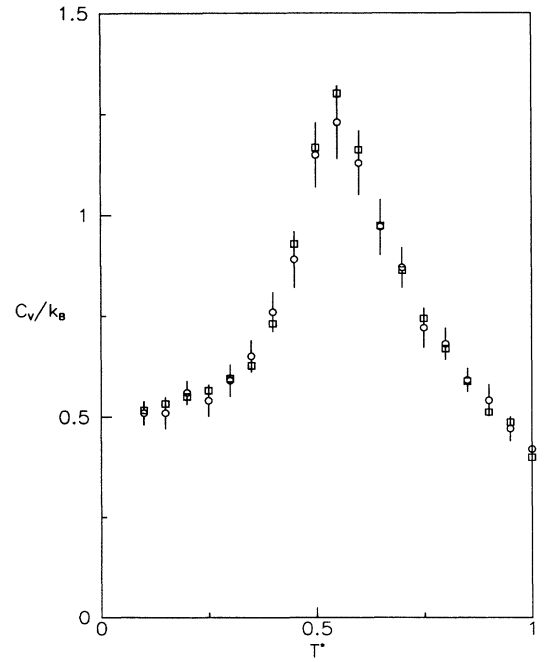

FIG. 2. Results for the configurational specific heat. (a) Circles: fluctuation quantities, with error bars. (b) Squares: results obtained by a least-squares fit and numerical differentiation of the potential energy.

and the corresponding order parameter $\bar{P}_2$ is defined via its positive eigenvalue; a detailed discussion of the computational aspects can be found in Refs. 36–39.

The temperature dependences of potential energy (Fig. 1) and configurational specific heat (Fig. 2) showed a smooth behavior, with a maximum of the specific heat about $T^*=0.55$; as an additional check, we repeated simulations at $T^*=0.5$, 0.55, and 0.6, using both $L=40$ 60, and found results, independent of the sample size to within the associated statistical errors. This behavior shows no hint of a transition. At $T^*=0.1$, results for potential energy and specific heat were found to be independent of the sample size, to within the associated statistical errors (see Table I); on the other hand, the ordering quantities kept decreasing with increasing sample size. Results for M_4 were fitted using the functional form

$$M_4=\lambda+\rho L^{-\tau}\ , \tag{15}$$

and the three parameters were determined by means of the general nonlinear least-squares program MINUIT from the CERN library. Including all sample sizes, we found a variance of 0.000 32 and the values $\lambda=0.013\pm0.004$, $\tau=0.045\pm0.002$; on the other hand, restriction to $L\geq40$ gave a variance of 0.000 079 and the value $\lambda=0.009\pm0.004$, $\tau=0.073\pm0.005$. The parameter ρ was found to be of the order of 1. Such numbers suggest M_4 to be actually zero in the thermodynamic limit. Finite-size order kept decreasing with increasing temperature (results are not shown here); for $L=50$, it disappears at $T^*\geq0.7$, as is also shown by the correlation function.

The correlation function is given by

$$G(r)=\langle \mathbf{u}_j\cdot\mathbf{u}_k\rangle \text{ as function of } r=|\mathbf{x}_j-\mathbf{x}_k|\ , \tag{16}$$

and for convenience of drawing we define the more

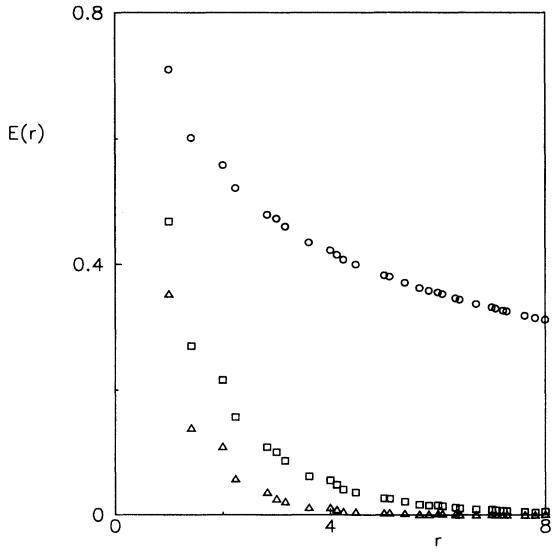

FIG. 3. Results for the staggered correlation function $E(r)$ at the temperatures $T^*=0.5$ (circles); $T^*=0.75$ (squares); $T^*=1$ (triangles); the correlation functions are defined in the text.

smoothly varying quantity (staggered correlation function)

$$E(r)=\sigma(\mathbf{x}_j)\sigma(\mathbf{x}_k)\langle \mathbf{u}_j\cdot\mathbf{u}_k\rangle=(-1)^{r^2}G(r)\ . \tag{17}$$

The functions $E(r)$ obtained at three different temperatures are plotted in Fig. 3. At the lowest temperature investigated, $E(r)$ kept slowly decreasing with distance, but still showing a significant amount of finite-range order: we found $E(r)\approx 0.2$ at $r=20$.

On the basis of the present results, and in the absence of more stringent rigorous ones, we conjecture that the examined potential models produce orientational disorder at all finite temperatures in the thermodynamic limit.

ACKNOWLEDGMENTS

The present calculations were carried out, among other machines, on a Digital Equipment Corporation VAX 8350 computer, belonging to the Sezione di Pavia of Istituto Nazionale di Fisica Nucleare (INFN); computer time on a Cray Research machine was allocated by the Italian Consiglio Nazionale delle Ricerche (CNR). This work was partially supported by Gruppo Nazionale di Struttura della Materia, CNR and by Centro Interuniversitario di Struttura della Materia, Ministero della Pubblica Istruzione. The author wishes to thank Professor G. R. Luckhurst (Department of Chemistry, University of Southampton) for helpful discussions and suggestions.

*Electronic address (E-mail): ROMANO@PAVIA.INFN.IT.

[1]Ya. G. Sinai, *Theory of Phase Transition: Rigorous Results* (Pergamon, Oxford, 1982).
[2]Y. Imry, Ann. Phys. (N.Y.) **51**, 1 (1969).
[3]C. Chiccoli, P. Pasini, and C. Zannoni, Liq. Cryst. **3**, 363 (1988).
[4]H. Kunz and C. E. Pfister, Commun. Math. Phys. **46**, 245 (1976).
[5]J. Fröhlich, R. Israel, E. H. Lieb, and B. Simon, Commun. Math. Phys. **62**, 1 (1978).
[6]C. E. Pfister, Commun. Math. Phys. **79**, 181 (1981).
[7]J. B. Rogers and C. J. Thompson, J. Stat. Phys. **25**, 669 (1981).
[8]B. Simon, J. Stat. Phys. **26**, 307 (1981).
[9]B. Simon and A. D. Sokal, J. Stat. Phys. **25**, 679 (1981).
[10]J. Fröhlich and T. Spencer, Commun. Math. Phys. **81**, 527 (1981).
[11]A Messager, S. Miracle-Sole, and J. Ruiz, Ann. Inst. Henri Poincaré, Phys. Théorique, **40**, 85 (1984).
[12]S. Romano, Phys. Rev. B **42**, 8647 (1990).
[13]E. Šimánek, Phys. Lett. A **119**, 477 (1987).
[14]G. S. Joyce, Phys. Rev. **146**, 349 (1966).
[15]G. S. Joyce, J. Phys. C **2**, 1531 (1969).
[16]G. S. Joyce, *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 2.
[17]M. Suzuki, Phys. Lett. **42A**, 5 (1972).
[18]M. E. Fisher, S. Ma, and G. G. Nickel, Phys. Rev. Lett. **29**, 917 (1972).
[19]S. Romano, Liq. Cryst. **3**, 1215 (1988); **4**, 483 (1989).
[20]S. Romano, Nuovo Cimento B **100**, 447 (1987).
[21]E. Dagotto and A. Moreo, Phys. Rev. B **37**, 7873 (1988).
[22]A. Caliri and D. C. Mattis, Phys. Lett. **106A**, 74 (1984).
[23]S. Romano, Phys. Rev. B **42**, 6739 (1990).
[24]D. Misra, Proc. Cambridge Philos. Soc. **36**, 173 (1943).
[25]M. Born and M. Bradburn, Proc. Cambridge Philos. Soc. **39**, 104 (1943).
[26]M. Bradburn, Proc. Cambridge Philos. Soc. **39**, 113 (1943).
[27]M. H. Cohen and F. Keffer, Phys. Rev. **99**, 1128 (1955).
[28]A. L. Fetter, Phys. Rev. B **11**, 2049 (1975).
[29]M. H. Lee and A. Bagchi, Phys. Rev. B **22**, 2645 (1980).
[30]*Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1964).
[31]M. L. Glasser, J. Math. Phys. **14**, 409 (1973); **14**, 701 (1973); **15**, 188 (1974).
[32]I. J. Zucker, J. Math. Phys. **15**, 187 (1974).
[33]A. Hautot, J. Math. Phys. **15**, 268 (1974).
[34]J. M. Ziman, *Principles of the Theory of Solids,* 2nd ed. (Cambridge University, Cambridge, 1972).
[35]M. P. Tosi, Solid State Phys. **16**, 1 (1964).
[36]C. Zannoni, in *The Molecular Physics of Liquid Crystals,* edited by G. R. Luckhurst and G. W. Gray (Academic, London, 1979) Chap. 3.
[37]C. Zannoni, *The Molecular Physics of Liquid Crystals* (Ref. 36), Chap. 9.
[38]U. Fabbri and C. Zannoni, Mol. Phys. **58**, 763 (1986).
[39]S. Romano, Nuovo Cimento D **9**, 409 (1987).