

Dipolar interaction and long-range order in the square planar rotator model

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A continuous manifold of inequivalent spin configuration minimize the energy of the square planar rotator model when the spins are coupled by dipolar interactions. This continuous degeneracy is accidental in nature and causes a soft mode at $\mathbf{q}=(2\pi/a)(1/2,1/2)$ in the simple spin-wave spectrum. Consequently no long-range order is obtained in simple spin-wave approximation in contrast with the expectation based on Monte Carlo simulation. The solution of the puzzle is found going beyond the harmonic approximation. Indeed a careful treatment of the magnon-magnon interaction replaces the accidental soft mode by a temperature-dependent gap so that long-range order is restored. Satisfactory agreement between renormalized spin-wave theory and Monte Carlo simulation is obtained in the low-temperature regime. Critical properties investigated by finite size scaling of Monte Carlo data differ from both mean-field and two-dimensional Ising model critical behavior.

I. INTRODUCTION

Two-dimensional (2D) spin systems with continuous symmetry and short-range interaction do not support long-range order (LRO).¹ However, different scenarios are found whether the spins are two-dimensional (planar rotator model) or three-dimensional vectors (Heisenberg model). Indeed the Heisenberg model with nearest neighbor (NN) exchange interaction is paramagnetic at any finite temperature, whereas the planar rotator model with NN exchange interaction² shows a Kosterlitz-Thouless phase transition at $T_{KT}=(0.895\pm 0.005)J$ (Ref. 3) with the low-temperature phase characterized by divergent susceptibility and algebraic decaying of the spin-spin correlation function.

When the spin-spin interaction is an isotropic long range interaction, a variety of different behaviors are expected. For instance, a ferromagnetic exchange coupling decaying as $1/r^3$ where r is the spin-spin distance, supports LRO as shown by renormalization-group (RG) analysis⁴ and confirmed by Monte Carlo (MC) simulation.⁵ On the contrary, an antiferromagnetic exchange coupling decaying with the same power law $1/r^3$ is expected to have no LRO on the basis of both MC simulation and simple spin-wave approximation.⁶

An interesting phenomenology characterizes the planar rotator model with pure dipole interaction, which is a long-range and anisotropic interaction. The ground state of a system of magnetic moments located at the sites of a simple cubic and of a square lattice was investigated by Belobrov *et al.*⁷ using the Luttinger and Tisza method.⁸ A continuous degeneracy of the ground state was found in both models. In particular, the ground state of the square planar rotator model was shown to consist of four sublattices where the magnetic moments of each sublattice make an angle α , $-\alpha$, $\pi+\alpha$, $\pi-\alpha$, with the x axis, α being arbitrary. The existence of a continuous degeneracy was pointed out also in the planar rotator model with pure dipole interaction on a honeycomb lattice.⁹ This model was investigated by the mean-field approximation and the continuous degeneracy was found to persist at finite temperature in zero external magnetic field. An ordered phase was found for $T < T_c$, however, it is well

known that the mean-field approximation provides LRO even in 2D planar and Heisenberg models with NN exchange interaction, where the absence of LRO is rigorously proved.¹

At finite temperature both square and honeycomb planar rotator models were investigated by Prakash and Henley¹⁰ who restricted the dipole interactions to nearest neighbors only, keeping the anisotropic nature of the true interaction. The free energy of both models was evaluated within the simple spin-wave approximation and symmetry-breaking terms were found at finite temperature so that *order by thermal disorder* was claimed. Other examples of order from thermal or quantum fluctuations, and from dilution are quoted in literature.¹¹ However, the simple spin-wave approximation, which is usually a reliable approach at low temperature, in this case leads to a divergent mean-square angular displacement because the ground state is affected by a continuous degeneracy. The breaking of the continuous degeneracy at finite temperature is a strong support to the existence of LRO whereas a divergent mean-square angular displacement implies the vanishing of the order parameter at any finite temperature.

The square planar rotator model with the full dipole interaction was studied by MC simulation in Ref. 12 and investigated by both simple spin-wave approximation and MC simulation in Refs. 13 and 14. MC simulation seems to support LRO as well as the degeneracy-breaking temperature-dependent terms of the free energy evaluated within the simple spin-wave approximation. Indeed thermal fluctuations select *columnar* spin configuration corresponding to alternate rows (columns) of parallel spins directed along the rows (columns) in agreement with MC results. However, the order parameter evaluated within the simple spin wave approximation is zero at any finite temperature.^{13,14} Higher order approximation is thought to overcome this apparent contradiction.^{13,15}

In this paper we perform a careful analysis of the spin-wave spectrum going beyond the simple spin-wave approximation. We introduce a renormalized spin-wave approximation which consists on accounting for cubic and quartic contributions of the Hamiltonian expanded in spin deviations and we find that the *accidental* soft mode in the simple spin-

wave spectrum (reminiscent of the continuous degeneracy of the ground state) is replaced by a temperature-dependent gap. Such a gap removes the divergence in the mean-square angular displacement and recovers LRO, even though the order parameter versus temperature has a singular behavior at very low temperature. We have checked this low-temperature singular behavior by MC simulation at variance with the linear behavior suggested in previous MC simulations.¹³

In order to test the renormalized spin-wave approximation we have performed the same calculation on a system with isotropic antiferromagnetic exchange coupling decaying as $1/r^3$. In this case no gap appears at finite temperature since the soft mode in the simple spin-wave spectrum is related to a *true* symmetry property of the Hamiltonian. This gapless mode leads to a divergent mean-square angular displacement in agreement with MC calculation.⁶

On the contrary, in the system with isotropic ferromagnetic exchange coupling decaying as $1/r^3$ LRO is assured by the linear dependence of the spectrum on the wave vector which implies a linear dependence of the mean-square angular displacement on the temperature in agreement with MC simulation.

We have evaluated the critical exponents for correlation length, staggered susceptibility and staggered magnetization by finite-size scaling of MC data. Assuming $\nu=1$ (Ref. 14) we obtain $\gamma=1.37\pm 0.07$ and $\beta=0.19\pm 0.04$. These critical exponents do not belong to any known universality class. This result could support the conjecture¹⁰ concerning the mapping of the present model into the two-dimensional planar model with symmetry-breaking perturbations¹⁶ for which a nonuniversal set of critical exponents is expected.

In Sec. II we apply the renormalized spin-wave approximation to the planar rotator model with dipolar interaction. In Sec. III we present the results obtained by MC simulation. Section IV contains summary and conclusions.

II. RENORMALIZED SPIN-WAVE THEORY

The Hamiltonian of the planar rotator model with pure dipolar interaction reads

$$\mathcal{H} = -\frac{1}{2} \frac{\mu^2}{a^3} \sum_{i,\mathbf{r}} \sum_{\alpha\beta} f^{\alpha\beta}(\mathbf{r}) S_i^\alpha S_{i+\mathbf{r}}^\beta, \quad (2.1)$$

where

$$f^{\alpha\beta}(\mathbf{r}) = \frac{a^3}{r^3} \left(3 \frac{r^\alpha r^\beta}{r^2} - \delta_{\alpha,\beta} \right). \quad (2.2)$$

In Eq. (2.1) μ is the magnetic moment; $\alpha, \beta = x, y$ label the two spin components; i labels the N sites of a square lattice; $\mathbf{r} = m_1 a \hat{u}_x + m_2 a \hat{u}_y$, with m_1, m_2 integers, is the generic lattice vector; a is the lattice constant. The ground-state spin configuration selected by thermal fluctuations is a columnar configuration.^{13,14} The two-component spins of planar rotator model are

$$S_i^x = S \cos(\mathbf{Q} \cdot \mathbf{r}_i + \psi_i), \quad S_i^y = S \sin(\mathbf{Q} \cdot \mathbf{r}_i + \psi_i), \quad (2.3)$$

where $\mathbf{Q} = (2\pi/a)(0, \frac{1}{2})$ is the order wave vector characterizing the columnar configuration and ψ_i is the angular dis-

placement from the ground state configuration at site i . We expand Hamiltonian (2.1) in powers of angular displacements retaining contributions up to fourth order. We introduce the Fourier transforms of angular displacements

$$\psi_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \psi_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}_i} \quad (2.4)$$

and we obtain the Hamiltonian

$$\mathcal{H} = E_0 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4 + \dots, \quad (2.5)$$

where

$$E_0 = -\frac{N}{2} \frac{\mu^2 S^2}{a^3} D^{xx}(\mathbf{Q}), \quad (2.6)$$

$$\mathcal{H}_2 = \frac{1}{2} \frac{\mu^2 S^2}{a^3} \sum_{\mathbf{q}} [D^{xx}(\mathbf{Q}) - D^{yy}(\mathbf{Q} - \mathbf{q})] \psi_{\mathbf{q}} \psi_{-\mathbf{q}}, \quad (2.7)$$

$$\begin{aligned} \mathcal{H}_3 = & -\frac{1}{2} \frac{\mu^2 S^2}{a^3} \frac{1}{\sqrt{N}} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} \delta_{\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3, 0} \\ & \times D^{xy}(\mathbf{Q} - \mathbf{q}_1) \psi_{\mathbf{q}_1} \psi_{\mathbf{q}_2} \psi_{\mathbf{q}_3}, \end{aligned} \quad (2.8)$$

$$\begin{aligned} \mathcal{H}_4 = & -\frac{1}{24} \frac{\mu^2 S^2}{a^3} \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3 \mathbf{q}_4} \delta_{\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4, 0} \\ & \times [D^{xx}(\mathbf{Q}) + 3D^{xx}(\mathbf{Q} + \mathbf{q}_3 + \mathbf{q}_4) - 4D^{yy}(\mathbf{Q} - \mathbf{q}_1)] \\ & \times \psi_{\mathbf{q}_1} \psi_{\mathbf{q}_2} \psi_{\mathbf{q}_3} \psi_{\mathbf{q}_4}, \end{aligned} \quad (2.9)$$

with

$$D^{\alpha\beta}(\mathbf{q}) = \sum_{\mathbf{r} \neq 0} f^{\alpha\beta}(\mathbf{r}) \cos(\mathbf{q} \cdot \mathbf{r}). \quad (2.10)$$

The simple spin-wave (SSW) spectrum is $\omega_{\text{SSW}}(\mathbf{q}) = (\mu^2 S^2 / 2a^3) \epsilon_{\mathbf{q}}$, where

$$\epsilon_{\mathbf{q}} = D^{xx}(\mathbf{Q}) - D^{yy}(\mathbf{Q} - \mathbf{q}). \quad (2.11)$$

Note that the SSW spectrum vanishes at $\mathbf{q}_0 = (2\pi/a)(\frac{1}{2}, \frac{1}{2})$. Indeed

$$\begin{aligned} \epsilon_{\mathbf{q}_0} = & \sum'_{m_1 m_2} \frac{1}{(m_1^2 + m_2^2)^{3/2}} \left[\left(3 \frac{m_1^2}{m_1^2 + m_2^2} - 1 \right) \right. \\ & \left. \times \cos(m_2 \pi) - \left(3 \frac{m_2^2}{m_1^2 + m_2^2} - 1 \right) \cos(m_1 \pi) \right] = 0, \end{aligned} \quad (2.12)$$

where the prime in the sum means that the term $m_1 = m_2 = 0$ has to be excluded. The soft mode excitation at \mathbf{q}_0 modifies the columnar ground state into the configuration given by

$$S_{m_1, m_2}^x \approx S \cos(m_2 \pi) \cos \alpha, \quad S_{m_1, m_2}^y \approx S \cos(m_1 \pi) \sin \alpha, \quad (2.13)$$

with α arbitrary.¹⁴ This configuration, shown in Fig. 2 of Ref. 15, corresponds to one of the continuous degenerate

ground states. The order parameter in SSW approximation is zero for any finite temperature. This fact claims for new investigations with respect to the selection of a columnar ground-state configuration out of the manifold of continuous degeneracy due to thermal fluctuations.^{13,14} To go beyond the SSW approximation we consider the cumulant expansion

$$\begin{aligned} \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle &= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} (\mathcal{H}_3 + \mathcal{H}_4 + \dots)^n \rangle_0^c \\ &= \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle_0 - \beta \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \mathcal{H}_4 \rangle_0^c \\ &\quad + \frac{1}{2} \beta^2 \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \mathcal{H}_3^2 \rangle_0^c + \dots, \end{aligned} \quad (2.14)$$

where

$$\langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle_0 = \frac{t}{\epsilon_{\mathbf{q}}} \quad (2.15)$$

is the SSW propagator of the noninteracting system and $t = k_B T a^3 / \mu^2 S^2$ is a reduced temperature.

The last two terms of Eq. (2.14) can be evaluated using Eqs. (2.8) and (2.9). One obtains

$$\begin{aligned} \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \mathcal{H}_4 \rangle_0^c &= -\frac{\mu^2 S^2}{a^3} \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle_0^2 \frac{1}{N} \sum_{\mathbf{k}} [D^{xx}(\mathbf{Q}) \\ &\quad + D^{xx}(\mathbf{Q} + \mathbf{q} - \mathbf{k}) - D^{yy}(\mathbf{Q} - \mathbf{q}) \\ &\quad - D^{yy}(\mathbf{Q} - \mathbf{k})] \langle \psi_{\mathbf{k}} \psi_{-\mathbf{k}} \rangle_0 \end{aligned} \quad (2.16)$$

and

$$\begin{aligned} \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \mathcal{H}_3^2 \rangle_0^c &= \left(\frac{\mu^2 S^2}{a^3} \right)^2 \langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle_0^2 \frac{1}{N} \sum_{\mathbf{k}} [D^{xy}(\mathbf{Q} - \mathbf{q})^2 \\ &\quad + 4D^{xy}(\mathbf{Q} - \mathbf{q})D^{xy}(\mathbf{Q} - \mathbf{k}) + 2D^{xy}(\mathbf{Q} - \mathbf{k})^2 \\ &\quad + 2D^{xy}(\mathbf{Q} - \mathbf{k})D^{xy}(\mathbf{Q} - \mathbf{k} + \mathbf{q})] \\ &\quad \times \langle \psi_{\mathbf{k}} \psi_{-\mathbf{k}} \rangle_0 \langle \psi_{\mathbf{k} - \mathbf{q}} \psi_{-\mathbf{k} + \mathbf{q}} \rangle_0. \end{aligned} \quad (2.17)$$

The propagator of the interacting system reads

$$\langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle = \frac{1}{\langle \psi_{\mathbf{q}} \psi_{-\mathbf{q}} \rangle_0^{-1} - \Sigma_{\mathbf{q}}} = \frac{t}{\epsilon_{\mathbf{q}} - t \Sigma_{\mathbf{q}}}, \quad (2.18)$$

where the proper self-energy $\Sigma_{\mathbf{q}}$ is easily obtained from Eqs. (2.16) and (2.17)

$$\begin{aligned} \Sigma_{\mathbf{q}} &= \frac{1}{N} \sum_{\mathbf{k}} [D^{xx}(\mathbf{Q}) + D^{xx}(\mathbf{Q} + \mathbf{q} - \mathbf{k}) - D^{yy}(\mathbf{Q} - \mathbf{q}) - D^{yy}(\mathbf{Q} \\ &\quad - \mathbf{k})] \frac{1}{\epsilon_{\mathbf{k}}} + \frac{1}{2N} \sum_{\mathbf{k}} [D^{xy}(\mathbf{Q} - \mathbf{q})^2 \\ &\quad + 4D^{xy}(\mathbf{Q} - \mathbf{q})D^{xy}(\mathbf{Q} - \mathbf{k}) + 2D^{xy} \\ &\quad \times (\mathbf{Q} - \mathbf{k})^2 + 2D^{xy}(\mathbf{Q} - \mathbf{k})D^{xy}(\mathbf{Q} - \mathbf{k} + \mathbf{q})] \frac{1}{\epsilon_{\mathbf{k}}} \frac{1}{\epsilon_{\mathbf{k} - \mathbf{q}}}. \end{aligned} \quad (2.19)$$

The renormalized spin-wave (RSW) spectrum is $\omega_{\text{RSW}}(\mathbf{q}) = (\mu^2 S^2 / 2a^3) \tilde{\epsilon}_{\mathbf{q}}$, where

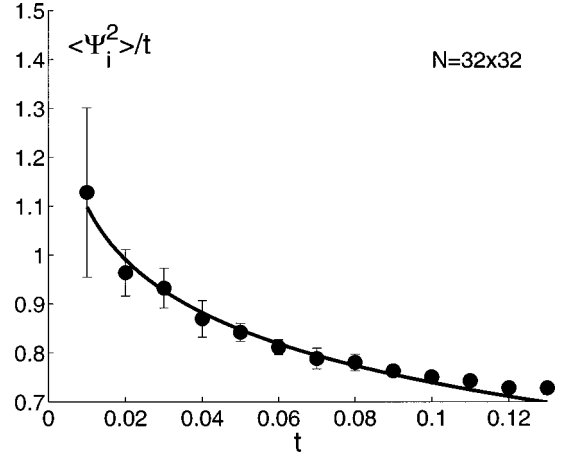


FIG. 1. Mean square angular displacement versus temperature. The continuous curve is the analytic result (2.23). Full circles are MC data for a 32×32 lattice.

$$\tilde{\epsilon}_{\mathbf{q}} = \epsilon_{\mathbf{q}} - t \Sigma_{\mathbf{q}}. \quad (2.20)$$

The value of the self-energy at $\mathbf{q} = \mathbf{q}_0$ is

$$\begin{aligned} \Sigma_{\mathbf{q}_0} &= \frac{1}{N} \sum_{\mathbf{k}} [D^{xx}(\mathbf{Q} + \mathbf{q}_0 - \mathbf{k}) - D^{yy}(\mathbf{Q} - \mathbf{k})] \frac{1}{\epsilon_{\mathbf{k}}} \\ &\quad + \frac{1}{N} \sum_{\mathbf{k}} D^{xy}(\mathbf{Q} - \mathbf{k}) [D^{xy}(\mathbf{Q} - \mathbf{k}) \\ &\quad + D^{xy}(\mathbf{Q} - \mathbf{k} + \mathbf{q}_0)] \frac{1}{\epsilon_{\mathbf{k}}} \frac{1}{\epsilon_{\mathbf{k} - \mathbf{q}_0}} \\ &= -0.575, \end{aligned} \quad (2.21)$$

so that $\tilde{\epsilon}_{\mathbf{q}_0} = 0.575t$. The gap at $\mathbf{q} = \mathbf{q}_0$ is originated by thermal fluctuations and increases as temperature increases. This behavior is very peculiar. As far as we know, this is the first example of a gap in the elementary excitation spectrum originated by thermal fluctuations. Usually the energy gap is reduced rather than increased by thermal fluctuations. A calculation of the renormalized spectrum in the neighborhood of \mathbf{q}_0 gives

$$\epsilon_{\mathbf{q} \rightarrow \mathbf{q}_0} \approx 0.575t + 0.150(\pi - aq_x)^2 + 1.786(\pi - aq_y)^2 \quad (2.22)$$

and the mean-square angular displacement becomes

$$\langle \psi_i^2 \rangle = \frac{t}{N} \sum_{\mathbf{k}} \frac{1}{\epsilon_{\mathbf{k}}} \approx -0.156t \ln t + ct, \quad (2.23)$$

where c is a constant coming from the regular contribution to the sum. As one can see from Eq. (2.23) at low temperature $\langle \psi_i^2 \rangle / t$ diverges logarithmically as shown by the continuous curve in Fig. 1. Note that the same quantity evaluated in systems with conventional LRO is a constant since in that case only the regular contribution in the sum (2.23) is present. The order parameter is

$$\begin{aligned} \langle \cos \psi_i \rangle &= \cos(\mathbf{Q} \cdot \mathbf{r}_i) e^{-(1/2)\langle \psi_i^2 \rangle} \\ &\approx \cos(m_2 \pi) \exp[0.0882t \ln t - ct/2]. \end{aligned} \quad (2.24)$$

Note the infinite slope of the order parameter for $t \rightarrow 0$. In this limit the energy cost to create a spin wave of wave vector $\mathbf{q} \sim \mathbf{q}_0$ is vanishing so that a large number of spin waves can be excited. However interaction between spin waves originates a gap in the spectrum that increases at increasing temperature and LRO is restored.

For comparison we consider the planar isotropic antiferromagnet where the spin-spin coupling decays as $1/r^3$ where r is the spin-spin distance. The Hamiltonian reads

$$\mathcal{H} = \frac{1}{2} \sum_{\substack{i, \mathbf{r} \\ \mathbf{r} \neq 0}} J(\mathbf{r}) \cos(\mathbf{Q} \cdot \mathbf{r} + \psi_i - \psi_{i+\mathbf{r}}), \quad (2.25)$$

where $J(\mathbf{r}) = J(a^3/r^3)$ and $\mathbf{Q} = (2\pi/a)(\frac{1}{2}, \frac{1}{2})$. Expansion of Hamiltonian (2.25) gives

$$\mathcal{H} = E_0 + \mathcal{H}_2 + \mathcal{H}_4 + \dots, \quad (2.26)$$

where

$$E_0 = \frac{N}{2} J(\mathbf{Q}), \quad (2.27)$$

$$\mathcal{H}_2 = \frac{1}{2} \sum_{\mathbf{q}} [J(\mathbf{Q} - \mathbf{q}) - J(\mathbf{Q})] \psi_{\mathbf{q}} \psi_{-\mathbf{q}}, \quad (2.28)$$

$$\begin{aligned} \mathcal{H}_4 = & \frac{1}{24} \frac{1}{N} \sum_{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4} \delta_{\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4, 0} [J(\mathbf{Q}) - 2J(\mathbf{Q} + \mathbf{q}_4) \\ & + 3J(\mathbf{Q} + \mathbf{q}_3 + \mathbf{q}_4) - 2J(\mathbf{Q} - \mathbf{q}_1)] \psi_{\mathbf{q}_1} \psi_{\mathbf{q}_2} \psi_{\mathbf{q}_3} \psi_{\mathbf{q}_4}, \end{aligned} \quad (2.29)$$

with

$$J(\mathbf{q}) = \sum_{\mathbf{r} \neq 0} J \frac{a^3}{r^3} \cos(\mathbf{q} \cdot \mathbf{r}). \quad (2.30)$$

Note that SSW approximation gives an elementary excitation energy $\omega_{\text{SSW}}(\mathbf{q}) = J\epsilon_{\mathbf{q}}$ where

$$\epsilon_{\mathbf{q}} = [J(\mathbf{Q} - \mathbf{q}) - J(\mathbf{Q})]/J \quad (2.31)$$

that vanishes quadratically as $q \rightarrow 0$. Indeed one has $\epsilon_{\mathbf{q}} \approx 0.40(aq)^2$. The RSW spectrum is given by $\omega_{\text{RSW}}(\mathbf{q}) = J\tilde{\epsilon}_{\mathbf{q}}$, where

$$\tilde{\epsilon}_{\mathbf{q}} = \epsilon_{\mathbf{q}} + t \Sigma_{\mathbf{q}}, \quad (2.32)$$

with $t = k_B T/J$ and

$$\begin{aligned} \Sigma_{\mathbf{q}} = & \frac{1}{JN} \sum_{\mathbf{k}} [J(\mathbf{Q}) - J(\mathbf{Q} - \mathbf{k}) + J(\mathbf{Q} - \mathbf{q} - \mathbf{k}) \\ & - J(\mathbf{Q} - \mathbf{q})] \frac{1}{\epsilon_{\mathbf{k}}}. \end{aligned} \quad (2.33)$$

In the long wavelength limit Eq. (2.32) gives

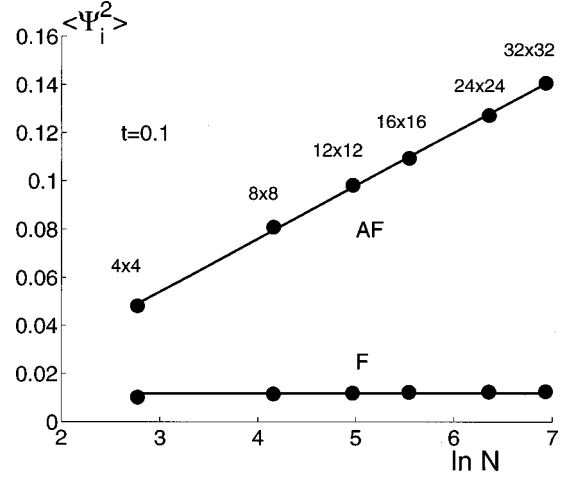


FIG. 2. Mean square angular displacement at $t=0.1$ versus $\ln N$ for square planar models with ferromagnetic (F) and antiferromagnetic (AF) isotropic long-range interactions decaying as $1/r^3$.

$$\tilde{\epsilon}_{\mathbf{q}} = (0.40 + ct)(aq)^2. \quad (2.34)$$

It is straightforward to prove that the leading order in temperature of the mean-square angular displacement obtained by RSW approximation is the same as that obtained by SSW approximation

$$\langle \psi_i^2 \rangle = \frac{t}{N} \sum_{\mathbf{k}} \frac{1}{\tilde{\epsilon}_{\mathbf{k}}} \approx \frac{t}{N} \sum_{\mathbf{k}} \frac{1}{\epsilon_{\mathbf{k}}} \approx 0.196t \ln N, \quad (2.35)$$

so that the absence of LRO expected on the basis of SSW approximation⁶ is confirmed by RSW approximation. Indeed the soft mode at $\mathbf{q}=0$ in the planar isotropic antiferromagnet is not suppressed by thermal fluctuations as one expects on account of the rotational invariance of Hamiltonian (2.25).

III. MONTE CARLO SIMULATION

We have performed MC simulation to get the thermodynamic properties of the model over the whole range of temperature. In particular, we have evaluated the temperature dependence of the mean-square angular displacement in order to compare the results of MC simulation with the analytic result at low temperature. As shown in Fig. 1 MC data (full circles) fit very well the analytic result given in Eq. (2.23) obtained by renormalized spin-wave theory (continuous curve). MC data are taken from a simulation on a sample 32×32 averaging over 10^3 configurations after having disregarded 10^5 steps for equilibration. The approach of periodic ‘‘images’’ is adopted.¹⁷ This approach, which is based on a periodic arrangement of MC cells, seems to be the most convenient to treat systems with long-range interactions. Note that the singular behavior of the mean-square angular displacement is caught by MC simulation only if the region of low temperature ($0.01 < t < 0.1$) is carefully investigated. This peculiar behavior escaped previous MC analysis.^{12,13}

In Fig. 2 we give the size dependence of the mean-square angular displacement at $t=0.1$ for the ferromagnetic and antiferromagnetic square planar model with isotropic long-range interaction decaying as $1/r^3$. The existence of LRO in the ferromagnetic model is proved by the size independence of the mean-square angular displacement. On the contrary

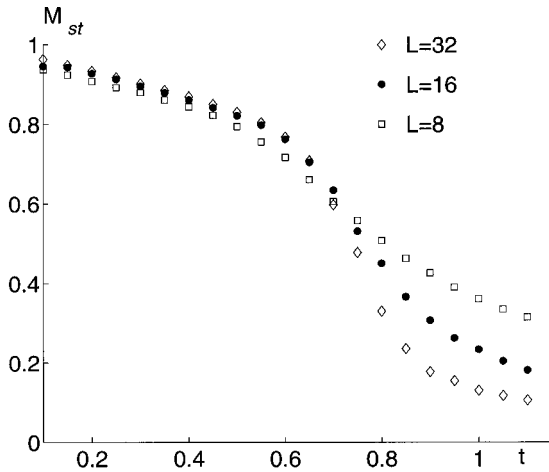


FIG. 3. Staggered magnetization versus temperature for different lattice sizes.

the absence of LRO in the antiferromagnetic model is clearly pointed out by the size dependence of the mean-square angular displacement which agrees very well with the analytic result of Eq. (2.35).

In Fig. 3 we show the staggered magnetization versus temperature of the square planar rotator model with pure dipolar interaction for $t > 0.1$. For $t < 0.1$ we have verified that the staggered magnetization is well reproduced by $M_s = 1 + 0.095t \ln t - 0.2t$ (Ref. 15) in good agreement with the analytic result of Eq. (2.24). Figures 1 and 3 of the present paper should be compared with Figs. 7, 12, 13 of Ref. 13 where MC results obtained for samples up to 128×128 are shown. A linear dependence of the staggered magnetization versus temperature is suggested: $M_s = 1 - 0.32t$ (note that our reduced temperature t is $T/2$ of Ref. 13). The same fit can be obtained looking at Fig. 3 in which the order parameter versus temperature is shown for $t > 0.1$. On the contrary, if we push the investigation out into the very low-temperature region as shown in Fig. 1, the singular behavior is recovered.

In Fig. 4 the staggered susceptibility is plotted against temperature for several lattice sizes in good agreement with Fig. 8 of Ref. 13.

Finally we try to get some insight on the critical behavior of the square planar model with dipolar interaction. This is

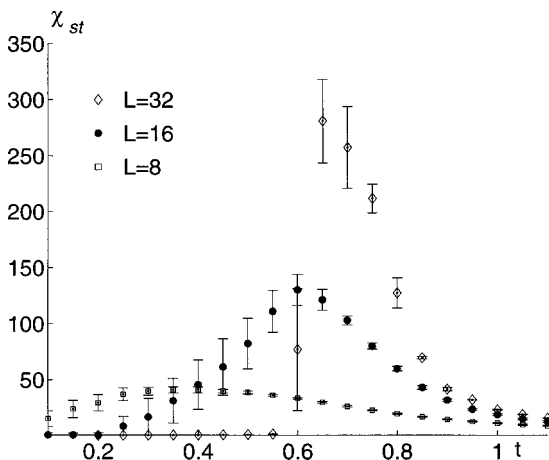


FIG. 4. Staggered susceptibility versus temperature for different lattice sizes.

an intriguing point. The RG analysis in $4-\epsilon$ dimensions¹⁸ was performed for models where spins are coupled by exchange and dipolar interactions under the hypothesis that the exchange is dominant with respect to the dipolar interaction. For antiferromagnetic spin configuration the critical exponents are the same as those found in absence of dipolar forces for both Heisenberg and Ising models. These results are relevant in 3D models with dominant exchange interaction but their extrapolation to models with pure dipole interactions, in particular to two-dimensional systems, is not obvious.

MC simulations on 3D Ising model¹⁷ partially support the RG results since no change in the behavior of magnetization and specific heat was observed when the ratio between short- and long-range interaction is changed. However no estimation of critical exponents was attempted.

For a simple cubic Ising model with pure dipolar interaction high-temperature series expansion¹⁹ provides a critical exponent of the staggered susceptibility $\gamma = 1.14$ which differs from both the mean-field exponent $\gamma = 1$ and the critical exponent $\gamma = 1.25$ of the Ising model with NN exchange interaction.

Very little is known about the critical properties of 2D lattices with spins coupled by pure dipolar interactions. In particular, no analytic evaluation of critical exponents was attempted. MC simulation performed on the square Ising model²⁰ leads to the conclusion that critical exponents are the same (within the numerical uncertainty) as those of the square Ising model with NN exchange interaction.

In the square planar rotator model we find that the dipole interaction supports LRO whereas the planar model with NN exchange interaction does not order at any finite temperature even though the existence of a topological phase transition, known as Kosterlitz-Thouless phase transition,² is proved. This fact prevents any comparison with the critical behavior of the corresponding NN model. Therefore we try to get the critical exponents by a finite-size scaling of our MC results. This procedure gives very good results for the NN Ising model and it has been successfully used to evaluate the critical exponents of the Ising model with dipole interaction.²⁰

We have verified that the choice $\nu = 1$ is consistent with MC data. As shown in Fig. 9 of Ref. 14 one finds that the relationship $t_c(L) - t_c \sim 1/L$, which implies $\nu = 1$, is consistent with the lattice size dependence of the temperature of the maximum of the staggered susceptibility or of the specific heat. Assuming $\nu = 1$ the value of γ is given by the slope of the straight line obtained by plotting the maximum of the staggered susceptibility versus the lattice size on a log-log scale. Mean values of the staggered susceptibility are evaluated averaging over 10 distinct simulations for a 32×32 lattice up to 100 distinct simulations for a 8×8 lattice. In Fig. 5 we show the least-squares linear interpolation of the data obtaining $\gamma = 1.37 \pm 0.07$.

We have also evaluated the critical exponent of the staggered magnetization β in different ways. In Fig. 6 we show the staggered magnetization (evaluated at the temperature of the maximum of the staggered susceptibility) versus the lattice size on a log-log scale. The slope of the least-squares linear interpolation of the data gives $\beta = 0.19 \pm 0.04$. A similar result is obtained by the scaling of the staggered magnetization evaluated at the critical temperature $t_c = 0.75$. Finally

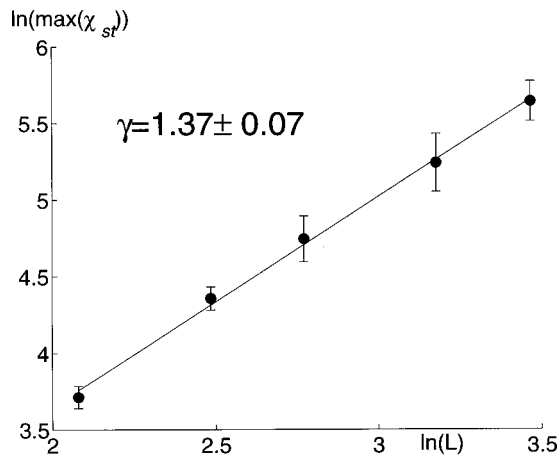


FIG. 5. Critical exponent γ of the staggered susceptibility obtained by finite-size scaling of MC data worked out on $L \times L$ samples.

the value of β deduced by the scaling of the staggered magnetization evaluated at the temperature at which the specific heat has its maximum, is in substantial agreement with the above result even though the error bars are much larger since the peak of the specific heat is less sharp than that of the susceptibility.

The critical exponents we have obtained differ from the mean field exponents as well as from those of the square Ising model with NN interaction. The square planar model with pure dipole interaction was conjectured to fall in the universality class of the square planar model with NN exchange interaction in presence of symmetry-breaking perturbations.¹⁰ If so the critical exponents of the present model should be the same as those of the $p=4$ model investigated in Ref. 16 which should display conventional power-law singularities, but with nonuniversal critical exponents. The critical exponents should depend on the symmetry-breaking field intensity h_4 . De'Bell *et al.*¹³ have noted that a NN square planar model with $h_4 \sim 0.2, 0.3$ shows similarities with the pure dipole square planar model. All these facts could explain why the critical exponents of the present model are unusual.

IV. SUMMARY AND CONCLUSIONS

Poor information is found in literature about the thermal behavior of spin systems where the spins are coupled by pure dipole interaction. Mostly, renormalization group analysis¹⁸ and MC simulation¹⁷ refer to 3D Ising or Heisenberg models in which the dipole interaction is weak with respect to the dominant NN exchange interaction.

Even less is known about 2D models. MC simulation was performed on the square Ising²⁰ and planar¹² model with pure dipole interaction. Nothing is known about the critical exponents of the planar rotator model with pure dipole interaction. We have investigated the thermodynamical properties of this model by both low-temperature expansion and MC simulation.

The ground-state configuration is affected by continuous degeneracy corresponding to four interpenetrating sublattices

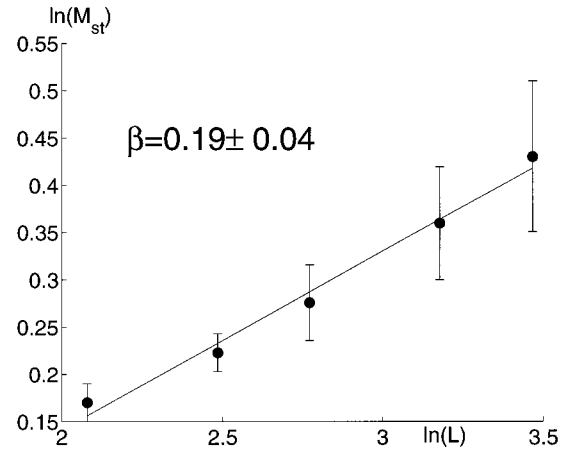


FIG. 6. Critical exponent β of the staggered magnetization obtained by finite-size scaling of MC data worked out on $L \times L$ samples.

making angles $\alpha, -\alpha, \pi + \alpha, \pi - \alpha$ with a reference axis, α being arbitrary. This continuous degeneracy is not related to the symmetry of the Hamiltonian and the simple spin-wave spectrum shows an *accidental* soft mode at $\mathbf{q} = (2\pi/\alpha)(\frac{1}{2}, \frac{1}{2})$ in the neighborhood of which the excitation energy is quadratic. For this reason the simple spin-wave theory leads to a contradictory result. Thermal contributions to the free energy select a *columnar* configuration where rows ($\alpha = 0$) or columns ($\alpha = \pi/2$) of parallel spins alternate. Thermal contributions to the magnetization reduce to zero the order parameter at any finite temperature.

We have solved this apparent contrasting result using the renormalized simple spin-wave approximation which accounts for interactions between spin waves. Indeed the accidental soft mode is replaced by a temperature-dependent gap [see Eq. (2.22)] that prevents the divergence of the mean-square angular displacement. Singular behavior of the order parameter is pointed out. We have checked this behavior, which escaped previous MC simulation,^{12,13} pushing our MC simulation into the range $0.01 < t < 0.1$. An excellent agreement between our analytic result and MC simulation is found. The staggered magnetization and the staggered susceptibility agree with previous MC data¹³ for $t > 0.1$.

We have performed finite-size scaling analysis of the maximum of the staggered susceptibility and of the staggered magnetization evaluated at the temperature of the maximum of the susceptibility leading to unusual values of the critical exponents $\gamma = 1.37$ and $\beta = 0.19$. An interesting conjecture¹⁰ about the mapping of the square planar rotator model with pure dipole interaction into the corresponding NN model with symmetry-breaking perturbation¹⁶ could explain the unusual critical exponents we have found.

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