Long-range order in 2*D* Heisenberg model with frustration

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Indications of the possible existence of a spin-liquid state have been found for a 2*D* Heisenberg model with frustration at values of the $\alpha = J_2/J_1$ near 0.6.

The spin subsystem of the insulating state of a CuO_2 plane of a high-T_c superconductor can be described well by a 2*D* Heisenberg model on a square lattice with an antiferromagnetic interaction of nearest $S = 1/2$ spins.[1] Substantial progress in the study of this model was achieved in Refs. 2–5, where it was shown that there is an exponentially small (along T) gap in the spectrum of spin excitations and that a long-range order arises at $T = 0$. Experiments have revealed that the long-range order is lost upon spin doping of the CuO_2 plane.[1] It is believed that the doping of the plane with holes leads to a frustration, i.e., to an interaction between remote spins.[6] The 2*D* model has thus been the subject of active research recently in connection with the possible existence of a spin-liquid state.[7] In this letter we are reporting results of a study of a model with frustration in the limit $T \to 0$; these results indicate the possible realization of a spin-liquid state.

The Hamiltonian of the model is

$$H = 1/2 J_1 \Sigma_{\mathbf{n},\mathbf{g}} \mathbf{S}_{\mathbf{n}} \mathbf{S}_{\mathbf{n}+\mathbf{g}} + 1/2 J_2 \Sigma_{\mathbf{n},\mathbf{d}} \mathbf{S}_{\mathbf{n}} \mathbf{S}_{\mathbf{n}+\mathbf{d}} , \tag{1}$$

where $J_1, J_2 > 0$ describe the interaction between the nearest neighbors (the vectors $\mathbf{g}$) and the next-nearest neighbors ($\mathbf{d} = \pm \mathbf{g}_x \pm \mathbf{g}_y$) on the square lattice.

For Hamiltonian (1) in the classical limit ($S \gg 1$) we know that at $\alpha = J_2/J_1 < 1/2$ (case I) there is a two-sublattice state, while at $\alpha > 1/2$ there is a stripe state (case II).[8] In the quantum limit ($S = 1/2$), these cases correspond to different vacuum states: case I to $S_n^z = (1/2)(-1)^n$, and case II to $S_n^z = (1/2)(-1)^{n_x}$. We write the spin operators in terms of boson operators for these vacuum states, using a Dyson-Maleev antiferromagnetic transformation.[5]

In case I, the Hamiltonian becomes

$$H = H_1 + H_2^a + H_2^b$$

$$H_1 = -\frac{1}{2} J_1 N + \frac{1}{2} J_1 \sum_{\langle \mathbf{nm} \rangle}$$

$$\times \{ a_{\mathbf{n}}^+ a_{\mathbf{n}} + b_{\mathbf{m}}^+ b_{\mathbf{m}} - a_{\mathbf{n}}^+ b_{\mathbf{m}}^+ - a_{\mathbf{n}} b_{\mathbf{m}} + a_{\mathbf{n}}^+ (b_{\mathbf{m}}^+ - a_{\mathbf{n}})^2 b_{\mathbf{m}} \} \tag{2}$$

$$\mathbf{m} = \mathbf{n} + \mathbf{g}, \ \mathbf{n} \in A, \ \mathbf{m} \in B$$

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$$H_2^a = \frac{1}{4}J_2N - \frac{1}{2}J_2 \sum_{\langle \mathbf{n}_1\mathbf{n}_2\rangle}$$

$$\times \{a^+_{\mathbf{n}_1}a_{\mathbf{n}_1} + a^+_{\mathbf{n}_2}a_{\mathbf{n}_2} - a^+_{\mathbf{n}_1}a_{\mathbf{n}_2} - a^+_{\mathbf{n}_2}a_{\mathbf{n}_1} + a^+_{\mathbf{n}_1}a^+_{\mathbf{n}_2}(a_{\mathbf{n}_1} - a_{\mathbf{n}_2})^2\}.$$

$$\mathbf{n}_2 = \mathbf{n}_1 + \mathbf{d};\ \mathbf{n}_1, \mathbf{n}_2 \in A.$$

Here H_2^b, which describes the interaction of spins on sublattice B, is similar to H_2^a.

As in Ref. 5, we consider the Hamiltonian H given by (2) in the mean-field approximation with the auxiliary condition $\langle S_n^z\rangle = 0$, in order to satisfy the Mermin-Wagner theorem[9] at $T \neq 0$. We introduce the following expectation values:

$$Q = \langle a^+_{\mathbf{n}} b^+_{\mathbf{n}+\mathbf{g}}\rangle = \langle a_{\mathbf{n}} b_{\mathbf{n}+\mathbf{g}}\rangle; \quad \Delta = \langle a^+_{\mathbf{n}} a_{\mathbf{n}+\mathbf{d}}\rangle;$$

$$\langle a^+_{\mathbf{n}} a_{\mathbf{n}}\rangle = \langle b^+_{\mathbf{m}} b_{\mathbf{m}}\rangle = \frac{1}{2}. \tag{3}$$

The last equality is equivalent to the requirement $\langle S_n^z\rangle = 0$ and is taken into account through the introduction of a "chemical potential" λ. After the expectation values in (3) are singled out, and after a transformation is made to the momentum representation, Hamiltonian (2) can be diagonalized easily through a standard spin-wave u–v transformation. As a result, the spectrum of excitations, $\omega_{\mathbf{k}}$, self-consistent equations (3), and the ground-state energy E_0^{I} per site become

$$\omega_{\mathbf{k}} = [\epsilon_{\mathbf{k}}^2 - (4QJ_1\gamma_{\mathbf{gk}})^2]^{1/2}, \qquad \epsilon_{\mathbf{k}} = \lambda + 4J_1Q - 4J_2\Delta(1 - \gamma_{\mathbf{dk}}), \tag{4}$$

$$\gamma_{\mathbf{gk}} = \frac{1}{2}(\cos k_x g + \cos k_y g), \quad \gamma_{\mathbf{dk}} = \cos k_x g \cos k_y g; \quad E_0^{\mathrm{I}} = -2(J_1Q^2 - J_2\Delta^2),$$

$$Q = 2N^{-1}\sum_{\mathbf{k}} 4Q\gamma^2_{\mathbf{gk}}\omega_k^{-1}(\nu_k + \frac{1}{2}); \qquad \Delta = 2N^{-1}\sum_{\mathbf{k}} \epsilon_k \gamma_{\mathbf{dk}}\omega_{\mathbf{k}}^{-1}(\nu_{\mathbf{k}} + \frac{1}{2}),$$

$$2N^{-1}\sum_{\mathbf{k}}\{\epsilon_{\mathbf{k}}\omega_{\mathbf{k}}^{-1}(\nu_{\mathbf{k}} + \frac{1}{2}) - \frac{1}{2}\} = \frac{1}{2}. \tag{5}$$

Here $\Sigma_{\mathbf{k}}$ means a summation over the magnetic Brillouin zone, $\nu_{\mathbf{k}} = \nu(\omega_{\mathbf{k}})$ is the Bose function, and $g = |\mathbf{g}|$ is the lattice constant.

In addition, as in Refs. 2–5, system (5) has a solution with an exponentially small gap $\lambda = \exp(-A/T)$, where A is a constant as $T \to 0$. The finite value of $A(T=0)$ is interpreted by analogy with the Bose condensation of excitations with $k = 0$ (Refs. 3 and 4). It gives rise to a long-range order at $T = 0$. In our case we have

$$\langle S_n S_{n+l}\rangle = (-1)^{|l|}(m_0^{\mathrm{I}} + 0(l^{-1}))^2, \quad m_0^{\mathrm{I}} = \frac{A}{2\pi(J_1Q - 2J_2\Delta)}, \qquad g \ll l \ll \zeta,$$

$$\zeta = \exp(A/T), \qquad T \to 0, \tag{6}$$

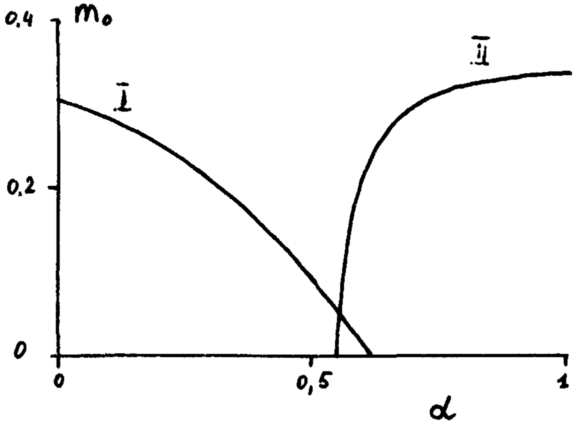

FIG. 1. The effective spin $m_0^{\mathrm{I,II}}$ as a function of α.

where m_0^{I} is the effective spin, ζ is the correlation length, and A, Q, and Δ are functions of α. A numerical solution of system (5) in the limit $T\to 0$ yields the values of m_0^{I} and $E_0^{\mathrm{I}}(\alpha)$ ($J_1 = 1$), shown in Figs. 1 and 2. It turns out that at $\alpha \approx 0.61$ the quantities A and m_0^{I} vanish; i.e., the long-range order disappears.

In case II we introduce the expectation values

$$q = \langle a_{\mathbf{n}}^{+} b_{\mathbf{n}+\mathbf{d}}^{+} \rangle, \qquad \rho_x = \langle a_{\mathbf{n}}^{+} b_{\mathbf{n}+\mathbf{g}_x}^{+} \rangle, \qquad \rho_y = \langle a_{\mathbf{n}}^{+} a_{\mathbf{n}+\mathbf{g}_y} \rangle, \tag{7}$$

which are determined by the structure of vacuum state II: ferromagnetic along the Y direction and antiferromagnetic along the X direction. The system of self-consistent equations which arises is analogous to system (5) and leads to

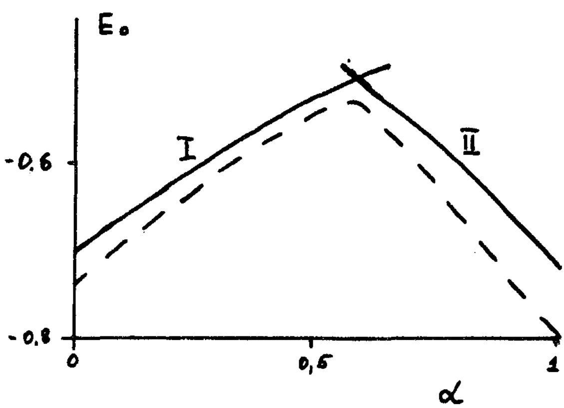

FIG. 2. Ground-state energy of the two phases, $E_0^{\mathrm{I,II}}$, as a function of α. Dashed line—$E_0(\alpha)$ from Ref. 11.

$$\omega_{\mathbf{k}} = [\epsilon_{\mathbf{k}}^2 - (4J_2 q\gamma_{\mathbf{dk}} + 2J_1\rho_x \cos k_x g)^2]^{1/2},$$

$$\epsilon_{\mathbf{k}} = \lambda + 4J_2 q + 2J_1\rho_x - 2J_1\rho_y (1-\cos k_y g), \quad (8)$$

$$E_0^{\mathrm{II}} = -2J_2 q^2 - J_1(\rho_x^2 - \rho_y^2).$$

The corresponding energies E_0^{II} and effective spin m_0^{II} are shown in Figs. 1 and 2. At $\alpha \approx 0.55$, the long-range order disappears on the large-α side.

For both phases, the form of ω_{k} in (4) and (8) is qualitatively the same as the spectrum in the approximation of linear spin waves.[10] For $S=1/2$, however, this approximation exaggerates the role of quantum fluctuations and leads to the conclusion that there is no solution in a region of finite size along α near $\alpha = 0.5$. In our analysis, the transition from one phase to the other occurs at $\alpha \approx 0.55$–0.6. Points $m_0 \to 0$ corresponds to metastable phases, which lie near a stable phase ($\Delta E \approx 0.01\, J_1$). This behavior agrees well with the results of a numerical diagonalization of a 4×4 cluster,[11] whose energy is shown in Fig. 1. Periodic boundary conditions for a cluster reduce E_0 from the exact value for an infinite system, primarily at $\alpha > 0.5$. In each limit, $\alpha \to 0$ ($\alpha \to \infty$), the energy E_0^{I} (E_0^{II}) agrees well with the known value[12] 0.667 $J_1(J_2)$. The presence at $\alpha \approx 0.6$ of two phases, spaced closely along the energy scale, with small values of m_0, indicates an instability of the long-range order with respect to the formation of a possible chiral spin-liquid state.[8] A finite, temperature-independent gap in the ω_{k} spectrum should correspond to this state.

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