Spin-wave interaction effects in the Néel phase of the J_1-J_2-J_3 model

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Treating the residual spin-wave interaction as a perturbation to the mean-field Hamiltonian, we compute the stability region of the Néel phase in the J_1-J_2-J_3 model. The phase boundary found within the second-order approximation lies between the mean-field boundary and the classical boundary.

The question of how the strong quantum fluctuations alter the classical picture of two-dimensional antiferromagnets has attracted much attention in the last years.[1,2] As a rule, quantum fluctuations work against ordering but in some cases they can stabilize ordered phases in a classically forbidden area.[3] Recently, an enhancement of the stability region of the Néel state over the classical case, perhaps as a combined effect of fluctuations and frustration, has been predicted in quantum frustrated antiferromagnets on a square lattice by mean-field-type theories (MFT).[4–7] On the other hand, several approaches, including linear spin-wave theory[8–10] (SWT) and series expansions,[11] lead to destruction of the Néel order at critical frustration appreciably smaller than that in the classical theory.

Further investigations[6,12–15] have been devoted to checking the reliability of approximations made in SWT and MFT. Along this direction, it has been found out[6,12–14] that $1/S$ expansions of SWT are well-behaved series in the square-lattice antiferromagnets only at small frustration. No way to improve systematically the linear SWT results at moderate frustration of these systems has been found yet. This fact makes questionable the predictions of SWT for the stability region of the Néel state in frustrated square-lattice antiferromagnets.

The other widely discussed results for the Néel state of these systems, namely the MFT results, can be affected by the fluctuations omitted in MFT. In the perturbation approach developed in our previous work[15] for investigation of the spin-$\frac{1}{2}$ J_1-J_2 model, MFT has been recognized as a zero-order approximation (an ideal gas of renormalized spin waves). Calculating the first nonvanishing corrections to the energy and magnetization caused by the residual spin-wave interaction in ordered phases, we have shown,[15] in particular, that the corrections to magnetization, though being small, reduce essentially the Néel state stability region predicted by MFT (Ref. 16) in the spin-$\frac{1}{2}$ J_1-J_2 model. We have found[15] for the critical frustration the value $\alpha_c = 0.52$ ($\alpha = J_2/J_1$) which is very close to the classical value 0.50 (MFT gives[4–6] $\alpha_c \simeq 0.62$). The agreement of this result with the numerical estimates[17–19] of α_c supports the suggestion that essential spin-wave interaction effects in frustrated antiferromagnets can be evaluated by a finite-order perturbation theory.

Here we study spin-wave interaction effects in the Néel phase of the more general J_1-J_2-J_3 model of a frustrated antiferromagnet where MFT also predicts[20] a significant enhancement of the stability region as compared to the classical case. The model is defined by the Hamiltonian

$$H = J_1 \sum_{\langle \mathrm{n} \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_2 \sum_{\langle \mathrm{nn} \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_3 \sum_{\langle \mathrm{nnn} \rangle} \boldsymbol{S}_i \boldsymbol{S}_j. \quad (1)$$

Positive J_1, J_2, and J_3 measure, respectively, the strength of interaction between nearest (n), next-nearest (nn), and next-next-nearest (nnn) neighbors on a square lattice. Consideration of the nn and nnn couplings in Eq. (1) is motivated, in particular, by the recent suggestion[21] that these interactions model to some extent the effects of holes in lightly doped CuO_2 planes of the cooper-oxide materials.

Following the scheme of Ref. 15, within the Dyson-Maleev (DM) formalism, we eliminate, by a Bogoliubov transformation, the quadratic part of the interaction term. This leads us to the DM Hamiltonian in the form

$$H_{\mathrm{DM}} = W_0 + H_0 + V_{\mathrm{DM}}, \quad (2)$$

where W_0 is a constant, H_0 represents an ideal gas of spin waves, and V_{DM} is a quartic normal-ordered operator describing the spin-wave interaction. It should be noticed that the elementary excitations of system (1) considered here are not the conventional magnons investigated in SWT. An essential part—namely, the quadratic part—of the interaction between SWT magnons is incorporated in the zero-order Hamiltonian H_0. The perturbation scheme above H_0 provides expansions of the ground-state characteristics in powers of the residual spin-wave interaction instead of the $1/S$ expansions.

The DM vertices of the J_1-J_2-J_3 model can be written as

$$\Phi^{(\nu)} = \Phi_{12}^{(\nu)} + \Phi_3^{(\nu)}, \quad \nu = 1, 2, \ldots, 9,$$

where $\Phi_{12}^{(\nu)}$ is the J_1-J_2 DM vertex[15] and $\Phi_3^{(\nu)}$ is the part caused by the J_3 term in Eq. (1). The parameters of the Bogoliubov transformation are defined by the equations

$$a = \frac{S + R_3 - R_2}{S + R_1 - R_2}, \quad b = \frac{S + R_4 - R_2}{S + R_1 - R_2},$$

where

$$R_1 = \frac{2}{N}\sum \gamma_k u_k v_k, \quad R_2 = \frac{2}{N}\sum v_k^2, \quad R_3 = \frac{2}{N}\sum \eta_k v_k^2, \quad R_4 = \frac{2}{N}\sum \widetilde{\gamma}_k v_k^2,$$

and

$$\gamma_k = \tfrac{1}{2}\left(\cos k_x + \cos k_y\right), \quad \widetilde{\gamma}_k = \tfrac{1}{2}\left(\cos 2k_x + \cos 2k_y\right), \quad \eta_k = \cos k_x \cos k_y,$$

$$u_k = \sqrt{\tfrac{1+\epsilon_k}{2\epsilon_k}}, \quad v_k = \mathrm{sgn}\left(f_k\right)\sqrt{\tfrac{1-\epsilon_k}{2\epsilon_k}}, \quad \epsilon_k = \sqrt{1-\left(\gamma_k/f_k\right)^2},$$

$$f_k = 1 - \alpha a\left(1-\eta_k\right) - \alpha_1 b\left(1-\widetilde{\gamma}_k\right), \quad \alpha = J_2/J_1, \quad \alpha_1 = J_3/J_1.$$

It can be proved that the description of the Néel state of model (1) based on the zero-order Hamiltonian H_0 [Eq. (2)] coincides with the description given by the Schwinger-boson mean-field theory (SBMFT).[20] In the limiting case $J_3 = 0$ (the J_1-J_2 model) the H_0 theory coincides with the modified spin-wave theory[4–6] (MSWT) as well. Hence, the interaction term V_{DM} describes the effects omitted in MFT. We treat this term by the second-order perturbation theory and obtain the results discussed below.

In Fig. 1 we present the magnetization m of the Néel state for the $S = \frac{1}{2}$ J_1-J_2-J_3 model in two cases: (i) $J_2 = 0$ (the J_1-J_3 model) and (ii) $J_2 = 2J_3$ [model (1) with this relation between exchange integrals is believed to be the most relevant effective spin model for doped CuO_2 planes].[20,21,14] The second-order results are displayed by solid lines and the zero-order approximation (MFT) corresponds to the dashed lines. As is seen, the residual spin-wave interaction increases m at a small frustration but this interaction melts the ordering near the MFT boundary. In the second-order approximation we obtain the phase boundary points $\alpha_{1c} \simeq 0.35$ and $\alpha_c \simeq 0.32$ for the (i) and (ii) cases, respectively. These results should be compared with the MFT predictions $\alpha_{1c} \simeq 0.39$ (Ref. 14) and $\alpha_c \simeq 0.35$ (Ref. 20). The classical theory yields[9,14] smaller values: $\alpha_c = \alpha_{1c} = 0.25$. It is also worth noticing that the second-order value $\alpha_c \simeq 0.35$ of the critical frustration in the J_1-J_3 model coincides with what has been obtained by numerical calculations on small clusters.[19]

The reduction of the MFT stability region of the Néel state in the J_1-J_2-J_3 model is smaller than in the J_1-J_2 model. This is seen in Fig. 2 where we present the stability region in the whole (α, α_1) plane. In general, within the second-order approximation, a noticeable enhancement of the Néel state stability region over the classical case is revealed everywhere except the vicinity of the point $J_3 = 0$.

The residual spin-wave interaction melts the Néel ordering even if $S > \frac{1}{2}$. The second-order corrections vanish only in the limit $S \to \infty$ (see Fig. 3). In this limit both MFT and perturbation theory stick with the classical one in a way displayed for the (ii) case in Fig. 3.

This figure represents a part of the phase diagram of model (1) with $J_2 = 2J_3$. Within the SBMFT, the full phase diagram of this model has been recently calculated by Ceccatto *et al.*[20] They predicted a small window between the Néel and spiral phases in the $S = \frac{1}{2}$ system and overlap between the two phases for the other physical S to exist. Neglecting corrections to the spiral phase,[22] we

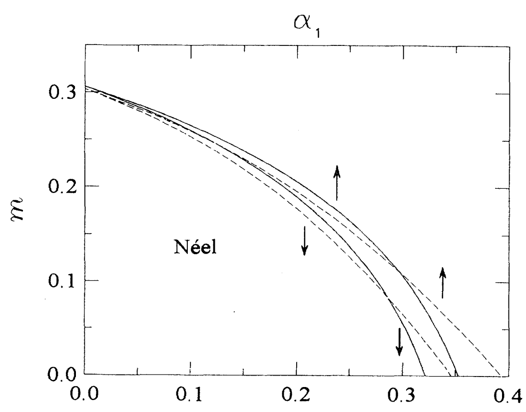

FIG. 1. Staggered magnetization of the Néel state of the spin-$\frac{1}{2}$ J_1-J_2-J_3 model: $m(\alpha_1)$ in the case $J_2 = 0$ and $m(\alpha)$ in the case $J_2 = 2J_3$ ($\alpha = J_2/J_1$, $\alpha_1 = J_3/J_1$). The zero-order results (SBMFT) (Ref. 20) are shown by dashed lines and the second-order results correspond to solid lines.

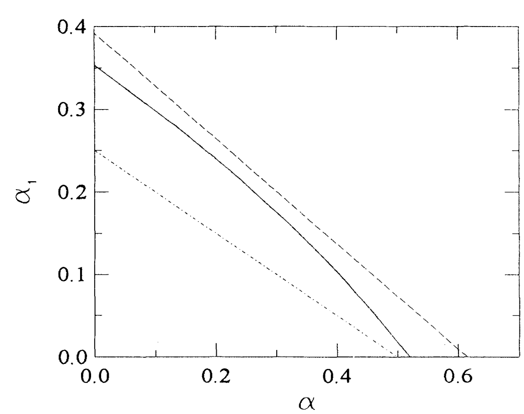

FIG. 2. Stability region of the Néel state of the $S = \frac{1}{2}$ J_1-J_2-J_3 model in the (α, α_1) plane according to the classical theory (dash-dotted line), SBMFT (dashed line), and present theory (solid line).

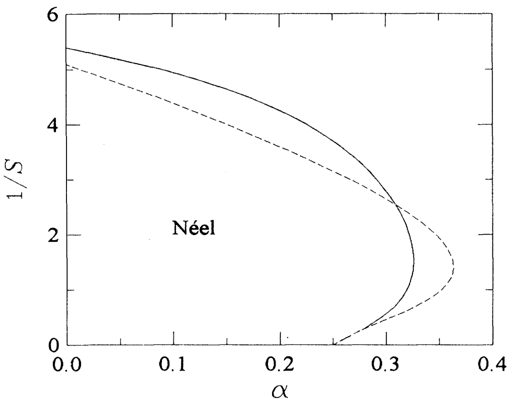

FIG. 3. Néel phase boundary in the $(1/S, \alpha)$ plane for model (1) with $J_2 = 2J_3$: SBMFT (Ref. 20), dashed line; present theory, solid line.

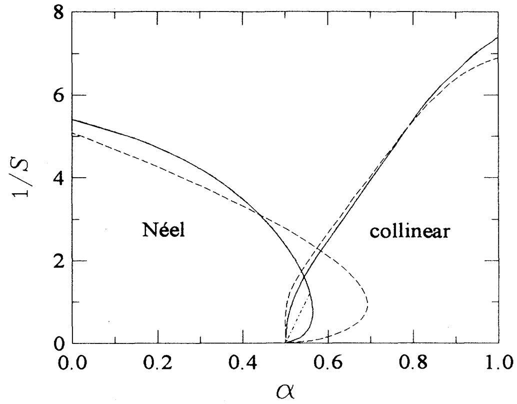

FIG. 4. Phase diagram of the J_1-J_2 model: zero-order theory [MSWT (Refs. 4 and 6), SBMFT (Ref. 5)], dashed lines; second-order theory, solid lines. Below the dash-dotted line the collinear state has a lower energy than the Néel state.

find that the correction to the Néel state stability region makes the window between the Néel and spiral phases for $S = \frac{1}{2}$ wider and almost washes out the overlap between ordered phases for larger S.

A more complete second-order description of the $(1/S$, frustration) phase diagram we obtain in the J_1-J_2 model. By calculating the corrections to both Néel and collinear phases we find a window (see Fig. 4) between the two phases for any $S < S_0 \simeq 0.63$ (MFT predicts[4–6] $S_0 \simeq 0.42$) and a noticeable overlap for larger S. Hence, within the second-order approximation, a disordered phase is possible to appear in the J_1-J_2 model only in the strong quantum limit $S = \frac{1}{2}$. From the results presented in Fig. 4 we may also conclude that spin-wave interaction effects are more pronounced in the Néel phase than those in the collinear phase.

The overlap area between the ordered phases should be regarded as a region of metastability of the Néel or collinear phase. We computed the line (the dash-dotted line in Fig. 4) along which $E(\text{Néel}) = E(\text{collinear})$, $E = E_0 + \Delta E$. The corrections ΔE turned out to be very small and this line is practically the same as that in the zero-order approximation.

In conclusion, we have found a noticeable reduction of the MFT stability region of the Néel state in the J_1-J_2-J_3 model occurring due to interaction effects. The reduced region remains, however, wider than the classical one. By comparing our results with available numerical estimates we have presented some evidence that the proposed second-order theory satisfactorily describes the Néel state of the complicated spin model, Eq. (1).

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[22] Presumably these corrections can be investigated by some (nontrivial) modification of the present method. We expect the spin-wave interaction effects in the spiral phase to be similar to those in the collinear phase of the J_1-J_2 model (see Ref. 15 and Fig. 4 in the main text of the present paper).