Theory of the Néel and collinear phases in the J_1-J_2 model of a spin-$\frac{1}{2}$ square-lattice frustrated antiferromagnet

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We present a perturbation scheme for evaluating the ground-state characteristics of Néel and collinear phases of the spin-$\frac{1}{2}$ J_1-J_2 model. Using the Dyson-Maleev formalism and performing a canonical transformation to exclude strong interaction between bosons, we convert the Hamiltonian of the J_1-J_2 model to the Hamiltonian $H_{\rm DM}=H_0+V_{\rm DM}$, where H_0 represents a noninteracting gas of quasiparticles and $V_{\rm DM}$ is a normal-ordered quartic operator. The description, based on the zero-order Hamiltonian H_0, turns out to be equivalent to the description of ordered phases, obtained earlier in the framework of modified spin-wave theory (MSWT). We carry out perturbation-type calculations up to second order in $V_{\rm DM}$ for the ground-state energy and magnetization and obtain small corrections in a wide range of the frustration parameter α ($=J_z/J_1$). It is shown that near the phase boundaries the spin-wave interaction causes an essential melting effect. The corrected value of magnetization of the Néel (collinear) phase goes to zero at $\alpha \simeq 0.52$ ($\alpha \simeq 0.57$). Thus, within a second-order approximation a window $0.52 < \alpha < 0.57$ instead of the MSWT overlap between Néel and collinear phases is found.

I. INTRODUCTION

The Hamiltonian for a square-lattice frustrated Heisenberg antiferromagnet, namely,

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{\langle lm \rangle} \mathbf{S}_l \mathbf{S}_m \;, \tag{1}$$

where positive J_1 and J_2 correspond to the nearest-neighbor (NN) and next-nearest-neighbor (NNN) coupling constant between spins, has attracted much attention in recent years.[1-12] It is believed that the investigation of the ground state and excitations of $S=\frac{1}{2}$ square-lattice frustrated models may lead to a better understanding of the nature of high-temperature superconductivity. Semiquantitative arguments about how the effect of doping can be described by including further couplings into the quantum Heisenberg model, the couplings being proportional to the doping of cooper oxide materials, have been presented in Ref. 12.

The classical ground state of the model (1) is Néel ordered up to $\alpha = J_2/J_1 = 0.5$. For $\alpha > 0.5$, J_2 dominates and the system separates into two sublattices, each of them having Néel order. The classical energy is independent of the angle between the two sublattices, and there is a continuous degeneracy between all canted states. In systems with large frustration, zero-point fluctuations favor the collinear phase, namely, the phase with stripe ordering. In the spin-$\frac{1}{2}$ model (1), which will be discussed in this paper, the quantum fluctuations can destroy classical structures and some other type of ground state may be possible. Several states, interesting for high-T_c superconductivity, have been proposed for the ground state of this NNN model at an intermediate range of the parameter α (see Ref. 10 and references therein).

Recently, the frustrated Heisenberg model (1) has been studied by various approximate and numerical methods, including conventional spin-wave theory (SWT),[1] modified spin-wave theory (MSWT),[2,3] symmetric-sublattice spin-wave theory (SSSWT),[4] Schwinger-boson mean-field theory (SBMFT),[5] exact diagonalization technique on small systems[6,7] finite-size scaling,[8] renormalization-group methods,[9] variational approaches,[11] and so on. There exist, however, a significant discrepancy between published results for the ground-state characteristics of the model (1). For example, whereas mean-field theories[2,3,5] predict an overlap between Néel and collinear phases, SWT (Ref. 1) and other approaches[7] lead to the existence of a rather large window between these phases. As a matter of fact, it is not clear yet if Néel and stripe orders are stabilized or not by quantum fluctuations and if there is some room for other states, ordered or disordered, in the J_1-J_2 model. More consistent methods, which will permit one to control approximations in the calculations of fundamental characteristics of frustrated models, are needed.

In the last few years, many authors[9,13-20] have demonstrated how precise analytical estimates of the ground-state characteristics of the NN Heisenberg model may be obtained by calculation of corrections within the framework of SWT. The so-called third-order spin-wave results for the ground-state energy,[16,17] magnetization,[16] spin-wave velocity,[15,16] spin-stiffness constant,[16] and transverse susceptibility[16] coincide very well with the most precise Green-function Monte Carlo and series expansion estimates. However, spin-wave expansions turned out not to be well-behaved series[2,8,9] for model (1). In order to develop a consistent method for investigation of frustrated antiferromagnets, it is useful to reveal and analyze the reasons for this breakdown of standard SWT in the description of the J_1-J_2 model.

Let us start the analysis with the spin-wave expansions for the basic characteristics of the square-lattice NN Heisenberg model, where the ground-state energy per bond,[16,17] $\mathcal{E}=E_0/2N$, is

$$\mathcal{E}=-S^2-0.157\,947S-0.006\,237+0.000\,107S^{-1}+O(S^{-2}) \tag{2a}$$

and magnetization[16] m is

$$m=S-0.196\,602+0.000\,866S^{-2}+O(S^{-3}) . \tag{2b}$$

Expansions for the spin-wave velocity,[15,16] spin-stiffness constant,[16] and transverse susceptibility[16] have a similar structure.

The last terms in the series (2) are very small even at $S=\frac{1}{2}$. Therefore one may suppose that the effective expansion parameter in (2) cannot be simply $1/S$, $1/zS$, or $\langle n\rangle/zS$ ($z=4$ is the number of neighbors; $\langle n\rangle\simeq 0.2$ is the average number of spin flips on one site), as is commonly assumed,[20] but it is instead a more subtle quantity, which we expect to be proportional to the interaction between spin waves.

The series (2) may be rewritten as a power series of the spin-wave interaction. In the Dyson-Maleev (DM) formalism, the Hamiltonian of the NN Heisenberg model, after introducing α and β bosons by the standard procedure, takes the form[13–17] $H_{\mathrm{DM}}=H_0+V_{\mathrm{DM}}$, where H_0 describes noninteracting gas and the interaction V_{DM} is a normal-ordered quartic term. Then, introducing a formal parameter λ in H_{DM}, $H_{\mathrm{DM}}=H_0+\lambda V_{\mathrm{DM}}$, and accounting for the Hartree-Fock renormalization of the spin-wave energy in the formulas of third-order SWT, we write, in the case of $S=\frac{1}{2}$, the series (2) as

$$\mathcal{E}=-0.335\,211+0.000\,185\lambda^2+O(\lambda^3) \tag{3a}$$

and

$$m=0.303\,398+0.002\,583\lambda^2+O(\lambda^3) . \tag{3b}$$

From Eqs. (3) it is seen that the corrections, caused by the interaction, are small at $\lambda=1$. Therefore the α and β bosons, defined by standard SWT relations, seem to be well-behaved quasiparticles in a NN antiferromagnet, namely, quasiparticles with very weak interaction between them. In this case the precise estimates of the ground-state characteristics can be obtained in a systematic way, calculating the corrections, caused by the interaction.

In the frustrated antiferromagnet, the large $O(1/S)$ correction to m, calculated in Refs. 2, 8, and 9, signals for the existence of a strong interaction between bosons in the standard SWT scheme. A strong interaction between bosons in this scheme can be established even without calculating corrections. Indeed, it is easy to show that the interaction term in standard SWT of the frustrated model (1) involves a quadratic part

$$\tilde{H}_2=\sum_k Q_k(\alpha_k\beta_k+\alpha_k^\dagger\beta_k^\dagger) , \tag{4}$$

which is comparable with the zero-order Hamiltonian at $S\sim 1$ and $\alpha\sim 1$. It can be proven (see Sec. III) that it is precisely $\tilde{H}_2$ that causes the large $O(1/S)$ correction to the magnetization in the standard SWT scheme. Then it is natural to ask if this strong interaction $\tilde{H}_2$ can be excluded by introducing new, better-behaved quasiparticles. A positive answer to this question is given in this work for the Néel and collinear phases of the J_1-J_2 model.

In the case of a Néel or stripe-ordered ground state, using the DM formalism and performing a canonical transformation to exclude the quadratic part of the interaction between bosons, we convert the Hamiltonian (1) to the Hamiltonian $H_{\mathrm{DM}}=H_0+V_{\mathrm{DM}}$, H_0 being a noninteracting gas of quasiparticles and V_{DM} being a quartic normal-ordered term. We show that the description, based on the zero-order Hamiltonian H_0, is equivalent to the well-known[2,3] MSWT description of ordered phases of the J_1-J_2 model. We perform perturbation-type calculations up to second order of V_{DM} for the ground-state energy $\mathcal{E}$ and magnetization m and show that the proposed theory is self-consistent and presents an efficient perturbation scheme for evaluating the characteristics of Néel and collinear phases of model (1).

The paper is organized as follows. In Sec. II we introduce the basic formalism and derive the zero-order results. In Sec. III we compute corrections to the ground-state energy and magnetization. Section IV contains a short discussion.

II. FORMALISM AND ZERO-ORDER APPROXIMATION

For brevity, we will present below the equations in the case of Néel ordering. The formulas for the collinear phase can be derived in a similar way.

A. Heisenberg Hamiltonian in the DM boson representation

To deal with the Hamiltonian (1), we use the DM formalism, which is the most tractable in terms of the number of well-behaved interaction vertices.[13,14] For small α we assume that the Néel-ordered square lattice of spins is divided into A and B sublattices. Having introduced bosons through the DM relations, we perform a Bogoliubov transformation and obtain H_{DM} as a sum of a diagonal quadratic term, a normal-ordered quartic term, and a nondiagonal $\tilde{H}_2$-like term [see Eq. (4)]. Following the line discussed in Sec. I, we require Q_k to be zero. This brings us to the equation[23] for parameters of Bogoliubov transformation u_k and v_k:

$$\begin{aligned}Q_k=&4S\{\gamma_k(u_k^2+v_k^2)-2u_kv_k[1-\alpha(1-\eta_k)]\}\\&+4(R_1-R_2)[\gamma_k(u_k^2+v_k^2)-2u_kv_k]\\&-8u_kv_k\alpha(R_2-R_3)(1-\eta_k)\\=&0 .\end{aligned} \tag{5}$$

The quantities R_i are defined as

$$\begin{gathered}R_1=\frac{2}{N}\sum_k\gamma_ku_kv_k,\quad R_2=\frac{2}{N}\sum_k v_k^2,\quad R_3=\frac{2}{N}\sum_k\eta_kv_k^2 ,\\ \gamma_k=\tfrac{1}{2}(\cos k_x+\cos k_y),\quad \eta_k=\cos k_x\cos k_y .\end{gathered} \tag{6}$$

The second equation for u_k and v_k has a standard form:

$$u_k^2 - v_k^2 = 1 . \tag{7}$$

The Bogoliubov transformation, determined by Eqs. (5) and (7), can be performed only if a solution of Eqs. (5) and (7) exists. In the case considered here, the analysis of this problem turns out to be very simple. Equations (5) and (7), after some algebra, can be rewritten as an equation for one parameter $\tilde{\alpha}$:

$$\tilde{\alpha} = \frac{S + R_3 - R_2}{S + R_1 - R_2} ,$$

$$u_k = [(1+\varepsilon_k)/2\varepsilon_k]^{1/2}, \quad v_k = [(1-\varepsilon_k)/2\varepsilon_k]^{1/2} ,$$

$$\varepsilon_k = (1 - \gamma_k^2 / f_k^2)^{1/2}, \quad f_k = 1 - \tilde{\alpha}\alpha(1-\eta_k) . \tag{8}$$

Equation (8) has been earlier obtained in Ref. 2, where MSWT of the Néel phase of model (1) has been developed. It has been analyzed numerically, and its solution $\tilde{\alpha}(\alpha)$ has been tabulated there. It is worth emphasizing that this equation has been derived in Ref. 2 as a self-consistent equation on the basis of the well-known Takashi assumptions,[21] which include a mean-field-type decoupling of quartic terms and a variational procedure for the minimization of the free energy at an additional constraint $\langle S_i^z \rangle = 0$.

Having the solution of Eq. (8), we write the Hamiltonian $H_{\rm DM}$ of the Néel phase in the J_1-J_2 model as

$$H_{\rm DM} = W_0 + H_0 + V_{\rm DM} . \tag{9}$$

The constant term is

$$W_0 = 2N\mathcal{E}_0 = 2N[-(S+R_1-R_2)^2 + \alpha(S+R_2-R_3)^2] . \tag{10}$$

The quadratic part of $H_{\rm DM}$ has a diagonal form

$$H_0 = \sum_k E_k(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) , \tag{11}$$

where the spin-wave energy can be written as

$$E_k = 4(S + R_1 - R_2) f_k \varepsilon_k . \tag{12}$$

The normal-ordered quartic operator in (9) is given by the expression

$$V_{\rm DM} = -\frac{2}{N} \sum_{(1234)} \Delta(1+2-3-4)[\Phi^{(1)}\alpha_1\alpha_2\beta_3\beta_4 + \Phi^{(2)}\alpha_3^\dagger\alpha_4^\dagger\beta_1^\dagger\beta_2^\dagger - 2\Phi^{(3)}\alpha_3^\dagger\beta_4\alpha_1\alpha_2 - 2\Phi^{(4)}\alpha_4^\dagger\beta_1^\dagger\beta_2^\dagger\beta_3$$
$$- 2\Phi^{(5)}\beta_2^\dagger\beta_3\beta_4\alpha_1 - 2\Phi^{(6)}\alpha_3^\dagger\alpha_4^\dagger\beta_1^\dagger\alpha_2 + \Phi^{(7)}\beta_1^\dagger\beta_2^\dagger\beta_3\beta_4$$
$$+ \Phi^{(8)}\alpha_3^\dagger\alpha_4^\dagger\alpha_1\alpha_2 + \Phi^{(9)}\alpha_4^\dagger\alpha_2\beta_1^\dagger\beta_3] . \tag{13}$$

The explicit expressions for the vertex functions $\Phi^{(i)}(1234)$ of the Néel phase are given in Appendix A.

The Hamiltonian (9) will be treated by employing perturbation theory, the interaction part $V_{\rm DM}$ being the perturbation.

B. Zero-order approximation

The quadratic part of $H_{\rm DM}$, H_0 from Eq. (11), describes a gas of noninteracting spin waves of two different species having the same dispersion (12). The magnetization m_0 of such a noninteracting gas can be expressed as

$$m_0 = S - R_2 . \tag{14}$$

From Eqs. (10), (12), and (14), it follows that the ground-state energy $\mathcal{E}_0$, spin-wave energy E_k, and magnetization m_0 are determined in the same way, as in MSWT.[2,3] Thus the MSWT of the Néel phase in model (1) turns out to be a zero-order theory of the Hamiltonian (9).

The MSWT results are presented in the literature,[2,3] and we shall briefly mention only the main features of the relations (10) and (14) (see also Tables I and II). The ground-state energy $\mathcal{E}_0$ is an increasing function of α, $\mathcal{E}_0 \simeq -0.3352$ at $\alpha=0$ and $\mathcal{E}_0 = -0.2346$ at $\alpha=0.60$. The magnetization m_0 vanishes when α has reached 0.62 instead of the classical point $\alpha=0.5$. Thus, according to MSWT, the Néel ordering of the ground state of the J_1-J_2 model is stabilized by quantum fluctuations.

In the following section, we try to answer how the interaction between spin waves changes these zero-order results.

III. FIRST- AND SECOND-ORDER CORRECTIONS TO $\mathcal{E}$ and m

A. First-order corrections

It is easy to show that the first-order corrections to $\mathcal{E}$ and m, caused by the interaction (13), vanish. The normal ordering of the quartic terms in (13) leads to the result $\Delta E_0^{(1)} = 0$, because $\langle 0 | V_{\rm DM} | 0 \rangle = 0$, $|0\rangle$ being the ground state of the unperturbed Hamiltonian H_0. We may prove that $m^{(1)} \equiv 0$ in the following way. The perturbed ground-state function $|\psi\rangle$ in the lowest order of the interaction $V_{\rm DM}$ has the form

$$|\psi\rangle = |0\rangle + |\psi_1\rangle + O(V_{\rm DM}^2) ,$$

where $|\psi_1\rangle$, as can be easily seen from the structure of $V_{\rm DM}$ in (13), includes only four-particle states $\alpha_1^\dagger\alpha_2^\dagger\beta_3^\dagger\beta_4^\dagger|0\rangle$ ($V_{\rm DM}$ does not contain a nondiagonal quadratic term). Therefore the operator of the sublattice magnetization, namely,

$$\hat{m}=S-\frac{2}{N}\sum_k v_k^2-\frac{1}{N}\sum_k (u_k^2+v_k^2)(\alpha_k^\dagger\alpha_k+\beta_k^\dagger\beta_k)+\frac{2}{N}\sum_k u_kv_k(\alpha_k\beta_k+\alpha_k^\dagger\beta_k^\dagger)\ , \tag{15}$$

does not connect the states $|0\rangle$ and $|\psi_1\rangle$, and consequently, $\langle 0|\hat{m}|\psi_1\rangle=0$ and $m^{(1)}\equiv 0$. This simple analysis proves also that the large $O(1/S)$ correction to m, evaluated by the Holstein-Primakoff transformation and SWT for model (1) in Refs. 2, 8, and 9 is caused only by a nondiagonal quadratic term in the Hamiltonian.

B. Second-order corrections

We shall perform the calculation of second-order corrections to the ground-state energy and magnetization of the Néel phase of the J_1-J_2 model in a way similar to that used for the evaluation of the $O(1/S)$ correction to $\mathcal{E}$ and also for the $O(1/S^2)$ correction to m in SWT of the NN antiferromagnet.[14–17]

We begin with the calculation of the second-order correction to the ground-state energy. It is well known[22] that the expression for the second-order correction to E_0 in the case of the Hermitian operator of the interaction

$$\Delta E_0=-\sum_{(\rho)}\frac{\langle 0|V|\rho\rangle\langle\rho|V|0\rangle}{E_\rho} \tag{16}$$

may be applied as well to the case of the non-Hermitian interaction operator considered here, namely, $V_{\rm DM}$ from (13). In (16), $|0\rangle$ and $|\rho\rangle$ are the ground and excited states of H_0, respectively ($E_0^{(0)}=0$). Further analysis repeats the analysis performed in Ref. 17 for an unfrustrated model, and we shall only give the final result for ΔE_0:

$$\frac{\Delta E_0}{2N}=-(2/N)^3\sum_{(1234)}\Delta(1+2-3-4)\times\frac{\Phi^{(1)}(1234)\Phi^{(2)}(3412)}{E_1+E_2+E_3+E_4}\ . \tag{17}$$

The explicit expressions for $\Phi^{(i)}$ are given in Appendix A [Eqs. (A1), (A2), and (A7)]. The spin-wave energy E_k is obtained in Eq. (12).

The second-order correction $m^{(2)}\equiv\Delta m$ to the magnetization can be defined as

$$\Delta m=-\frac{1}{N}\left[\frac{\partial\Delta E_0}{\partial h}\right]_{h\to 0}\ , \tag{18}$$

where ΔE_0 is the second-order correction to the ground-state energy of the antiferromagnet (1) in the presence of a staggered magnetic field h. In terms of α and β bosons, the corresponding Hamiltonian has the form

$$H_{\rm DM}(h)=H_{\rm DM}-h\hat{M}\ , \tag{19}$$

where $H_{\rm DM}$ is given by Eq. (9) and $\hat{M}=N\hat{m}$; $\hat{m}$ is defined in Eq. (15). After some manipulations (the details are presented in Appendix B), we obtain the following expression for Δm:

$$\Delta m=\Delta m^{(\rm I)}+\Delta m^{(\rm II)}\ , \tag{20a}$$

where

$$\Delta m^{(\rm I)}=-\frac{16}{N^3}\sum_{(1234)}\Delta(1+2-3-4)\frac{\Phi^{(1)}(1234)\Phi^{(2)}(3412)}{(E_1+E_2+E_3+E_4)^2}\left[\frac{1}{\varepsilon_1}+\frac{1}{\varepsilon_2}+\frac{1}{\varepsilon_3}+\frac{1}{\varepsilon_4}\right] \tag{20b}$$

and

$$\Delta m^{(\rm II)}=-\frac{64}{N^3}(S+R_1-R_2)\sum_{(1234)}\Delta(1+2-3-4)\frac{F(1234)}{E_1+E_2+E_3+E_4}\ . \tag{20c}$$

The function $F(1234)$ is defined as

$$F(1234)=\Phi^{(1)}(1234)\left[\frac{\gamma(1)}{E_1^2}\Phi^{(4)}(3412)+\frac{\gamma(4)}{E_4^2}\Phi^{(6)}(3412)\right]+\left[\frac{\gamma(2)}{E_2^2}\Phi^{(5)}(1234)+\frac{\gamma(3)}{E_3^2}\Phi^{(3)}(1234)\right]\Phi^{(2)}(3412)\ . \tag{20d}$$

The vertex functions $\Phi^{(i)}$ are determined by Eqs. (A1)–(A7) in Appendix A. Equations (20) are consistent with the formula for the $O(1/S^2)$ correction to the magnetization of the unfrustrated model, obtained earlier by Castilla and Chakravarty[14] and by Hamer, Zheng, and Arndt.[16]

The investigation of the long-wavelength singularities of the integrands in (17) and (20) can be most easily studied by using the parametrization of the DM vertices, proposed in Ref. 13. By using this parametrization, one can prove that $|\Delta E_0|<\infty$ and $|\Delta m|<\infty$; i.e., the calculation of ΔE_0 and Δm in the DM formalism does not lead to a divergence.

We calculated numerically the six-dimensional integrals in Eqs. (17) and (20) in a wide range of parameter α by the method used in our paper[17] for the calculation of the $O(1/S)$ correction to the ground-state energy of the Heisenberg model. The results for $\Delta\mathcal{E}$ ($=\Delta E_0/2N$) and Δm are presented in Tables I and II, respectively.

Having obtained the corrections $\Delta\mathcal{E}$ and Δm, we can

TABLE I. Ground-state energy of the Néel phase ($\alpha \leq 0.53$) and collinear phase ($\alpha \geq 0.57$): zero-order result $\mathscr{E}_0$, correction $\Delta\mathscr{E}$, and corrected value $\mathscr{E}=\mathscr{E}_0+\Delta\mathscr{E}$, $S=\frac{1}{2}$.

α	$\mathscr{E}_0$	$\Delta\mathscr{E}$	$\mathscr{E}$
0.00	−0.335 21	0.000 18	−0.335 03
0.10	−0.315 43	0.000 38	−0.315 06
0.20	−0.296 52	0.000 61	−0.295 91
0.30	−0.278 70	0.000 85	−0.277 85
0.40	−0.262 24	0.000 87	−0.261 36
0.45	−0.254 62	0.000 64	−0.253 98
0.50	−0.247 46	0.000 05	−0.247 40
0.51	−0.246 08	−0.000 12	−0.246 21
0.52	−0.244 73	−0.000 33	−0.245 06
0.53	−0.243 40	−0.000 56	−0.243 96
0.57	−0.231 90	−0.003 54	−0.235 44
0.60	−0.236 04	−0.001 21	−0.237 25
0.70	−0.258 21	−0.000 09	−0.258 31
0.80	−0.285 84	−0.000 00	−0.285 84
0.90	−0.315 72	−0.000 04	−0.315 76
1.00	−0.346 78	−0.000 10	−0.346 88

write the following expressions for the ground-state energy and magnetization of the Néel phase of the J_1-J_2 model:

$$\begin{aligned} \mathscr{E} &= \mathscr{E}_0+\Delta\mathscr{E}+O(V_{\mathrm{DM}}^3)\,, \\ m &= m_0+\Delta m+O(V_{\mathrm{DM}}^3)\,, \end{aligned} \tag{21}$$

where $\mathscr{E}_0$ and m_0 are, respectively, the ground-state energy (10) and magnetization (14) of the noninteracting gas, described by the Hamiltonian H_0. For $\alpha=0$, Eqs. (21) coincide with Eqs. (3).

In a similar way, we investigated the collinear phase of the spin-$\frac{1}{2}$ J_1-J_2 model as well. The results for $\Delta\mathscr{E}$ and Δm are presented in Tables I and III.

TABLE II. Zero-order magnetization m_0, correction Δm, and corrected magnetization $m=m_0+\Delta m$ of the Néel phase for various α.

α	m_0	Δm	m
0.00	0.3034	0.0026	0.3060
0.10	0.2782	0.0044	0.2826
0.20	0.2465	0.0064	0.2529
0.30	0.2061	0.0070(1)	0.2131(1)
0.40	0.1544	−0.0011(2)	0.1533(2)
0.44	0.1301	−0.0120(1)	0.1181(1)
0.45	0.1237	−0.0160(1)	0.1077(1)
0.46	0.1171	−0.0207	0.0964
0.47	0.1104	−0.0261	0.0843
0.48	0.1036	−0.0324	0.0712
0.49	0.0966	−0.0398(1)	0.0568(1)
0.50	0.0895	−0.0482(2)	0.0413(2)
0.51	0.0823	−0.0579(3)	0.0244(3)
0.52	0.0750	−0.0691(4)	0.0059(4)
0.53	0.0675	−0.0818(5)	−0.0143(5)

TABLE III. Zero-order magnetization m_0, correction Δm, and corrected magnetization $m=m_0+\Delta m$ of the collinear phase for various α.

α	m_0	Δm	m
0.565	0.1074	−0.1373(33)	−0.0299(33)
0.57	0.1298	−0.1003(20)	0.0295(20)
0.58	0.1639	−0.0589(9)	0.1050(9)
0.59	0.1894	−0.0374(4)	0.1520(4)
0.60	0.2095	−0.0250(2)	0.1845(2)
0.61	0.2259	−0.0174(1)	0.2084(1)
0.62	0.2393	−0.0126(1)	0.2268(1)
0.63	0.2507	−0.0093	0.2414
0.70	0.2963	−0.0020	0.2942
0.80	0.3206	−0.0011	0.3195
0.90	0.3298	−0.0015	0.3283
1.00	0.3334	−0.0021	0.3313
2.00	0.3273	−0.0051(1)	0.3222(1)
50.00	0.3045	0.0025	0.3070
∞	0.3034	0.0026	0.3060

IV. DISCUSSION

We see from the tables that the corrections $\Delta\mathscr{E}$ and Δm are small in a wide range of parameter space. This provides some evidence that the quasiparticles, introduced in the proposed scheme, are well-behaved quasiparticles.

The correction Δm for the Néel state (see Table II) is positive at small α. At $\alpha \simeq 0.38$, Δm changes its sign and continues to decrease with increasing α, but it remains relatively small up to $\alpha \simeq 0.48$. The corrected value of the magnetization goes to zero at $\alpha \simeq 0.52$, which is substantially smaller than the MSWT result[2,3] $\alpha \simeq 0.62$. The magnetization $m=m_0+\Delta m$ of the collinear phase (see Table III) vanishes at $\alpha \simeq 0.57$, which is higher than the MSWT result[2,3] $\alpha \simeq 0.55$. A significant melting effect ($|\Delta m| \sim m_0 \sim 0.1$) produced by the interaction between the spin waves in the collinear phase is clearly seen near $\alpha \simeq 0.57$.

Thus we conclude that mean-field-type theories overestimate the stability of the ordered phases in the spin-$\frac{1}{2}$ J_1-J_2 model. The same conclusion has been drawn recently by Ferrer.[24] He analyzed some features of the Schwinger-boson mean-field theory and supposed that there is a spin-liquid phase in a very small region near $\alpha \simeq 0.6$ for the $S=\frac{1}{2}$ J_1-J_2 model.

Within the second-order approximation, we have shown the existence of a window $0.52<\alpha<0.57$ instead of MSWT overlap between the Néel and collinear phases of the spin-$\frac{1}{2}$ J_1-J_2 model. In principle, more precise estimates of the phase boundaries can be obtained by the evaluation of higher-order corrections. Other methods should be employed to clarify the order of the phase transitions.

To conclude, we have found that near the boundaries of the Néel and collinear phases the spin waves interact in a complicated way, melt the ordering, and create the possibility of the appearance of a new ground state in the window between these phases. On the basis of exact-diagonalization data, some evidence of the existence of a nonclassical state in the spin-$\frac{1}{2}$ J_1-J_2 model at $\alpha \simeq 0.5$ has been presented earlier in Refs. 6, 10, and 25. Finite-size scaling analysis, performed by Schultz and Ziman,[7] leads to an intermediate phase between $\alpha \simeq 0.4$ and $\alpha \simeq 0.65$. This interval is much wider than the one obtained here. The nature of the nonclassical states in the J_1-J_2 model is actually still controversial.[1–10,24–28]

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APPENDIX A: DYSON-MALEEV VERTICES (NÉEL PHASE)

When we write the bare operators a_k and b_k in terms of the new operators α_k and β_k, $H_{\rm DM}$ is transformed into a complicated form. After the normal ordering of each term is performed, we obtain the expressions (5), (6), and (9)–(13). The vertex functions $\Phi^{(i)}(1234)$, $i=1,2,\ldots,6$, used in the calculations in the present work, can be written in the form

$$\begin{aligned}\Phi^{(1)}(1234)=&\gamma(4-1)v_1u_2v_3u_4+\gamma(4-2)u_1v_2v_3u_4+\gamma(3-1)v_1u_2u_3v_4+\gamma(3-2)u_1v_2u_3v_4\\&-\gamma(4)u_1u_2v_3u_4-\gamma(3)u_1u_2u_3v_4-\gamma(4-1-2)v_1v_2v_3u_4-\gamma(3-1-2)v_1v_2u_3v_4\\&-\alpha Q(u_1u_2v_3v_4+v_1v_2u_3u_4)\ ,\end{aligned}\tag{A1}$$

$$\begin{aligned}\Phi^{(2)}(1234)=&\gamma(4-2)v_1u_2u_3v_4+\gamma(3-2)v_1u_2v_3u_4+\gamma(4-1)u_1v_2u_3v_4+\gamma(3-1)u_1v_2v_3u_4\\&-\gamma(3)v_1v_2v_3u_4-\gamma(4)v_1v_2u_3v_4-\gamma(4-2-1)u_1u_2u_3v_4-\gamma(3-2-1)u_1u_2v_3u_4\\&-\alpha Q(u_1u_2v_3v_4+v_1v_2u_3u_4)\ ,\end{aligned}\tag{A2}$$

$$\begin{aligned}\Phi^{(3)}(1234)=&\gamma(4-1)v_1u_2u_3u_4+\gamma(3-1)v_1u_2v_3v_4+\gamma(4-2)u_1v_2u_3u_4+\gamma(3-2)u_1v_2v_3v_4\\&-\gamma(4)u_1u_2u_3u_4-\gamma(3)u_1u_2v_3v_4-\gamma(4-1-2)v_1v_2u_3u_4-\gamma(3-1-2)v_1v_2v_3v_4\\&-\alpha Q(u_1u_2u_3v_4+v_1v_2v_3u_4)\ ,\end{aligned}\tag{A3}$$

$$\begin{aligned}\Phi^{(4)}(1234)=&\gamma(3-1)u_1v_2u_3u_4+\gamma(4-1)u_1v_2v_3v_4+\gamma(3-2)v_1u_2u_3u_4+\gamma(4-2)v_1u_2v_3v_4\\&-\gamma(3)v_1v_2u_3u_4-\gamma(4)v_1v_2v_3v_4-\gamma(4-1-2)u_1u_2v_3u_4-\gamma(3-1-2)u_1u_2u_3u_4\\&-\alpha Q(u_1u_2u_3v_4+v_1v_2v_3u_4)\ ,\end{aligned}\tag{A4}$$

$$\begin{aligned}\Phi^{(5)}(1234)=&\gamma(4-1)v_1v_2v_3u_4+\gamma(4-2)u_1u_2v_3u_4+\gamma(3-1)v_1v_2u_3v_4+\gamma(3-2)u_1u_2u_3v_4\\&-\gamma(4)u_1v_2v_3u_4-\gamma(3)u_1v_2u_3v_4-\gamma(4-1-2)v_1u_2v_3u_4-\gamma(3-1-2)v_1u_2u_3v_4\\&-\alpha Q(u_1v_2v_3v_4+v_1u_2u_3u_4)\ ,\end{aligned}\tag{A5}$$

$$\begin{aligned}\Phi^{(6)}(1234)=&\gamma(4-1)u_1u_2u_3v_4+\gamma(4-2)v_1v_2u_3v_4+\gamma(3-1)u_1u_2v_3u_4+\gamma(3-2)v_1v_2v_3u_4\\&-\gamma(4)v_1u_2u_3v_4-\gamma(3)v_1u_2v_3u_4-\gamma(4-1-2)u_1v_2u_3v_4-\gamma(3-1-2)u_1v_2v_3u_4\\&-\alpha Q(u_1v_2v_3v_4+v_1u_2u_3u_4)\ ,\end{aligned}\tag{A6}$$

where

$$Q=\eta(3-2)+\eta(4-2)-\eta(3)-\eta(4)\ .\tag{A7}$$

At $\alpha=0$, these expressions reduce to the expressions of DM vertices[15] for the NN Heisenberg model. The expressions (A1)–(A6) are presented in a form permitting the correct treatment of the umklapp processes.

APPENDIX B: DERIVATION OF THE FORMULAS (20)

In the staggered magnetic field h, the four-particle states $|\rho\rangle=\alpha_1^\dagger\alpha_2^\dagger\beta_3^\dagger\beta_4^\dagger|0\rangle$, contributing to the second-order correction ΔE_0 [Eq. (16)], change their functions and energies. According to the usual perturbation theory, in the case of the perturbation $\hat{m}$ [Eq. (15)], we can write the new states and their energies as

$$\begin{aligned}&|\tilde\rho\rangle=|\rho\rangle+h\sum_{(2)}c_2|2\rangle+h\sum_{(6)}c_6|6\rangle+O(h^2)\ ,\\&|\tilde 0\rangle=|0\rangle+h\sum_{(2)}d_2|2\rangle+O(h^2)\ ,\\&\tilde E_k-\tilde E_0=E_k+hE_k^{(1)}+O(h^2)\ .\end{aligned}\tag{B1}$$

Here $|2\rangle\equiv\alpha_q^\dagger\beta_q^\dagger|0\rangle$ is a two-particle excited state of H_0, $|6\rangle$ is a six-particle state; c_2, d_2, and c_6 may be calculated by formulas like (B4). The correction to E_k is

$$E_k^{(1)} = u_k^2 + v_k^2 = \frac{1}{\varepsilon_k} . \tag{B2}$$

Using (B1) and Eq. (9) for the perturbed matrix elements $\langle \tilde{0} | V_{\text{DM}} | \tilde{\rho} \rangle$ and $\langle \tilde{\rho} | V_{\text{DM}} | \tilde{0} \rangle$, one can write

$$\begin{aligned} \langle \tilde{0} | V_{\text{DM}} | \tilde{\rho} \rangle &= \langle 0 | V_{\text{DM}} | \rho \rangle \\ &\quad + h \sum_{(2)} d_2 \langle 2 | V_{\text{DM}} | \rho \rangle + O(h^2) , \\ \langle \tilde{\rho} | V_{\text{DM}} | \tilde{0} \rangle &= \langle \rho | V_{\text{DM}} | 0 \rangle \\ &\quad + h \sum_{(2)} d_2 \langle \rho | V_{\text{DM}} | 2 \rangle + O(h^2) . \end{aligned} \tag{B3}$$

The coefficient d_2 is easily calculated as

$$d_2 = \frac{\langle 2 | \hat{M} | 0 \rangle}{E_0 - E_2} = \frac{2 u_q v_q}{2 E_q} = \frac{2 \gamma_q}{E_q^2} (S + R_1 - R_2) . \tag{B4}$$

After that, taking the corresponding DM vertices and carrying out the summation in (B3), we obtain from Eqs. (16), (18), and (B2)–(B4) formulas (20) for Δm.

[1] P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).

[2] J. H. Xu and C. S. Ting, Phys. Rev. B **42**, 6861 (1990).

[3] H. Nishimori and Y. Saika, J. Phys. Soc. Jpn. **59**, 4454 (1990); A. F. Barabanov and O. A. Stary'h, Pis'ma Zh. Eksp. Teor. Fiz. **51**, 271 (1990) [JETP Lett. **51**, 311 (1990)]; T. Oguchi and H. Kitatani, J. Phys. Soc. Jpn. **59**, 3322 (1990).

[4] J. E. Hirsh and S. Tang, Phys. Rev. B **39**, 2887 (1989).

[5] F. Mila, D. Poilblanc, and C. Bruder, Phys. Rev. B **43**, 7891 (1991).

[6] E. Dagotto and A. Moreo, Phys. Rev. Lett. **63**, 2148 (1989).

[7] H. J. Schulz and T. A. L. Ziman, Europhys. Lett. **18**, 355 (1992).

[8] Q. F. Zhong and S. Sorella, Europhys. Lett. **21**, 629 (1993).

[9] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989).

[10] A. Moreo, E. Dagotto, Th. Jolicoeur, and J. Riera, Phys. Rev. B **42**, 6283 (1990); E. Dagotto, Int. J. Mod. Phys. B **5**, 77 (1991).

[11] N. B. Ivanov and J. Richter (unpublished).

[12] M. Inui, S. Doniach, and M. Gabay, Phys. Rev. B **38**, 6631 (1988); J. Annett, R. Martin, A. McMahan, and S. Satpathy, *ibid.* **40**, 2640 (1989).

[13] P. Kopietz, Phys. Rev. B **41**, 9228 (1990).

[14] G. E. Castilla and S. Chakravarty, Phys. Rev. B **43**, 13 687 (1991).

[15] C. M. Canali, and S. M. Girvin, Phys. Rev. B **45**, 7127 (1992); C. M. Canali, S. M. Girvin, and M. Wallin, *ibid.* **45**, 10 131 (1992).

[16] C. J. Hamer, Zheng Weihong, and P. Arndt, Phys. Rev. B **46**, 6276 (1992).

[17] I. G. Gochev, Phys. Rev. B **47**, 1096 (1993).

[18] Zheng Weihong and C. J. Hamer, Phys. Rev. B **47**, 7961 (1993).

[19] J. Igarashi and A. Watabel, Phys. Rev. B **43**, 13 456 (1991).

[20] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

[21] M. Takahasi, Phys. Rev. Lett. **58**, 168 (1987); Phys. Rev. B **40**, 2494 (1989).

[22] D. Mattis, *The Theory of Magnetism* (Harper and Row, New York, 1982).

[23] In standard SWT the corresponding equation for u_k and v_k has another form and Bogoliubov transformation in this case diagonalizes the quadratic in bare operators a_k, b_k part of the Hamiltonian.

[24] J. Ferrer, Phys. Rev. B **47**, 8769 (1993).

[25] H. A. Ceccatto, C. J. Gazza, and A. E. Trumper, Phys. Rev. B **45**, 7832 (1992).

[26] P. Chandra, P. Coleman, and A. I. Larkin, J. Phys. Condens. Matter **2**, 7933 (1990).

[27] S. Sachdev and N. Read, Phys. Rev. Lett. **66**, 1773 (1991).

[28] L. B. Ioffe and A. I. Larkin, Int. J. Mod. Phys. B **2**, 203 (1988).