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ORDER, DISORDER, AND PHASE TRANSITIONS IN CONDENSED SYSTEMS

A Quantum Spin Liquid in a Two-Layer Triangular Antiferromagnet

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Abstract—The possibility of implementing a quantum-spin-liquid-type state in a two-layer triangular spin-1/2 antiferromagnet at $T = 0$ is investigated. The ratio of intra- to interlayer exchange constants (j) is found under which a transition from the classical state with 120° triangular order to a quantum state with zero magnetization per site occurs; in this case, the spins of adjacent layers form singlets that are separated from triplet excitations by an energy gap. Compared with an analogous system with the square lattice, the range of j in which the classical ordered state is realized turns out to be an order of magnitude smaller due to the effects of frustration; in this case, the behavior of thermodynamic quantities is analogous, on the whole, to that in two-layer square lattices; a difference manifests itself in the behavior of the gap in the spectrum of quasiparticles in an external magnetic field h. For small fields h, a j–h phase diagram is constructed that determines the domains in which the 120° and the singlet phases exist. It is established that, in the neighborhood of the second-order phase transition, the contribution, to the thermodynamic quantities, of longitudinal spin fluctuations, which are disregarded in the spin-wave description, is comparable to the contribution of transverse fluctuations. © *2005 Pleiades Publishing, Inc.*

1. INTRODUCTION

It is well known that the formation of a spin gap between a lower singlet state and excited magnetic levels in magnets leads to the situation when there is now magnetic ordering in these magnets at low temperatures. Moreover, the phenomenon of high-temperature superconductivity is likely to have a spin-gap nature. Therefore, a large number of model objects and real compounds possessing the above properties have recently been studied [1–19]. Quantum phenomena most clearly manifest themselves in low-dimensional systems, systems with small coordination number, low-spin systems, and frustrated systems [20–26]. Frustrations, in particular, create or enhance the degeneracy of the ground state [27], thus giving rise to new types of ordering as a result of competition between quantum phenomena and weak perturbations of different nature; on the other hand, they lead to the effective damping of coupling, thus significantly changing the domain where a quantum-disordered phase can be realized.

In the present paper, we consider conditions under which singlet and magnetic phases arise, as well as the thermodynamic properties of a system consisting of two layers of a triangular ferromagnet. Theoretical interest in bilayer systems has been stimulated in part by experimental factors. Experiments show that certain high-temperature semiconductors contain pairs of CuO_2 layers separated from other layers by nonmagnetic interlayers [28, 29]. Layers with a triangular lattice formed by ferromagnetic He^3 have also been deposited in experiments [30].

Investigations in two-dimensional triangular Heisenberg antiferromagnets have shown [31–34] that, at $T = 0$, long-range ordering exists even in spin-1/2 systems; in this case, the magnetization per site is half the classical magnetization and has virtually the same value as that in square lattices [35, 36]. At the same time, it is well known that, under certain relations between intra- and interlayer exchange constants, the interaction between layers in two-layer square antiferromagnets may lead to the transition to a singlet state with complete quantum reduction of the spin [37–39].

The possibility of quantum behavior in bilayer antiferromagnets is clear from the following considerations. In a bilayer system consisting of Heisenberg 1/2 spins with the intralayer exchange constant J_1 and the interlayer constant J_2, in the limiting case of $J_1 = 0$, we have a system of noninteracting dimers in which one of the following four states is realized at each site: a singlet or one of three triplet states, whose energies differ from the ground-state energy by the value of the exchange constant J_2. Obviously, the inclusion of the weak intralayer exchange J_1 does not substantially change the situation: the width of the gap is not equal to J_2 as in the case of noninteracting dimers but is on the

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order of J_2 (a confirmation of this fact is given in the text; see formula (14) below). Therefore, for a weak interlayer exchange ($J_2 \ll J_1$), the gap is small, the triplet states at every site are populated, and the mean magnetization is different from zero and, in a bilayer triangular antiferromagnet, should correspond to the classical 120° ordering. In the limit of large J_2 ($J_2 \gg J_1$), the triplet magnetic levels are separated from the ground state by a too large gap, and the system should live in a singlet state with zero magnetization per site.

The Hamiltonian of the model ($J_1, J_2 \geq 0$) is given by

$$\begin{aligned} H &= J_1 \sum_{\langle i,j\rangle} \mathbf{S}_{1i}\mathbf{S}_{1j} + J_1 \sum_{\langle i,j\rangle} \mathbf{S}_{2i}\mathbf{S}_{2j} \\ &+ J_2 \sum_i \mathbf{S}_{1i}\mathbf{S}_{2i} + J_2 \sum_i \mathbf{S}_{2i}\mathbf{S}_{1i}, \end{aligned} \tag{1}$$

where $\langle i, j\rangle$ is a pair of nearest neighbors in each layer and 1 and 2 are the layer numbers. The apparent redundancy in the last terms is due to the fact that, under a systematic enumeration in $\sum_{\langle i,j\rangle}$, each interacting pair of spins is counted twice, while, in $\sum_i$, it is counted once. A pair of nearest-neighbor spins of adjacent layers is called a dimer.

2. SPIN-WAVE CALCULATIONS

We carried out standard spin-wave calculations in the ordered triangular phase with the use of the Holstein–Primakov transformation from spin operators to the operators of creation and annihilation of magnon deviations from the 120° triangular order. We established that the excitation spectrum consists of two branches each of which contains a Goldstone boson: the first branch contains this boson at a wavevector of $\mathbf{k} = (0, 0)$, which corresponds to fermionic ordering, and the second, at $\mathbf{k} = \mathbf{q} = (4\pi/3, 0)$, which corresponds to the 120° triangular order:

$$\begin{aligned} E_{k1}^{\mathrm{HP}} &= 3J_1 S\sqrt{(1-\nu_k)(1+2\nu_k+2j)}, \\ E_{k2}^{\mathrm{HP}} &= 3J_1 S\sqrt{(1+2\nu_k)(1-\nu_k+2j)} > E_{k1}^{\mathrm{HP}}, \end{aligned} \tag{2}$$

$$\nu_k \equiv \frac{1}{3}\left(\cos k_x + 2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}}{2}k_y\right), \quad j \equiv \frac{J_2}{3J_1}. \tag{3}$$

In the first order in $1/S$, we obtained the magnetization per site and the velocity of spin waves in the neighborhood of a symmetry wavevector $\mathbf{k} = \mathbf{q}$ (here, N is the number of dimers).

$$\begin{aligned} N_0 &= S + \frac{1}{2} - \frac{S}{2N}\sum_{\alpha,k} \frac{3J_1 + J_2 + 3J_1\nu_k/2}{2E_{k\alpha}^{\mathrm{HP}}}, \\ c &= \frac{3\sqrt{3}}{2\sqrt{2}} J_1 S\sqrt{1+\frac{4}{9}\frac{J_2}{J_1}}. \end{aligned} \tag{4}$$

3. BOND-OPERATOR REPRESENTATION

In another limiting case, a spin-wave description is inapplicable to a singlet phase with zero magnetization per site; therefore, we used the bond-operator representation, which was first introduced in [35] and was later applied to Heisenberg models with a competing interaction [2, 5, 36] and to two-layer antiferromagnets with a square lattice [38, 39]. We introduce a system of dimer states

$$\begin{aligned} |t_a\rangle &= \uparrow\uparrow = |1, 1\rangle, \\ |t_b\rangle &= -\downarrow\downarrow = |1, -1\rangle, \\ |t_c\rangle &= \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) = |1, 0\rangle, \\ |0\rangle &= \frac{-1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) = |0, 0\rangle \end{aligned} \tag{5}$$

and three bosons a, b, and c that describe a transition from the singlet state $|0\rangle$ to one of the three triplet states:

$$a^+|0\rangle = |t_a\rangle, \quad b^+|0\rangle = |t_b\rangle, \quad c^+|0\rangle = |t_c\rangle. \tag{6}$$

The creation and annihilation operators of the singlet state are defined as

$$s^+|0\rangle = |0\rangle, \quad s|0\rangle = |0\rangle. \tag{7}$$

The operators s^+ and s thus defined are equal to each other and to a constant:

$$s^+ = s \equiv u,$$

which indicates that the singlet state is a condensed state. The operator u defined by the normalization condition allows us to rule out the existence of several triplet excitations at a single site. At a given moment, one of the four states is realized at a site and the operator of the total number of particles at the site is 1:

$$s^+s + a^+a + b^+b + c^+c = 1.$$

Therefore,

$$\begin{aligned} s^+s = u^2 &= 1 - a^+a - b^+b - c^+c \Rightarrow u \\ &= \sqrt{1-(a^+a + b^+b + c^+c)}. \end{aligned} \tag{8}$$

In terms of the new operators, the components of the

ferro- and antiferromagnetism vectors

$$\mathbf{M} = \mathbf{S}_1 + \mathbf{S}_2, \quad \mathbf{L} = \mathbf{S}_1 - \mathbf{S}_2$$

of the dimer are expressed as

$$\begin{aligned} M^z &= a^+a - b^+b, \quad M^+ = \sqrt{2}(a^+c - c^+b), \\ M^- &= \sqrt{2}(c^+a - b^+c), \quad L^z = -(c^+u + uc), \\ L^+ &= \sqrt{2}(a^+u + ub), \quad L^- = \sqrt{2}(b^+u + ua). \end{aligned} \tag{9}$$

Following [38], we introduce a parameter λ in the root of the operator u,

$$u = \sqrt{1 - \lambda(a^+a + b^+b + c^+c)},$$

which allows us to expand u in the approximation of $\lambda \ll 1$. Then, similar to the $1/S$ expansion in the usual spin-wave theory, we set $\lambda = 1$ in the final results. In order that the spin commutation relations

$$\begin{aligned} [M^\alpha, M^\beta] = i\varepsilon_{\alpha\beta\gamma}M^\gamma, \quad [L^\alpha, L^\beta] = i\varepsilon_{\alpha\beta\gamma}M^\gamma, \\ [M^\alpha, L^\beta] = i\varepsilon_{\alpha\beta\gamma}L^\gamma \end{aligned} \tag{10}$$

remain unchanged, we introduce the factor $1/\sqrt{\lambda}$ into the three components of the vector $\mathbf{L}$:

$$\begin{aligned} L^z &= -(c^+u + uc)/\sqrt{\lambda}, \\ L^+ &= \sqrt{2}(a^+u + ub)/\sqrt{\lambda}, \\ L^- &= \sqrt{2}(b^+u + ua)/\sqrt{\lambda}. \end{aligned} \tag{11}$$

Substituting (9) and (11) into the initial Hamiltonian (1) and taking into account that the relation

$$\mathbf{S}_1\mathbf{S}_2 = -\frac{3}{4} + a^+a + b^+b + c^+c$$

holds for a dimer with $S = 1/2$, we obtain ($J^*_{ij} \equiv J_{ij}/\lambda$)

$$\begin{aligned} H = &-\frac{3}{2}J_2N + 2J_2\sum_i (a_i^+a_i + b_i^+b_i + c_i^+c_i) \\ &+ \sum_{ij}\Big\{ J_{ij}(c_i^+a_i - b_i^+c_i)(a_j^+c_j - c_j^+b_j) \\ &+ J^*_{ij}(b_i^+u_i + u_ia_i)(a_j^+u_j + u_jb_j) \\ &+ \frac{1}{2}J^*_{ij}(c_i^+u_i + u_ic_i)(c_j^+u_j + u_jc_j) \\ &+ \frac{1}{2}J_{ij}(a_i^+a_i - b_i^+b_i)(a_j^+a_j - b_j^+b_j)\Big\}, \end{aligned} \tag{12}$$

where the operators a, b, and c satisfy the boson permutation relations

$$\begin{aligned} [a_i, a_j^+] = \delta_{ij}, \quad [a_i^+, a_j^+] = 0, \\ [a_i, a_j] = 0, \quad [a_i, b_j] = 0, \text{ etc.} \end{aligned}$$

4. THE SPECTRUM OF A DISORDERED PHASE

In a disordered state, the bosons a, b, and c are equivalent and a quadratic form of Hamiltonian (12) is expressed as ($u \approx 1$)

$$\begin{aligned} H = &-\frac{9}{2}J_2N + \sum_k A_k(a_k^+a_k + b_k^+b_k + c_k^+c_k \\ &+ a_{-k}a_{-k}^+ + b_{-k}b_{-k}^+ + c_{-k}c_{-k}^+) \\ &+ \sum_k B_k(a_k^+b_{-k}^+ + b_k^+a_{-k}^+ + b_{-k}a_k \\ &+ a_{-k}b_k + c_k^+c_{-k}^+ + c_{-k}c_k), \\ A_k = 3J_1^*(j + \nu_k), \quad B_k = 3J_1^*\nu_k, \quad j \equiv &\frac{J_2}{3J_1^*}. \end{aligned} \tag{13}$$

The stability domain of the singlet phase can be determined by analyzing the excitation spectrum of quasiparticles. The excitation spectrum of a disordered state is determined without taking quantum corrections into account by the diagonalization of the quadratic form. In view of the equivalence of the bosons a, b, and c, the spectrum is triply degenerate and has a gap at the wavevector $\mathbf{q}$ of the 120° triangular order:

$$\begin{aligned} E_k &= \sqrt{A_k^2 - B_k^2} = J_2\sqrt{1 + \frac{1}{j}2\nu_k}, \\ \Delta_{abc} &= J_2\sqrt{1 - 1/j} = E_k(\mathbf{k} = \mathbf{q}). \end{aligned} \tag{14}$$

As explained in the Introduction, the gap in the spectrum of elementary excitations of a disordered phase (including the domain $J_2 \gg J_1$) is on the order of J_2 and is equal to the exact value of J_2 in the case of noninteracting dimers ($J_1 = 0$).

When $j > 1$, the spectrum is everywhere real; when $j < 1$, the spectrum becomes partially imaginary: the system should pass to a new state. At the point of the phase transition, $j = 1$, the gap in the spectrum vanishes; therefore, the energy of excitations associated with the formation of the 120° triangular order vanishes. A Goldstone boson $E_k(\mathbf{k} = \mathbf{q}) = 0$ arises that points to the symmetry reduction associated with the condensation of the new state—the 120° triangular order—for $j < 1$. Thus, in this approximation, the 120° triangular order is stable in the domain of $j < 1$, while the singlet phase is

stable for $j > 1$. The velocity of spin waves at the transition point is $c = (3/2)J_1^*$.

5. MODIFICATION OF OPERATORS IN THE 120° PHASE

In the ordered phase, the operators a, b, and c are modified so as to guarantee that the mean value of the spin at a site corresponds to the 120° triangular order. This can be done by separating the mean value of operators of kind c at the wavevector $\mathbf{k} = \mathbf{q}$. If we set

$$\langle c_q \rangle = \sqrt{N}\alpha \Leftrightarrow c_k\sqrt{N}\alpha\delta_{kq} + \varepsilon_k, \tag{15}$$

then, for the mean value of the spin at a site in the second layer, we obtain

$$\langle S_{2i}^z \rangle = \frac{\sqrt{\beta(1-\beta)}}{\lambda}\cos qR_i \equiv N_0^{\text{mid}}\cos qR_i,$$

where $\beta \equiv \lambda\alpha^2$. One can see that $\langle S_{2i}^z \rangle$ behaves as a projection of the modulus N_0^{mid} onto the z axis at an angle $\alpha_i = qR_i$, where α_i is changed by $4\pi/3 \cdot 1 = 240° \Leftrightarrow -120°$ (rotation of the spin) under the transition from a certain site to the neighboring one ($R_i = 1$). At each site, the spins of the first layer are opposite, as it must be, to the spins of the second. Thus,

$$N_0^{\text{mid}} \equiv \frac{\sqrt{\beta(1-\beta)}}{\lambda}$$

is the mean value of the spin at a site in the zero approximation, and representation (15) guarantees the 120° triangular order.

The equilibrium value of β is determined from the minimum of the ground-state energy. In the mean-field approximation, the energy of the ground state and β ($\partial E_0/\partial\beta = 0$) are given by

$$\begin{aligned} E_0 &= -\frac{3}{2}J_2 N + 2J_2 N\frac{\beta}{\lambda} - 6J_1^* N\frac{\beta}{\lambda}(1-\beta), \\ \beta_0 &= \frac{1}{2}(1-j). \end{aligned} \tag{16}$$

Thus, the mean value of the operators c ($\sim\alpha$) and the mean value of the spin at a site make sense for $j < 1$, i.e., in the ordered phase; at the point $j = 1$ of the phase transition in the mean-field approximation, all the means vanish.

6. THE EXCITATION SPECTRUM OF THE ORDERED PHASE

To determine the excitation spectrum in the ordered phase, one should find a quadratic form of Hamiltonian (12) with regard to relations (15).

The Hamiltonian of the ordered phase can be represented as

$$H = E_0 + H_\perp + H_\parallel,$$

where $H_\perp$ is a part that is quadratic with respect to the operators a and b and $H_\parallel$ is a part that is quadratic with respect to the operators ε. $H_\parallel$ yields the spectrum of longitudinal fluctuations of the spin (the operators c and ε determine the mean value of the spin at a site), and $H_\perp$ determines the spectrum of transverse oscillations.

6.1. The Spectrum of Transverse Oscillations

Let us explain how we determine the quadratic form by the operators a and b ($H_\perp$). To this end, in Hamiltonian (12), it suffices to use, as u, the expression

$$u = \langle u \rangle = \sqrt{1-\beta}$$

in the terms that explicitly contain a, b, and u, and the approximation

$$u = 1 - \frac{\lambda}{2}(a^+a + b^+b)$$

in the terms containing c and u; for c in $H_\perp$, we everywhere use the mean value

$$c = \langle c \rangle.$$

As a result, after the transition to the k space, $H_\perp$ takes the form

$$\begin{aligned} H_\perp &= \sum_k A_k^\perp(a_k^+a_k + b_k^+b_k + a_{-k}a_{-k}^+ + b_{-k}b_{-k}^+) \\ &+ B_k^\perp(a_k^+b_{-k}^+ + b_k^+a_{-k}^+ + a_kb_{-k} + b_ka_{-k}), \\ \frac{A_k^\perp}{3J_1^*} &\equiv a_\perp = j + \beta + \nu_k\left(1 - \frac{3}{2}\beta\right), \\ \frac{B_k^\perp}{3J_1^*} &\equiv b_\perp = \nu_k\left(1 - \frac{\beta}{2}\right). \end{aligned} \tag{17}$$

The spectrum of transverse modes is doubly degenerate, is gapless, and contains a Goldstone mode with $\mathbf{k} = \mathbf{q}$ (for any j):

$$\begin{aligned} E_k^\perp &= \sqrt{A_k^{\perp^2} - B_k^{\perp^2}} = J_2\left(1 + \frac{\beta}{j}\right) \\ &\times \sqrt{\left(1 - \frac{\beta}{j+\beta}\nu_k\right)\left(1 + \frac{1-\beta}{j+\beta}2\nu_k\right)}, \end{aligned} \tag{18}$$

$$E_k^\perp(\beta_0) = \frac{3}{2}J_1^*(1+j)\sqrt{(1+2\nu_k)\left(1 - \frac{1-j}{1+j}\nu_k\right)}, \tag{19}$$

where $E_k^{\perp}(\beta_0)$ is the mean-field approximation. The presence of a Goldstone boson in the spectrum of oscillations in the plane of the layer is obviously associated with symmetry breaking due to the 120° Néel ordering in the plane of the layer for $j < 1$. The velocity of spin waves near $\mathbf{k} = \mathbf{q}$ is equal to

$$c = \frac{3}{2}J_1^*\sqrt{(1-\beta_0)\left(1-\frac{\beta_0}{2}\right)}.$$

6.2. The Spectrum of Longitudinal Oscillations

The terms that are quadratic in ε and form the Hamiltonian $H_{\parallel}$ are contained in the following components of Hamiltonian (12):

$$H_{\parallel} = 2J_2\sum_i \varepsilon_i^+\varepsilon_i + \frac{1}{2\lambda}\sum_{ij} J_{ij}\{(c_i^+u_i + u_ic_i)(c_j^+u_j + u_jc_j) - (c_{i0}^+u_{i0} + u_{i0}c_{i0})(c_{j0}^+u_{j0} + u_{j0}c_{j0})\},$$

where it suffices to apply the relations

$$u = \sqrt{1-\lambda c^+c}, \quad c = c_0 + \varepsilon,$$

and expand u in powers of λ. The condensate state that is included in the sum with minus sign is already taken into account in the ground-state energy (16). Upon separating the part quadratic in ε and passing to the k space, we obtain

$$H_{\parallel} = e_{\parallel}^0 + \sum_k \{A_k^{\parallel}(\varepsilon_k^+\varepsilon_k + \varepsilon_{-k}\varepsilon_{-k}^+) + B_k^{\parallel}(\varepsilon_k^+\varepsilon_{-k}^+ + \varepsilon_k\varepsilon_{-k})\}, \quad (20)$$

$$e_{\parallel}^0 = \frac{3}{2}J_1^*N\frac{\beta^2}{1-\beta},$$

$$\frac{A_k^{\parallel}}{3J_1^*} \equiv a_k^{\parallel} = j + 2\beta + \frac{\beta^2}{2(1-\beta)}(1+2\nu_k) + \nu_k(1-3\beta),$$

$$\frac{B_k^{\parallel}}{3J_1^*} \equiv b_k^{\parallel} = \beta + \frac{\beta^2}{2(1-\beta)}(1+2\nu_k) + \nu_k(1-3\beta).$$

The spectrum of longitudinal oscillations has a gap ($E_k^{\parallel}(\beta_0)$ is the mean-field approximation) and is represented as

$$E_k^{\parallel} = \sqrt{A_k^{\parallel 2} - B_k^{\parallel 2}} = 3J_1^*\sqrt{(j+\beta)\frac{j(1-\beta)-\beta(2\beta-3)}{1-\beta}\left[1+\frac{(2\beta-1)^2}{j(1-\beta)-\beta(2\beta-3)}2\nu_k\right]}, \quad (21)$$

$$E_k^{\parallel}(\beta_0) = 3J_1^*\sqrt{1+2\nu_k j^2},$$
$$\Delta_{\parallel}(\beta_0) = 6J_1^*\sqrt{\beta_0(1-\beta_0)} = E_k^{\parallel}(\mathbf{k}=\mathbf{q}). \quad (22)$$

The gap is closed at the phase-transition point $\beta_0 = 0$. In the neighborhood of the critical point ($\beta_0 \longrightarrow 0$), the value of the gap is small ($\Delta_{\parallel}(\beta_0) \sim \sqrt{\beta_0}$); therefore, in calculating various physical quantities, one may expect that the contribution of longitudinal fluctuations will be comparable to the contribution of transverse ones.

7. CORRELATION FUNCTIONS

We investigated the behavior of correlation functions between nearest-neighbor spins in a layer, $\langle \mathbf{S}_{ni}\mathbf{S}_{nj}\rangle$, and between the layers, $\langle \mathbf{S}_{1i}\mathbf{S}_{2i}\rangle$, in both phases:

$$\langle \mathbf{S}_{1i}\mathbf{S}_{1j}\rangle = \left\langle \frac{\mathbf{M}_i + \mathbf{L}_i}{2}\frac{\mathbf{M}_j + \mathbf{L}_j}{2}\right\rangle,$$
$$\langle \mathbf{S}_{2i}\mathbf{S}_{2j}\rangle = \left\langle \frac{\mathbf{M}_i - \mathbf{L}_i}{2}\frac{\mathbf{M}_j - \mathbf{L}_j}{2}\right\rangle, \quad (23)$$

where we used relations (9) and (11) and restricted the analysis to a quadratic approximation with respect to operators. For example, in a disordered phase, we obtained the following expression for $\langle \mathbf{S}_i\mathbf{S}_j\rangle^{1,2}$:

$$\langle \mathbf{S}_i\mathbf{S}_j\rangle^{1,2} = \frac{1}{4\lambda N}\sum_k 2\Big(\langle a_k^+b_{-k}^+\rangle + \langle a_kb_{-k}\rangle + \langle a_k^+a_k\rangle + \langle b_k^+b_k\rangle + \langle c_k^+c_k\rangle + \frac{1}{2}[\langle c_k^+c_{-k}^+\rangle + \langle c_kc_{-k}\rangle]\Big)\cos\mathbf{k}\Delta.$$

The mean values in this expression are obtained by a Bogolyubov transformation to new operators in terms of which the original Hamiltonian (the Hamiltonian of a disordered state in this case) is diagonal. As a result, these means contain constants and the operators of the number of particles of certain kinds with a definite value of $\mathbf{k}$; according to the Bose distribution, these operators are equal to zero in the case, which is considered here, of a magnon gas with a chemical potential of $\mu = 0$ at $T = 0$. The remaining correlation functions are

determined analogously. The results for a disordered phase look as follows ($j > 1$):

$$\langle \mathbf{S}_i\mathbf{S}_j\rangle^{1,2} = \frac{3}{4\lambda N}\sum_k \frac{\cos\mathbf{k}\Delta}{\sqrt{1+\frac{2\nu_k}{j}}},$$
$$\langle \mathbf{S}_{1i}\mathbf{S}_{2i}\rangle = -\frac{9}{4} + \frac{3}{2N}\sum_k \frac{1+\frac{\nu_k}{j}}{\sqrt{1+\frac{2\nu_k}{j}}}. \quad (24)$$

We do not present analytical results for the ordered phase ($j < 1$) in view of their awkwardness. A detailed account of all the results discussed can be found in [40]. The behavior of correlation functions is shown in Fig. 1. As it should be, in the limit of $j \longrightarrow \infty$, the correlation between spins of the same dimer $\langle \mathbf{S}_{1i}\mathbf{S}_{2i}\rangle$ have the asymptotics –3/4, while intralayer correlations $\langle \mathbf{S}_i\mathbf{S}_j\rangle$ tend to zero. At the transition point, the correlation functions are continuous. In the limit of $j = 0$, the terms in $\langle \mathbf{S}_i\mathbf{S}_j\rangle$ that are attributed to the longitudinal fluctuations total zero; i.e., they make zero contribution. In contrast to modified spin-wave methods, the correlations between spins in a layer in the singlet phase have a finite value and increase as approaching the phase-transition point ($j = 1$). The correlations between spins in adjacent layers decrease with j and reach a value of –0.47, which is less than that in the modified spin-wave theory.

8. GROUND-STATE ENERGY WITH REGARD TO FLUCTUATIONS

After the diagonalization, the components $H_\perp$ and $H_\parallel$ of the Hamiltonian of the ordered phase have a standard form that allows us to calculate the ground-state energy E with regard to fluctuation corrections,

$$H_\perp = \sum_k E_k^\perp(\alpha_k^+\alpha_k + \beta_k^+\beta_k + \alpha_{-k}\alpha_{-k}^+ + \beta_{-k}\beta_{-k}^+) + 2\sum_k (E_k^\perp - A_k^\perp),$$
$$H_\parallel = e_\parallel^0 + \sum_k E_k^\parallel(\gamma_k^+\gamma_k + \gamma_{-k}\gamma_{-k}^+) + \sum_k (E_k^\parallel - A_k^\parallel), \quad (25)$$
$$E = E_0 + e_\parallel^0 + 2\sum_k (E_k^\perp - A_k^\perp) + \sum_k (E_k^\parallel - A_k^\parallel),$$

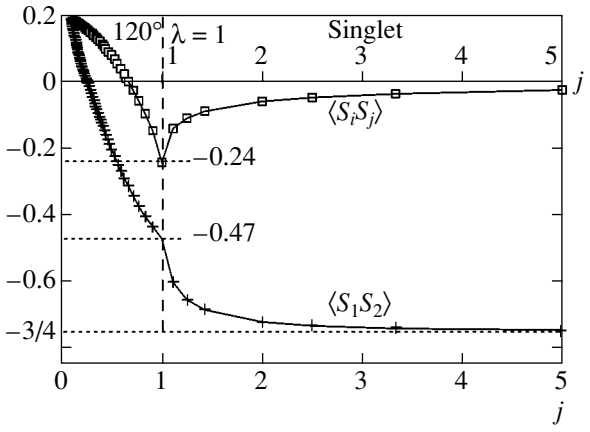

Fig. 1. Correlation functions between nearest-neighbor spins (the mean-field approximation).

and to refine the equilibrium value of the parameter β ($\partial E/\partial\beta = 0$). An equation for the equilibrium β has a self-consistent form:

$$\beta = \beta_0 - \lambda Z_b(\beta),$$
$$Z_b(\beta) = Z_1(\beta) + Z_2(\beta) + Z_3(\beta) + Z_4(\beta) + Z_5(\beta), \quad (26)$$
$$Z_1(\beta) = \frac{\beta(2-\beta)}{8(1-\beta)^2},$$
$$Z_2(\beta) = \frac{1}{N6J_1^*}\sum_k \frac{\partial A_k^\perp}{\partial\beta}\left(\frac{A_k^\perp}{E_k^\perp} - 1\right),$$
$$Z_3(\beta) = -\frac{1}{N6J_1^*}\sum_k \frac{\partial B_k^\perp}{\partial\beta}\frac{B_k^\perp}{E_k^\perp},$$
$$Z_4(\beta) = \frac{1}{N12J_1^*}\sum_k \frac{\partial A_k^\parallel}{\partial\beta}\left(\frac{A_k^\parallel}{E_k^\parallel} - 1\right),$$
$$Z_5(\beta) = -\frac{1}{N12J_1^*}\sum_k \frac{\partial B_k^\parallel}{\partial\beta}\frac{B_k^\parallel}{E_k^\parallel}.$$

We calculated $Z_b(\beta)$ to a first approximation by transforming the exact values of β and then used the mean-field approximation β_0 for β. The roots of the equation are determined by the method of interval bisection with an accuracy of 0.01. A family of functions $\beta(j)$ that correspond to different λ is shown in Fig. 2. One can see that there exists an asymptote

$$\beta = \beta_0 = \frac{1}{2}(1-j)$$

as $\lambda \longrightarrow 0$. A characteristic feature of these functions for large values of λ is the two-valuedness of $\beta(j)$ in the

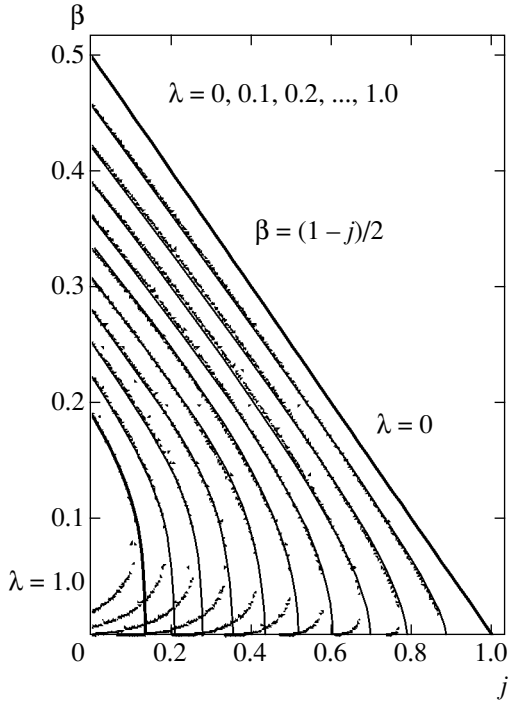

Fig. 2. Equilibrium β with regard to quantum corrections. The dots represent a solution to the self-consistent equation (26) for λ = 0.1, …, 1.0; the solid curves represent an approximation that eliminates the unphysical two-valuedness of the function, which is associated with the divergence of Gaussian fluctuations near the phase transition (β ⟶ 0). The point at which β vanishes for the physical case of λ = 1 is $j = 0.132$.

region of small β, which is physically meaningless. Such results are attributed to Gaussian fluctuations that indefinitely increase as the phase transition (β ⟶ 0) is approached; this fact was discussed in detail in [38]. Therefore, using the values of β that were calculated away from the phase transition, we approximate the functions in the neighborhood of the phase transition (β ≈ 0) so as to avoid the two-valuedness (Fig. 2). According to this approximation, the point at which β vanishes for λ = 1 is given by $j = J_2/3J_1 = 0.132$; i.e., $J_2/J_1 = 0.4$. In a similar system with a square lattice, the point of transition to a disordered phase corresponds to the values of J_2/J_1 ranging from 1.86 to 4.5 depending on the computation method [38, 39]. As expected, the classical 120° state triangular ordered decays much faster than that in the square system: the domain of values of j in which the ordered state is realized is less by an order of magnitude. Such a significant difference may be attributed in part to the in-plane frustratedness of bonds. For equal J_1 and J_2 in square and triangular systems, the effective interaction of two spins in the plane of the triangular lattice $\tilde{J}_1$ proves to be weaker by a factor of two and the ratio J_2/J_1 at the transition point is effectively greater (approaching that in the square lattice), because the spin is not oriented according to the local energy minimum. It is qualitatively clear that an effective increase in J_2/J_1 leads to an increase in the gap between the singlet and the triplet levels, whereby the singlet orbital turns out to be populated earlier (in j) and the 120° triangular order is destroyed.

9. SPONTANEOUS MAGNETIZATION

The mean value of the spin at a site in the 120° phase is equal to

$$N_0 = \left|\langle S_1^z\rangle\right| = \left|\langle S_2^z\rangle\right| = \frac{1}{\sqrt{\lambda}}\langle c^+ u\rangle = \frac{1}{\sqrt{\lambda}} \times \langle(\alpha+\varepsilon^+)\sqrt{1-\lambda[a^+a + b^+b + (\alpha+\varepsilon^+)(\alpha+\varepsilon)]}\rangle. \quad (27)$$

Up to the terms that are quadratic in the operators, we have

$$N_0 = \frac{\alpha\sqrt{1-\beta}}{\sqrt{\lambda}} \times\Bigg[1 - \frac{\lambda}{2(1-\beta)}(\langle a_k^+ a_k\rangle + \langle b_k^+ b_k\rangle + \langle \varepsilon_k^+ \varepsilon_k\rangle) - \frac{\lambda}{2(1-\beta)}(\langle \varepsilon_k^+ \varepsilon_k\rangle + \langle \varepsilon_k^+ \varepsilon_{-k}^+\rangle) - \frac{\lambda\beta}{8(1-\beta)^2} \times(\langle \varepsilon_k \varepsilon_{-k}\rangle + \langle \varepsilon_k^+ \varepsilon_{-k}^+\rangle + \langle \varepsilon_k^+ \varepsilon_k\rangle + \langle \varepsilon_k \varepsilon_k^+\rangle)\Bigg]. \quad (28)$$

The means are determined by the Bogolyubov transformation, which was obtained in Section 7. As a result, we obtain

$$N_0 = \frac{\sqrt{\beta(1-\beta)}}{\lambda}(1 - \lambda Z_a(\beta)),$$

$$Z_a(\beta) = Z_6(\beta) + Z_7(\beta) + Z_8(\beta) + Z_9(\beta),$$

$$Z_6(\beta) = \frac{\beta}{8(1-\beta)^2},$$

$$Z_7(\beta) = -\frac{2-\beta}{8(1-\beta)^2}\frac{1}{N}\sum_k \frac{B_k^{\parallel}}{E_k^{\parallel}},$$

$$Z_8(\beta) = \frac{4-3\beta}{8(1-\beta)^2}\frac{1}{N}\sum_k\left(\frac{A_k^{\parallel}}{E_k^{\parallel}} - 1\right),$$

$$Z_9(\beta) = \frac{1}{2(1-\beta)}\frac{1}{N}\sum_k\left(\frac{A_k^{\perp}}{E_k^{\perp}} - 1\right). \quad (29)$$

Here,

$$\frac{\sqrt{\beta(1-\beta)}}{\lambda} = \frac{\langle c_0^+ u_0\rangle}{\sqrt{\lambda}}$$

is the approximation of magnetization without fluctuations.

An approximation of spontaneous magnetization, which is independent of the table of values of $\beta(j)$, can be obtained with the use of the first iterative approximation for β:

$$\beta \approx \beta_1 = \beta_0 - \lambda Z_b(\beta_0).$$

Then, setting

$$Z_a \approx Z_a(\beta_0), \quad Z_b \approx Z_b(\beta_0),$$

and taking into account that $\lambda \ll 1$, we obtain the approximation of magnetization that is shown in Fig. 3. This approximation has an significant drawback: the points at which N_0 and β vanish (the phase-transition point) do not coincide. However, it reveals the following characteristic feature of the function: the presence of a small maximum in the region of small j, which is especially manifest for medium values of λ; this behavior is analogous to that in two-layer square lattices [38].

We have established that, in the limit of $j = 0$, longitudinal waves do not contribute to the magnetization because the terms in Z_a that are associated with longitudinal fluctuations total zero. In the other limiting case, in the neighborhood of the phase transition ($\beta \longrightarrow 0$), the magnetization vanishes as $N_0 \propto \sqrt{\beta}$, and all the terms in $Z_a(\beta = 0)$, both transverse and longitudinal, prove to be of the same order of magnitude. Thus, longitudinal spin fluctuations, which are neglected in the spin-wave description, prove to be comparable with transverse fluctuations in the neighborhood of the phase transition.

It may seem that the obtained table of equilibrium values of $\beta(j)$ allows one to determine the exact behavior of magnetization. However, this is a fallacy, because the substitution of the values of $\beta(j)$ determined with regard to fluctuations into the integral functions $Z_a(\beta)$ and $Z_b(\beta)$, which contain the spectrum, and are calculated only in the quadratic approximation with respect to the operators of secondary quantization without taking quantum corrections into account, is an excess of accuracy. In the quadratic approximation, the spectrum is determined in the range of $j \in (0, 1)$, the point of the phase transition is $j = 1$, and the equilibrium value is $\beta = (1/2)(1-j)$. The substitution of the refined values of $\beta(j) < (1/2)(1-j)$, which are determined in the interval

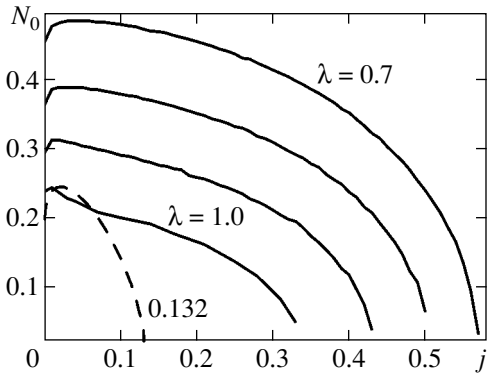

Fig. 3. Spontaneous magnetization with regard to fluctuations. The solid curves are obtained with the use of the first iterative approximation for β, and the dashed curve illustrates the approximate behavior corresponding to the table of equilibrium $\beta(j)$ for $\lambda = 1.0$.

of $j \in (0, 0.132)$, makes the spectra of the ordered phase partially imaginary (for example, the transverse spectrum is positive definite in the entire Brillouin zone only if $\beta \in ((1/2)(1-j), 1)$). Thus, a more accurate determination of the behavior of the magnetization and other quantities requires that one should either determine the excitation spectrum and the equilibrium β in the same consistent approximation, which is often associated with the elimination of unphysical states in higher orders of expansion in the operators, or apply the Monte Carlo method. We restricted ourselves to an approximate determination of the behavior that is based on the knowledge of the phase-transition point and the characteristic form of the function. An approximate behavior of magnetization is shown by a dashed line in Fig. 3. According to this figure, the magnetization vanishes simultaneously with $\beta(j)$ at $j = J_2/3J_1 = 0.132$. The calculations performed allow us to evaluate the mean value of the spin at a site; it ranges from about 1/4 to 0. Thus, the quantum reduction of the spin in the 120° triangular phase ranges from 50 to 100% depending on j.

10. INITIAL SUSCEPTIBILITY

We have calculated the initial susceptibility in a field $H = H_x$ that is perpendicular to the plane of the layers. Instead of the a and b bosons, it is convenient to use operators s and p in the field H_x,

$$s = \frac{a+b}{\sqrt{2}}, \quad p = \frac{a-b}{\sqrt{2}},$$

which satisfy the relation

$$a^+a + b^+b = s^+s + p^+p;$$

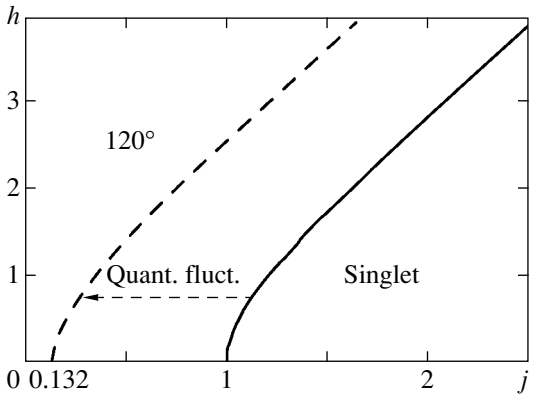

Fig. 4. *j–h* phase diagram for small *h*. The solid curve shows the position of the phase boundary in the mean-field approximation, and the dashed curve shows the same boundary with regard to fluctuations. As the field *h* increases, instead of the 120° structure [41], other seven phases become the ground state in the region of small *j*.

the ferro- and antiferromagnetism vectors are given by

$$M^x = c^+p + p^+c, \quad M^y = i(c^+s - s^+c),$$
$$M^z = s^+p + p^+s, \quad L^x = \frac{1}{\sqrt{\lambda}}(s^+u + us), \tag{30}$$
$$L^y = -\frac{i}{\sqrt{\lambda}}(p^+u - up), \quad L^z = -\frac{1}{\sqrt{\lambda}}(c^+u + uc).$$

The convenience of the new operators is associated with the fact that a field applied along the *x* axis induces the condensation of the *p* field alone, which occurs at the wavevector $\mathbf{k} = \mathbf{q}$. Indeed, the expected value of induced magnetization

$$\langle S_x(i)\rangle = M_\perp(i) = \langle c_i^+ p_i\rangle = \text{const}(i)$$

must not depend on a site; this fact imposes a constraint on the admissible form of the operators *p*. In the general case, we have

$$c_i^+ = \langle c_i^+\rangle + \varepsilon_i^+, \quad p_i = \langle p_i\rangle + \chi_i;$$

therefore,

$$M_\perp = \langle S_x\rangle = \langle c_i^+ p_i\rangle = \langle c_i^+\rangle\langle p_i\rangle + \langle \varepsilon_i^+\chi_i\rangle$$
$$\equiv M_\perp^0(i) + \Delta M_\perp(i) = \text{const}(i),$$
$$M_\perp^0(i) = \langle c_i^+\rangle\langle p_i\rangle = \alpha\exp(-iqR_i)\langle p_i\rangle \tag{31}$$
$$= \text{const}(i) \Rightarrow \langle p_i\rangle = \tilde{\alpha}\exp(iqR_i),$$
$$p_k = \sqrt{N}\tilde{\alpha}\delta_{kq} + \chi_k,$$
$$M_\perp^0 = \alpha\tilde{\alpha} = \frac{\sqrt{\beta\gamma}}{\lambda}, \quad \gamma \equiv \lambda\tilde{\alpha}^2;$$

i.e., bosons *c* and *p* condense at a wavevector $\mathbf{k} = \mathbf{q}$. The induced magnetization and the susceptibility are given by

$$M_\perp = \frac{\sqrt{\beta\gamma}}{\lambda} + \frac{1}{N}\sum_k \langle \varepsilon_k^+\chi_k\rangle \equiv M_\perp^0 + \Delta M_\perp,$$
$$\chi_\perp = \left.\frac{\partial M_\perp}{\partial H_x}\right|_{H_x = 0} \equiv \chi_\perp^0 + \Delta\chi_\perp. \tag{32}$$

The parameters β and γ can be determined from the minimum of the ground-state energy $\tilde{e}_0$ in a magnetic field. In the mean-field approximation ($h \equiv H_x/3J_1^*$), we have

$$\tilde{e}_0 \equiv \frac{\lambda E_0}{N} = -\frac{3}{2}J_2\lambda + 2J_2(\beta + \gamma)$$
$$-2H_x\sqrt{\beta\gamma} + 18J_1^*\beta\gamma - 6J_1^*\beta(1-\beta), \tag{33}$$

$$\gamma_0 = \beta_0\left[\frac{h}{2(j + 3\beta_0)}\right]^2,$$
$$j = 1 - 2\beta_0 + j\left[\frac{h}{2(j + 3\beta_0)}\right]^2. \tag{34}$$

On the curve

$$j_k = \frac{1}{2}[1 + \sqrt{1 + h^2}],$$

the parameters β_0 and γ_0 vanish simultaneously for $h \neq 0$. This function represents a curve of phase transitions in the mean-field approximation because the 120° triangular order vanishes in this case. Figure 4 shows the corresponding *j–h* phase diagram of the model. The dashed curve in this figure illustrates how the phase diagram changes when one takes into account the effect of quantum fluctuations. The magnetic field displaces, as it should, the point of phase transition to a disordered state to a domain of greater values of *j*. However, such behavior of the equilibrium curve is only characteristic of small *h*; as the magnetic field increases, the 120° triangular order is no longer the ground state, and the *j–h* phase plane exhibits an intricate structure in the region of small *j* and *h* and defines the existence domain of seven phases with different types of spin ordering [20, 41, 42]. Note that thermal fluctuations in purely two-dimensional systems lead to complete destruction of ordering at $h = 0$ due to the vanishing of the effective spin length (the Mermin–Wagner theorem). The temperature behavior of quasi-two-dimensional triangular antiferromagnets has recently been investigated in [43] with the example of $RuFe(MnO_4)_2$.

Using the obtained values of β_0 and γ_0, we determine the mean-field approximation to the induced magnetization and the initial susceptibility:

$$M_\perp^0(h \longrightarrow 0) = \left.\frac{\sqrt{\beta_0\gamma_0}}{\lambda}\right|_{h\to 0} = \frac{1}{2\lambda}\frac{(1-j)}{(3-j)}h,$$
$$\chi_\perp^0 = \frac{\partial M_\perp^0(h \longrightarrow 0)}{\partial H_x} = \frac{1}{6J_1}\frac{(1-j)}{(3-j)}. \quad (35)$$

In the limiting case of $j = 0$, we have $\chi_\perp^0 = 1/18J_1$, which coincides with the results for single-layer triangular lattices.

To calculate the fluctuation corrections to the magnetization,

$$\Delta M_\perp = \frac{1}{N}\sum_k \langle \varepsilon_k^+ \chi_k \rangle,$$

we should find the eigenfunctions of the Hamiltonian in a magnetic field; in the quadratic approximation, this Hamiltonian can be reduced to

$$H_h = E_0 + H_s + H_{cp},$$

where H_s and H_{cp} are the quadratic forms with respect to the s and $\varepsilon\chi$ operators, respectively. We have

$$H_s = \sum_k 2A_k^s s_k^+ s_k + B_k^s(s_k^+ s_{-k}^+ + s_k s_{-k}),$$
$$\frac{A_k^s}{3J_1^*} \equiv a_s = j + \beta + \nu_k\left(1 - \frac{3}{2}\beta - \frac{3}{2}\gamma\right), \quad (36)$$
$$\frac{B_k^s}{3J_1^*} \equiv b_s = \nu_k\left(1 - \frac{\beta}{2} - \frac{3}{2}\gamma\right).$$

The spectrum of s excitations has a gap,

$$E_k^s = 3J_1^*(j+\beta) \times \sqrt{\left(1 - \frac{\beta}{j+\beta}\nu_k\right)\left(1 + \frac{1-\beta-\frac{3}{2}\gamma}{j+\beta}2\nu_k\right)}, \quad (37)$$

$$\Delta_s = E_k^s(\mathbf{k} = \mathbf{q})|_{h\to 0} \longrightarrow 3J_1^*\frac{2-\beta_0}{4(1+\beta_0)}h. \quad (38)$$

In contrast to square lattices, the gap depends on j; moreover, it is closed in zero field. The spectrum of s excitations in zero field transforms into the spectrum of transverse oscillations of the ordered phase. We have

$$H_{cp} = -J_q^*\frac{\beta(\beta+\gamma)}{2(1-\beta-\gamma)}N + \sum_k \{2A_k^\varepsilon \varepsilon_k^+ \varepsilon_k + B_k^\varepsilon(\varepsilon_k^+ \varepsilon_{-k}^+ + \varepsilon_k \varepsilon_{-k}) + 2A_k^\chi \chi_k^+ \chi_k + B_k^\chi(\chi_k^+ \chi_{-k}^+ + \chi_k \chi_{-k}) + C_k(\varepsilon_k^+ \chi_k + \chi_k^+ \varepsilon_k) + D_k(\varepsilon_k^+ \chi_{-k}^+ + \varepsilon_k \chi_{-k})\}, \quad (39)$$

$$\frac{A_k^\varepsilon}{3J_1^*} \equiv a_\varepsilon = j + 2\beta + \frac{\beta^2}{2(1-\beta-\gamma)}(1+2\nu_k) + \nu_k\left(1 - 3\beta - \frac{3}{2}\gamma\right),$$

$$\frac{B_k^\varepsilon}{3J_1^*} \equiv \beta_\varepsilon = \beta + \frac{\beta^2}{2(1-\beta-\gamma)}(1+2\nu_k) + \nu_k\left(1 - 3\beta - \frac{3}{2}\gamma\right),$$

$$\frac{A_k^\chi}{3J_1^*} \equiv a_\chi = j + \beta + \frac{\beta\gamma}{2(1-\beta-\gamma)}(1+2\nu_k) + \nu_k\left(1 - \gamma - \frac{3}{2}\beta\right),$$

$$\frac{B_k^\chi}{3J_1^*} \equiv b_\chi = \frac{\beta\gamma}{2(1-\beta-\gamma)}(1+2\nu_k) + \nu_k\left(-1 + \gamma + \frac{\beta}{2}\right),$$

$$\frac{C_k}{3J_1^*} \equiv c = -h + \sqrt{\beta\gamma}\left[5 + \frac{\beta}{1-\beta-\gamma}(1+2\nu_k) - 3\nu_k\right],$$

$$\frac{D_k}{3J_1^*} \equiv d = \sqrt{\beta\gamma}\left[1 + \frac{\beta}{1-\beta-\gamma}(1+2\nu_k) - 3\nu_k\right].$$

An analytic expression for the spectrum of *cp* excitations in a magnetic field is given by

$$E_k^{cp} = 3J_1^*\sqrt{m \pm \sqrt{m^2 - \tilde{c}}},$$
$$m = \frac{1}{2}\left[a_\varepsilon^2 - b_\varepsilon^2 + a_\chi^2 - b_\chi^2 + \frac{1}{2}(c^2 - d^2)\right],$$
$$\tilde{c} = c_1 c_2, \quad (40)$$
$$c_1 = \frac{(c-d)^2}{4} - (a_\varepsilon - b_\varepsilon)(a_\chi - b_\chi),$$
$$c_2 = \frac{(c+d)^2}{4} - (a_\varepsilon + b_\varepsilon)(a_\chi + b_\chi).$$

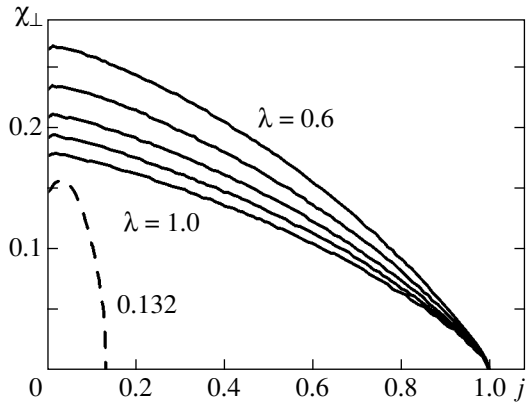

Fig. 5. Initial susceptibility. The solid curves are obtained with the use of the mean-field approximation for β, and the dashed curve represents an approximate behavior that corresponds to β(*j*) with regard to fluctuations: $\chi_\perp \sim \sqrt{\beta}$; therefore, β and $\chi_\perp$ vanish simultaneously at $j = 0.132$.

Unfortunately, this spectrum cannot be represented as a compact function of the variables (*j*, *h*), (β, γ), or others. The spectrum of *cp* excitations contains two branches. The lower branch contains a Goldstone boson for $\mathbf{k} = \mathbf{q}$ and, at $h = 0$, turns into the spectrum of transverse (*ab*) modes of the ordered phase. The upper branch has a gap and turns into the spectrum of longitudinal (*c*) oscillations at $h = 0$; the value of the gap in the mean-field approximation is

$$\Delta_{cp} = E^{cp}_{k(2)}(\mathbf{k} = \mathbf{q}) = 6J_1^*\sqrt{(j+\beta_0)(j-1+3\beta_0)}. \quad (41)$$

The diagonalization of H_s yields

$$H_s = \sum_k (E^s_k - A^s_k) + \sum_k 2E^s_k \gamma^+_k \gamma_k.$$

As $h \longrightarrow 0$, the diagonalization of H_{cp} leads to the following expression (ε_c and ε_p are the spectra for $h \longrightarrow 0$):

$$H_{cp} = E^0_{cp} + \sum_k [(\varepsilon_c - A^\varepsilon_k) + (\varepsilon_p - A^\chi_k) - O(h^2)] + 2\sum_k (\varepsilon_p a^+_k a_k + \varepsilon_c b^+_k b_k),$$
$$E^0_{cp} = 3J_1^*\frac{\beta(\beta+\gamma)}{2(1-\beta-\gamma)}N, \quad \varepsilon_c = \sqrt{A^{\varepsilon 2}_k - B^{\varepsilon 2}_k}, \quad \varepsilon_p = \sqrt{A^{\chi 2}_k - B^{\chi 2}_k}. \quad (42)$$

The ground-state energy in a magnetic field for $h \longrightarrow 0$,

$$E_h = E_0 + E^0_{cp} + \sum_k (E^s_k - A^s_k) + \sum_k [(\varepsilon_c - A^\varepsilon_k) + (\varepsilon_p - A^\chi_k) - O(h^2)], \quad (43)$$

allows us to determine the equilibrium values of β and γ (upon setting $\partial E_h/\partial\beta = 0$ and $\partial E_h/\partial\gamma = 0$). It suffices to refine one parameter, γ; the other parameter can be taken in the mean-field approximation because β and γ enter the equation

$$M_\perp = \frac{\sqrt{\beta\gamma}}{\lambda} + \Delta M_\perp$$

as a product. As a result, we obtain

$$\gamma = \beta\left[\frac{h}{2(j+3\beta)+\lambda\varphi}\right]^2,$$

where $\varphi = \varphi(\beta, \gamma, j, h)$ is an integral that contains the coefficients of the Hamiltonians H_s and H_{cp}.

Thus, taking into account a renormalized value of γ and diagonalizing transformations, we obtain the following expressions for the induced magnetization:

$$M_\perp = \frac{\sqrt{\beta_0\gamma}}{\lambda} + \Delta M_\perp$$

and the initial susceptibility,

$$\chi_\perp = \chi^0_\perp + \Delta\chi_\perp,$$

where the mean fluctuation components are given by (here, $h \longrightarrow 0$, $\beta = \beta_0$, and $j \approx 1 - 2\beta_0$)

$$M^0_\perp \approx \frac{\sqrt{\beta_0\gamma}}{\lambda} \approx h\frac{\beta_0}{\lambda[2(1+\beta_0)+\lambda\varphi(h=0)]},$$
$$\chi^0_\perp = \frac{1}{3J_1^*}\frac{\beta_0}{\lambda[2(1+\beta_0)+\lambda\varphi(h=0)]},$$
$$\Delta M_\perp = -h\frac{1}{4(1+\beta_0)}\frac{1}{N}\sum_k u^2_c u^2_p (x_c + x_p) \times \frac{[-2(1-\beta_0)+\beta_0 d'](x_c+x_p)+\beta_0 d'(1+x_c x_p)}{e_c + e_p}, \quad (44)$$

$$\Delta\chi_\perp = -\frac{1}{3J_1^*}\frac{1}{4(1+\beta_0)}\frac{1}{N}$$

$$\times\sum_k \frac{u_\parallel^2 u_\perp^2 (x_\parallel + x_\perp)}{e_\parallel + e_\perp}$$

$$\times\{[-2(1-\beta_0)+\beta_0 d']\,(x_\parallel + x_\perp) + \beta_0 d'(1 + x_\parallel x_\perp)\}.$$

Here,

$$u_i = \sqrt{\frac{1}{2}\left(\frac{a_i}{e_i}+1\right)}, \quad x_i = -\frac{b_i}{a_i + e_i},$$

$$e_i = \sqrt{a_i^2 - b_i^2} = \frac{\varepsilon_i}{3J_1^*}, \quad i = c(\varepsilon), p(\chi),$$

$$\alpha_{c(\varepsilon)}(h=0) = \alpha_k^\parallel, \quad \alpha_{p(\chi)}(h=0) = \alpha_k^\perp,$$

$$\alpha = a, e, u, x, \quad b_\varepsilon(h=0) = b_k^\parallel,$$

$$b_\chi(h=0) = -b_k^\perp, \quad d' \equiv 1 + \frac{\beta_0}{1-\beta_0}(1+2\nu_k) - 3\nu_k.$$

The form of the function $\chi_\perp$ is shown in Fig. 5. This function is nonmonotonic with a small maximum in the neighborhood of small j. The dashed line represents the behavior corresponding to the table of equilibrium values of $\beta(j)$.

In this paper, we did not consider the possibility of the formation of singlet pairs in a layer. In our view, consideration of this possibility should lead to vanishing of the spin at a site of $\chi_\perp$ for $j \approx 0$; thus, the interval of the 120° triangular phase will become even narrower.

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