

## Self-consistent spin-wave theory of layered Heisenberg magnets

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The versions of the self-consistent spin-wave theories (SSWT) of two-dimensional Heisenberg ferro- and antiferromagnets with a weak interlayer coupling and/or magnetic anisotropy, that are based on the nonlinear Dyson-Maleev, Schwinger, and combined boson-pseudofermion representations, are analyzed. Analytical results for the temperature dependences of (sublattice) magnetization and the short-range order parameter, and the critical points are obtained. The influence of external magnetic field is considered. Fluctuation corrections to SSWT are calculated within a random-phase approximation which takes into account correctly leading and next-leading logarithmic singularities. These corrections are demonstrated to improve radically the agreement with experimental data on layered perovskites and other systems. Thus an account of these fluctuations provides a quantitative theory of layered magnets. [S0163-1829(99)12025-3]

### I. INTRODUCTION

Investigation of low-dimensional magnetism is an important branch of modern solid-state physics. Experimental interest in this problem is connected with the magnetic properties of copper-oxide high- $T_c$  superconductors, organic compounds, ferromagnetic films, multilayers, and surfaces.<sup>1</sup>

As stated by the Mermin-Wagner theorem, two-dimensional (2D) isotropic magnets possess long-range order (LRO) only in the ground state. Unlike purely 2D Heisenberg magnets, real layered compounds have finite values of the magnetic ordering temperature  $T_M \ll |J|$  ( $J$  is the exchange integral) due to weak interlayer coupling and/or magnetic anisotropy. The smallness of transition temperature leads to some peculiar features of these systems. When crossing  $T_M$ , the short-range order (SRO) is not totally destroyed (in the 2D situation it is maintained up to  $T \sim |J|$ ), and a broad region above  $T_M$  with strong SRO exists. Corresponding experimental indications are provided by the data on elastic and inelastic neutron scattering: well-pronounced peaks of diffuse scattering were observed in  $\text{La}_2\text{CuO}_4$ ,<sup>2</sup>  $\text{Rb}_2\text{MnF}_4$  and  $\text{K}_2\text{NiF}_4$ ,<sup>3</sup> and well-defined spin waves in  $\text{K}_2\text{MnF}_4$  up to  $T \sim 2T_N$ .<sup>4</sup>

A great progress in the theory of the ground state and thermodynamic properties was made with the use of rigorous mathematical methods [quantum Monte Carlo and renormalization-group (RG) calculations]. At the same time, simple approaches, which yield an analytical description of a wide range of physical properties, are very useful for practical purposes. At low temperatures ( $T \ll T_M$ ) the standard spin-wave theory works satisfactorily. At higher temperatures corrections owing to spin-wave interactions become important. These corrections were treated self-consistently many years ago for the 3D Heisenberg model in Ref. 5 The same results were obtained within a variational approach for isotropic<sup>6</sup> and anisotropic<sup>7</sup> Heisenberg magnets.

For 2D magnets, close ideas were used recently by the ‘‘boson mean-field theory’’<sup>8,9</sup> which is based on the representation of spin operators through Schwinger bosons, and the ‘‘modified spin-wave theory’’<sup>10</sup> based on the Dyson-Maleev (DM) representation. Note that the former approach

differs drastically from the standard mean-field approximation in the Heisenberg model: it takes into account spin-wave excitations and is highly sensitive to the space dimensionality. The results of these theories are in a good agreement with the scaling consideration<sup>11,12</sup> and experimental data on spin excitations in  $\text{CuO}_2$  planes. Being generalized to the quasi-2D case (see, for example, Refs. 13–16), these approaches lead to the same results as Refs. 5–7. The approaches of Refs. 8–10 were also applied to frustrated 2D (Refs. 17–21) and 3D (Ref. 18) antiferromagnets.

In the approaches<sup>9,10</sup> LRO is described in terms of boson condensation, see also Ref. 22. To continue the region of applicability of the theory to disordered phase, a chemical potential of the Bose system (fictitious magnetic field) is introduced at  $T > T_M$ , which is determined from the condition of the vanishing of (staggered) magnetization. Introducing such a field can be more strictly justified within the projection operator technique.<sup>23</sup>

While the approach of Refs. 8,9 corresponds to  $N \rightarrow \infty$  limit of the generalized  $\text{SU}(N)$  Heisenberg model, the approach of Ref. 10 can be considered as the result of the self-consistent first-order  $1/S$  expansion, i.e., summation of all the bubble diagrams for the self-energy (see also Ref. 5). As argued in the present paper, this equivalence is preserved also between the first-order  $1/N$  expansion and second-order self-consistent  $1/S$  expansion and seems to take place in all the orders of perturbation theories discussed.

At the same time, the above-discussed approaches (we refer them to as the self-consistent spin-wave theories, SSWT) turn out to have some shortcomings. The first one is mainly technical: the Bose condensation picture is inapplicable for anisotropic systems, since they have a gap in the excitation spectrum. Further, the  $\text{SU}(N)$  symmetry in this case is broken, and the  $1/N$  expansion in the  $\text{SU}(N)$  model cannot be performed in principle. However, as it was mentioned, this expansion (and also the description of LRO in terms of the Bose condensate) is not the only way to SSWT.

The second shortcoming is much more essential. It concerns the description of thermodynamics at temperatures that are comparable with  $T_M$ . In particular, the description of the (sublattice) magnetization curve near the ordering point is

poor: the corresponding equation has two solutions, so that  $\bar{S}(T)$  does not vanish continuously (see, e.g., Refs. 5,16). Besides that, the transition points are strongly overestimated. These drawbacks are due to that at sufficiently high temperatures the higher-order processes connected with dynamical interaction between spin waves, and also kinematical interaction, should be taken into account.

The kinematical interaction is important in a wide temperature region only for systems where  $T_M$  is not small in comparison with  $|J|S^2$  (e.g., for 3D systems). This interaction can be, in principle, taken into account by the projection operator technique (see, e.g., Ref. 23). However, this technique is rather complicated and is not convenient for practical purposes. Another way to obtain the corrections owing to the kinematical interaction is the use of the Baryakhtar-Krivoruchko-Jablonsky (BKJ) representation<sup>24,25</sup> of spin operators via bosons and pseudofermions, which generalizes the DM representation (we do not know such a generalization for the Schwinger bosons). The introduction of pseudofermions gives, in principle, a possibility of excluding the contribution of unphysical states. These pseudofermions can be easily incorporated into the theory and, at least for 3D magnets, partially correct the above-mentioned drawbacks of the early versions of SSWT.

For layered systems with  $T_M \ll |J|S^2$  the kinematical interaction is less important (in fact, it works only in a narrow critical region near  $T_M$ ), but higher-order (in the dynamic interaction) contributions should be included. As will be shown in the present paper, an infinite random-phase approximation (RPA)-type series of diagrams are to be taken into account<sup>26</sup> (as already mentioned, this is equivalent to the first-order  $1/N$  expansion in the  $SU(N)$  model). Such a procedure permits us to describe the ‘‘2D-like’’ Heisenberg regime<sup>27,28</sup> where thermodynamics is determined by fluctuations of a 2D Heisenberg nature. These results enable one to obtain the correct expression for  $T_M$  up to some nonsingular constant in the denominator. At the same time, the true critical region, where the spin-wave picture of the spectrum is completely inadequate, turns out to be very narrow in the layered systems. A satisfactory description of this region is possible within the  $1/N$  expansion in the  $O(N)$  model (see Refs. 27,29). The latter model is based on a fluctuation rather than spin-wave picture of excitation spectrum. This circumstance provides important advantages at high temperatures, but leads to some difficulties at the description of the low- and intermediate-temperature regions. Therefore, the approach based on the  $SU(N)$  model ( $1/S$  expansion) is more appropriate at not too high temperatures.

In the present paper we formulate a version of the SSWT, which is to a large measure free from above-mentioned shortcomings and is a good starting point for further improvements. To this end we (i) use the BKJ representation to obtain the correct description at not too low temperatures (ii) discard the condition  $\bar{S}=0$  and do not describe LRO in terms of Bose condensate, which permits to us treat anisotropic systems. We also demonstrate (where possible) how our results can be obtained by the Schwinger boson method.<sup>9</sup> Further we calculate the corrections to SSWT for quasi-2D and easy-axis 2D magnets with small interlayer coupling or an-

isotropy using second-order spin-wave results in the self-consistent form.

The plan of the present paper is as follows. In Sec. II we describe the representation of spin operators by Schwinger and Baryakhtar-Krivoruchko-Yablonsky.<sup>24</sup> In Secs. III and IV we consider thermodynamics of quasi-2D and anisotropic 2D layered magnets within SSWT and construct an interpolation scheme between the 2D and 3D cases. In Sec. V we treat the problem of introducing the magnetic field into SSWT and calculating magnetic susceptibility. In Sec. VI we investigate fluctuation corrections to the SSWT results, in particular to the (sublattice) magnetization and ordering temperature, and compare the results of our calculations with experimental data.

## II. BOSON REPRESENTATIONS OF THE SPIN OPERATORS

We consider the anisotropic Heisenberg model

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j - \frac{1}{2} \eta \sum_{ij} J_{ij} S_i^z S_j^z - D \sum_i (S_i^z)^2, \quad (1)$$

where  $J_{ij}$  are the exchange integrals,  $\eta > 0$  and  $D > 0$  are the two-site and single-site easy-axis anisotropy parameters.

Consider first the Baryakhtar-Krivoruchko-Jablonsky representation<sup>24,25</sup>

$$\begin{aligned} S_i^+ &= \sqrt{2S} b_i, & S_i^z &= S - b_i^\dagger b_i - (2S+1) c_i^\dagger c_i, \\ S_i^- &= \sqrt{2S} \left( b_i^\dagger - \frac{1}{2S} b_i^\dagger b_i^\dagger b_i \right) - \frac{2(2S+1)}{\sqrt{2S}} b_i^\dagger c_i^\dagger c_i, \end{aligned} \quad (2)$$

where  $b_i^\dagger, b_i$  are the Bose ideal magnon operators, and  $c_i^\dagger, c_i$  are the auxiliary pseudofermion operators at the site  $i$  which take into account the kinematic interaction of spin waves. For the states  $|p\rangle$  in the physical subspace (with the boson occupation numbers  $N_i < 2S$  and pseudofermion occupation numbers  $F_i = 0$ ) we have  $c|p\rangle = 0$ , and the representation (2) reduces to the standard DM representation. The states  $|u_0\rangle$  with  $N_i > 2S$ ,  $F_i = 0$  and  $|u_1\rangle$  with  $F_i = 1$  are unphysical. As shown in Ref. 24, the partition function can be calculated as

$$\mathcal{Z} = \text{Sp} \left\{ \exp \left( -\beta H[b, b^\dagger, c, c^\dagger] - i\pi \sum_i c_i^\dagger c_i \right) \right\}, \quad (3)$$

where  $H[b, b^\dagger, c, c^\dagger]$  is the original spin Hamiltonian (1) written through the Bose and Fermi operators according to Eq. (2). Analogous relations take place for the averages of spin operators. It can be proved<sup>24</sup> that the contribution of states  $|u_0\rangle$  in Eq. (3) is exactly canceled by the contribution of the states  $|u_1\rangle$ .

Thus, unlike the DM representation, using the BKJ representation gives the possibility of excluding the contribution of the states with the boson occupation numbers  $N_i > 2S$  to thermodynamic quantities. It should be noted that this property relates to the exact Hamiltonian of the boson-pseudofermion system  $H[b, b^\dagger, c, c^\dagger]$  only and does not necessarily hold for its approximate expressions. However, one could expect that the introduction of the Fermi operators extends the region of the applicability of approximate methods to not too low temperatures.

The factor  $\exp(-i\pi\Sigma_i c_i^\dagger c_i)$  in Eq. (3) results in that the distribution function of the pseudofermions becomes  $-N(E_f)$  where  $N(E) = 1/[\exp(E/T) - 1]$  is the Bose function,  $E_f$  is the excitation energy for pseudofermions [as follows from the representation (2), the  $c$  field has no dispersion].

In the case of a two-sublattice antiferromagnet we separate the lattice into  $A$  and  $B$  sublattices. On the sublattice  $A$  we use a representation that is similar to Eq. (2)

$$S_i^+ = \sqrt{2S}a_i, \quad S_i^z = S - a_i^\dagger a_i - (2S+1)c_i^\dagger c_i, \quad i \in A, \quad (4)$$

$$S_i^- = \sqrt{2S} \left( a_i^\dagger - \frac{1}{2S} a_i^\dagger a_i^\dagger a_i \right) - \frac{2(2S+1)}{\sqrt{2S}} a_i^\dagger c_i^\dagger c_i,$$

and on the sublattice  $B$  the ‘‘conjugate’’ representation:

$$S_i^+ = \sqrt{2S}b_i^\dagger, \quad S_i^z = -S + b_i^\dagger b_i + (2S+1)d_i^\dagger d_i, \quad i \in B, \quad (5)$$

$$S_i^- = \sqrt{2S} \left( b_i - \frac{1}{2S} b_i^\dagger b_i b_i \right) - \frac{2(2S+1)}{\sqrt{2S}} d_i^\dagger d_i b_i,$$

where  $a_i^\dagger, a_i$  and  $b_i^\dagger, b_i$  are the Bose operators, and  $c_i^\dagger, c_i$  and  $d_i^\dagger, d_i$  are the Fermi operators.

Another useful representation of spin operators is the Schwinger-boson representation

$$\mathbf{S}_i = \sum_{\sigma\sigma'} s_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} s_{i\sigma'}, \quad (6)$$

where  $\boldsymbol{\sigma}$  are the Pauli matrices,  $\sigma, \sigma' = \uparrow, \downarrow$ , so that

$$S_i^z = \frac{1}{2}(s_{i\uparrow}^\dagger s_{i\uparrow} - s_{i\downarrow}^\dagger s_{i\downarrow}), \quad S_i^+ = s_{i\uparrow}^\dagger s_{i\downarrow}, \quad S_i^- = s_{i\downarrow}^\dagger s_{i\uparrow}. \quad (7)$$

The constraint condition

$$s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow} = 2S \quad (8)$$

should be satisfied at each lattice site. Since the phases of  $s_{i\uparrow}$  and  $s_{i\downarrow}$  can be simultaneously changed,  $s_{i\sigma} \rightarrow s_{i\sigma} \exp(i\phi)$ , this representation possesses a gauge symmetry. The Schwinger-boson representation can be simply related with the Holstein-Primakoff representation if we fix the gauge by the condition of hermiticity for one of the operators  $s_{i\sigma}$ , say,  $s_{i\uparrow}$ , i.e.,  $s_{i\uparrow}^\dagger = s_{i\uparrow}$ . Then we have from Eq. (8)

$$s_{i\uparrow} = \sqrt{2S - s_{i\downarrow}^\dagger s_{i\downarrow}}, \quad (9)$$

and substituting this into Eq. (7) we obtain the Holstein-Primakoff representation. Thus the representations of the Schwinger bosons and by Holstein-Primakoff are equivalent. As well as for the BKJ representation, this equivalence can be violated in approximate treatments. Unlike the Holstein-Primakoff (or DM) representation, the Schwinger-boson representation can be easily generalized to an arbitrary number of boson ‘‘flavors’’  $N \geq 2$ , and the  $1/N$  expansion can be developed. At the same time, there is no natural way to take into account ‘‘roughly’’ the kinematical interaction by introducing the Fermi operators into this representation.

In the antiferromagnetic case we pass (following Ref. 8) to the local coordinate system by the replacement

$$s_{i\uparrow} \rightarrow -s_{i\downarrow}, \quad s_{i\downarrow} \rightarrow s_{i\uparrow}$$

at one of two sublattices.

### III. SSWT OF QUASI-2D MAGNETS

#### A. Self-consistent approach within the BKJ representation

In this section we consider the quasi-2D case with  $D = \eta_{ij} = 0$  and the exchange integrals  $J_{ij} = J$  for  $i, j$  being nearest neighbors in the same plane and  $J_{ij} = J'$  for  $i, j$  in different planes. First we use the BKJ representation. In the ferromagnetic (FM) case the Heisenberg Hamiltonian (1) takes the form

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \left[ [S - b_i^\dagger b_i - (2S+1)c_i^\dagger c_i] [S - b_j^\dagger b_j - (2S+1)c_j^\dagger c_j] + 2S \left( b_i^\dagger - \frac{1}{2S} b_i^\dagger b_i^\dagger b_i \right) b_j - 2(2S+1)b_i^\dagger b_j c_i^\dagger c_i \right] - \mu \sum_i [b_i^\dagger b_i + (2S+1)c_i^\dagger c_i]. \quad (10)$$

To satisfy the condition  $\bar{S} = 0$  in the paramagnetic phase we have introduced the Lagrange multiplier  $\mu$ . This multiplier corresponds to the constraint of the total number of bosons and pseudofermions at  $T > T_C$  and plays a role of common chemical potential  $\mu$  of the boson-pseudofermion system (for the pure boson system it was introduced in Refs. 30,10). At  $T < T_C$  we have  $\mu = 0$  since no restriction of boson and pseudofermion occupation numbers is needed here. Introducing the chemical potential, which gives the possibility of continuing the theory into the disordered phase, can be justified more strictly if one takes into account the kinematical interaction in a regular way.<sup>23</sup> Since the magnon number is not conserved at  $T < T_C$ , the Bose condensation which takes place in Refs. 9 and 10 does not occur in our approach.

Further, we perform decouplings of the quartic forms which occur in Eq. (10). Introducing the averages

$$\gamma = \bar{S} + \langle b_i^\dagger b_{i+\delta_\perp} \rangle, \quad \gamma' = \bar{S} + \langle b_i^\dagger b_{i+\delta_\parallel} \rangle, \quad (11)$$

we derive the quadratic Hamiltonian of the mean-field approximation in the form

$$H = \sum_{i\delta} J_\delta \gamma_\delta [b_i^\dagger b_i - b_{i+\delta}^\dagger b_{i+\delta} + (2S+1)c_i^\dagger c_i] - \mu \sum_i [b_i^\dagger b_i + (2S+1)c_i^\dagger c_i], \quad (12)$$

where  $\gamma_{\delta_\perp} = \gamma$  and  $\gamma_{\delta_\parallel} = \gamma'$ . From the definition of  $\gamma$ , Eq. (11), one finds the system of self-consistent equations

$$\gamma = \bar{S} + \sum_{\mathbf{k}} N_{\mathbf{k}} \cos k_x, \quad \gamma' = \bar{S} + \sum_{\mathbf{k}} N_{\mathbf{k}} \cos k_z, \quad (13)$$

which should be solved together with the condition

$$\bar{S} = S + (2S+1)N(E_f) - \sum_{\mathbf{k}} N_{\mathbf{k}}, \quad (14)$$

where  $N_{\mathbf{k}}=N(E_{\mathbf{k}})$  are the Bose occupation numbers,

$$E_f=(2S+1)(\Gamma_0-\mu), \quad (15)$$

$$E_{\mathbf{k}}=\Gamma_0-\Gamma_{\mathbf{k}}-\mu,$$

are the pseudofermion excitation energy, and the spin-wave spectrum, respectively,

$$\Gamma_{\mathbf{k}}=2[|J|\gamma(\cos k_x+\cos k_y)+|J'|\gamma'\cos k_z]. \quad (16)$$

Consider now the case of an antiferromagnet (AFM). Introducing the operators

$$B_i=\begin{cases} a_i & i \in A \\ b_i^\dagger & i \in B, \end{cases} \quad C_i=\begin{cases} c_i & i \in A \\ d_i & i \in B, \end{cases} \quad (17)$$

we derive

$$\begin{aligned} H_{\text{AF}}= & |J|\gamma \sum_{i,\delta_\perp} [B_i^\dagger B_i - B_{i+\delta}^\dagger B_i + (2S+1)C_i^\dagger C_i] \\ & + |J'|\gamma' \sum_{i,\delta_\parallel} [B_i^\dagger B_i - B_{i+\delta}^\dagger B_i + (2S+1)C_i^\dagger C_i] \\ & - \mu \sum_i [B_i^\dagger B_i + (2S+1)C_i^\dagger C_i], \end{aligned} \quad (18)$$

where

$$\gamma=\bar{S}+\langle a_i b_{i+\delta_\perp} \rangle, \quad \gamma'=\bar{S}+\langle a_i b_{i+\delta_\parallel} \rangle. \quad (19)$$

Diagonalizing this Hamiltonian one finds the self-consistent equations

$$\gamma=\bar{S}+\sum_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}}{2E_{\mathbf{k}}} \cos k_x \coth \frac{E_{\mathbf{k}}}{2T}, \quad (20)$$

$$\gamma'=\bar{S}+\sum_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}}{2E_{\mathbf{k}}} \cos k_z \coth \frac{E_{\mathbf{k}}}{2T},$$

$$\bar{S}=(S+1/2) \coth \frac{E_f}{2T} - \sum_{\mathbf{k}} \frac{\Gamma_0-\mu}{2E_{\mathbf{k}}} \coth \frac{E_{\mathbf{k}}}{2T},$$

where the antiferromagnetic spin-wave spectrum has the form

$$E_{\mathbf{k}}=\sqrt{(\Gamma_0-\mu)^2-\Gamma_{\mathbf{k}}^2} \quad (21)$$

with  $\Gamma_{\mathbf{k}}$  and  $E_f$  being the same as in the ferromagnetic case.

For both ferro- and antiferromagnetic cases, the calculation of spin-correlation functions<sup>10</sup> shows that  $\mu$  is directly connected with the correlation length  $\xi_\delta$  in the direction  $\delta$  by the relation

$$\xi_\delta^{-1}=\sqrt{-\mu/|J_\delta \gamma_\delta|}. \quad (22)$$

The parameters  $\gamma$  and  $\gamma'$  are also simply related to the spin-correlation function at the nearest-neighbor sites

$$|\langle \mathbf{S}_i \mathbf{S}_{i+\delta} \rangle|=\gamma_\delta^2, \quad (23)$$

and, therefore, play the role of SRO parameters. For the total energy we readily obtain

$$\mathcal{E}=-\frac{1}{2} \sum_{\delta} |J_{i,i+\delta}| \gamma_\delta^2 = -(2|J|\gamma^2 + |J'|\gamma'^2). \quad (24)$$

In the classical limit  $S \rightarrow \infty$  the SSWT equations are simplified. Supposing  $T \gg |J|S$  ( $T_M \sim |J|S^2$  in this case) the equations for both FM and AFM cases reduce to

$$\bar{S}/S = \coth(E_f/2T) - \frac{T}{S} \sum_{\mathbf{k}} \frac{1}{\Gamma_0 - \Gamma_{\mathbf{k}} - \mu},$$

$$\gamma = \bar{S} + T \sum_{\mathbf{k}} \frac{\cos k_x}{\Gamma_0 - \Gamma_{\mathbf{k}} - \mu},$$

$$\gamma' = \bar{S} + T \sum_{\mathbf{k}} \frac{\cos k_z}{\Gamma_0 - \Gamma_{\mathbf{k}} - \mu}. \quad (25)$$

For  $T < T_M$  ( $\mu=0$ ) the averaged (over nearest neighbors) SRO parameter

$$\gamma_{\text{ef}}(T) = (4J\gamma + 2J'\gamma')/J_0 \quad (26)$$

(but not the magnetization) satisfies the standard mean-field equation

$$\gamma_{\text{ef}}/S = B_\infty(J_0 \gamma_{\text{ef}} S/T), \quad (27)$$

where  $B_\infty(x) = \coth x - 1/x$  is the classical Brillouin function (Langevin function). The temperature  $T^*$  where  $\gamma_{\text{ef}}(T^*) = 0$  is higher than  $T_M$ , so that we have  $\gamma_{\text{ef}}(T_M) > 0$  and the behavior of  $\gamma_{\text{ef}}$  for  $T > T_M$  is more complicated in comparison with Eq. (27).

## B. Approximation of effective SRO parameter

Equations (13), (14), and (20) still demonstrate unphysical behavior of magnetization for  $T$  close to  $T_M$  at small enough  $J'/J$  (see below). Introducing the pseudofermion field does not improve the situation in this case: the transition temperature is already too small to be influenced by pseudofermion excitations with the energy of the order of  $|J|$ . As discussed in the Introduction, the dynamical spin-wave interaction should be treated more correctly in such a situation. A rough solution of this problem can be achieved by the replacement

$$\sum_{\delta} J_{i,i+\delta} \gamma_\delta (b_i^\dagger b_i - b_{i+\delta}^\dagger b_{i+\delta}) \rightarrow \gamma_{\text{ef}} \sum_{\delta} J_{i,i+\delta} (b_i^\dagger b_i - b_{i+\delta}^\dagger b_{i+\delta}), \quad (28)$$

where  $\gamma_{\text{ef}}$  is determined by Eq. (26). Then we obtain the spectrum

$$E_{\mathbf{q}} = \gamma_{\text{ef}}(J_0 - J_{\mathbf{q}}) - \mu, \quad \text{FM},$$

$$E_{\mathbf{q}} = \sqrt{(J_0 \gamma_{\text{ef}} - \mu)^2 - (J_{\mathbf{q}} \gamma_{\text{ef}})^2}, \quad \text{AFM}, \quad (29)$$

and the pseudofermion excitation energy

$$E_f = (2S+1)(\gamma_{\text{ef}} J_0 - \mu), \quad (30)$$

[here and hereafter we use the definition  $J_{\mathbf{q}} = \sum_{\delta} |J_\delta| \exp(i\mathbf{q}\cdot\boldsymbol{\delta})$ ]. The SSWT equations take the form

$$\bar{S} = S + (2S + 1)N(E_f) - \sum_{\mathbf{k}} N_{\mathbf{k}}, \quad (31)$$

$$\gamma_{\text{ef}} = \bar{S} + \frac{1}{J_0} \sum_{\mathbf{k}} J_{\mathbf{k}} N_{\mathbf{k}},$$

in the FM case and

$$\bar{S} = (S + 1/2) \coth \frac{E_f}{2T} - \gamma_{\text{ef}} \sum_{\mathbf{k}} \frac{J_0}{2E_{\mathbf{k}}} \coth \frac{E_{\mathbf{k}}}{2T}, \quad (32)$$

$$\gamma_{\text{ef}} = \bar{S} + \frac{\gamma_{\text{ef}}}{J_0} \sum_{\mathbf{k}} \frac{J_{\mathbf{k}}^2}{2E_{\mathbf{k}}} \coth \frac{E_{\mathbf{k}}}{2T},$$

in the AFM case. The approximation (28) is analogous to passing from the Hartree-Fock approximation to the local approximation in the spin-density-functional method for the electron gas. As it is known, taking into account screening effects, such approximations can lead to improving the results and eliminating the unphysical peculiarities. Note that the same equations (31) and (32) were obtained earlier in Ref. 31. However, when deriving these equations, the authors have used expressions for the spin Green's function which have incorrect  $\omega \rightarrow \infty$  asymptotics.

Another approach, which gives the possibility of improving the behavior of (sublattice) magnetization near  $T_M$ , is based on a variational principle and is considered in Appendix A. It leads to the same spin-wave spectrum (29), but the corresponding SSWT equations are somewhat different from Eqs. (31) and (32). However, numerical calculations show that this difference is very small (several percents of magnetization value), and further we will refer to both these approaches as the approximation of the effective SRO parameter.

### C. Temperature dependences of long- and short-range order parameters

In the two-dimensional case  $J' = 0$  the spectrum  $E_{\mathbf{k}}$  is independent of  $\gamma'$ , and two remaining equations for  $\bar{S}$  and  $\gamma$  differ from those of the approaches of Refs. 8 and 13 only by the presence of pseudofermion distribution function  $N(E_f)$ , which describes the kinematical interaction of spin waves. At  $T = 0$  we have  $\mu = 0$ , and  $\gamma = \bar{S} = S$  in the FM case and  $\gamma > S$ ,  $\bar{S} < S$  in the AFM case, which corresponds to magnetic ordering in the ground state. As well as in Refs. 8 and 13, Eqs. (13), (14), and (20) do not have at  $T > 0$  solutions with  $\mu = 0$ ,  $\bar{S} > 0$  since the integrals in Eqs. (13), (14), and (20) are logarithmically divergent in this case, and the only solution of these equations for  $J' = 0$  is  $\bar{S} = 0$ ,  $\mu < 0$ , which corresponds to a disordered phase.

At low temperatures  $T \ll |J|S^2$ , we can neglect the pseudofermion contribution (i.e., kinematical interaction of spin waves) and we completely reproduce the results of Refs. 8–10, 13. In particular, the correlation length has the exponential dependence

$$\xi = C_{\xi}^{\text{F}} \sqrt{J/T} \exp(2\pi JS^2/T) \quad (\text{FM}), \quad (33a)$$

$$\xi = C_{\xi}^{\text{AF}} (J/T) \exp(2\pi |J| \gamma_0 \bar{S}_0 / T) \quad (\text{AFM}), \quad (33b)$$

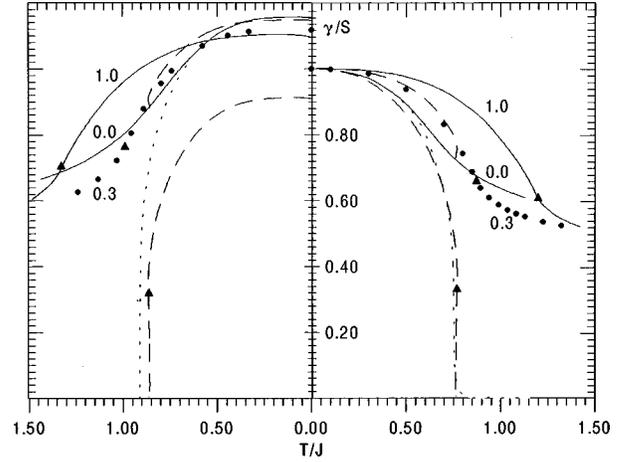


FIG. 1. Calculated temperature dependences of SRO parameters in  $S = 1/2$  quasi-2D ferro- (right-hand side) and antiferromagnets (left-hand side). The values of  $J'/J$  stand at the curves. Dots correspond to the 2D case ( $J'/J = 0$ ) without including the pseudofermion contribution, long-dashed lines and circles correspond to calculations from Eqs. (13), (14), (20) and (29), (32), respectively, for  $J'/J = 0.3$ . Triangles mark the ordering temperatures.

where

$$\bar{S}_0 = S - 0.1971, \quad \gamma_0 = S + 0.079 \quad (34)$$

are the 2D ground-state LRO and SRO parameters, and  $C_{\xi}^{\text{F,AF}}$  are  $S$ -dependent constants. The results (33) were obtained earlier within the one-loop RG approach.<sup>11,12</sup> The two-loop RG analysis changes the preexponential factor only: in the AFM case it becomes a temperature-independent constant<sup>11</sup> while in the FM case the factor is proportional to  $(T/J)^{1/2}$  (see Ref. 12).

With increasing  $T$  the role of the kinematical interaction increases and for  $T \sim JS^2$  we cannot neglect  $N(E_f)$ . The dependence  $\gamma(T)$  for  $J' = 0$  is shown and compared with the result of approaches<sup>9,10</sup> in Fig. 1. Unlike the approaches in Refs. 9, 10, Eqs. (13), (14), and (20) do not lead to the non-physical phase transition with vanishing of the SRO parameter, and the latter is finite at any temperatures. Note that for  $J' = 0$  Eqs. (29) and (32) give the same results.

In the presence of interlayer coupling, the integrals in the SSWT equations (13), (14), and (20) becomes convergent at finite  $T$  even at  $\mu = 0$ . For not too high temperatures  $T < T_M$  (the ordering temperature  $T_M$  will be calculated below) these equations have the solution with  $\bar{S} > 0$ , which corresponds to the ordered magnetic phase. For  $T > T_M$  we again have  $\bar{S} = 0$  and  $\mu < 0$  as well as in the 2D case at finite  $T$ .

Figures 1–4 show the results of the numerical solution of the equations of Secs. III A, III B for different values of the interlayer coupling. In the three-dimensional case ( $J' = J$ ) the (staggered) magnetization vanishes at  $T_C = 1.20J$  ( $T_N = 1.33|J|$ ) that is approximately by 20% higher than the corresponding value obtained from the high-temperature series expansion. At the same time, the ratio  $T_N/T_C = 1.20$  is in agreement with the results of this expansion. The SRO parameter  $\gamma$  demonstrates a sharp decrease in a narrow temperature region above  $T_M$  and then asymptotically goes to zero. One can see that  $\gamma_{\text{AFM}} > \gamma_{\text{FM}}$  due to the quantum fluc-

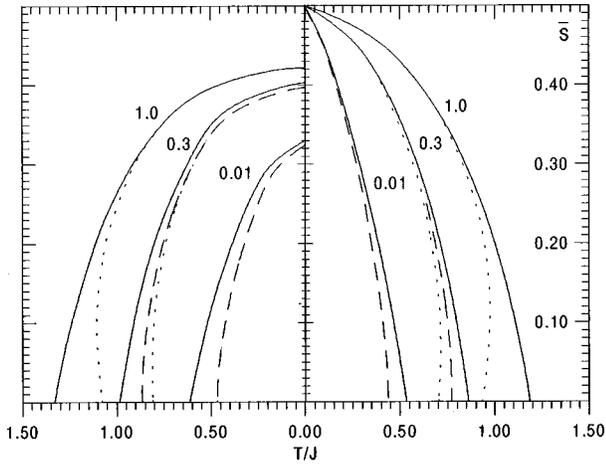


FIG. 2. Temperature dependence of the (staggered) magnetization  $\bar{S}$  for  $S=1/2$  quasi-2D ferro- (right-hand side) and antiferromagnets (left-hand side) with different values of  $J'/J$ . Short-dashed lines show the results without inclusion of pseudofermions, long-dashed lines in the presence of pseudofermions, and solid lines correspond to the approximation of the effective SRO parameter of Sec. III B. For  $J'/J=1$  the solid and long-dashed lines coincide exactly, and for  $J'/J=0.01$  long- and short-dashed lines coincide practically.

tuations. At the transition point we have  $\gamma_c \equiv \gamma(T_M) = 0.62$  for FM case and  $\gamma_c = 0.70$  for AFM case. The dependences  $\gamma(T)/S$  for 3D ferromagnets with different  $S$  are shown in Fig. 3. One can see that the value  $\gamma_c/S$  rapidly decreases with increasing  $S$ , reaching  $\gamma_c = 0.39$  at  $S \rightarrow \infty$ . Thus at  $S = 1/2$  strong quantum fluctuations are present even at  $T = T_M$ .

Consider now the quasi-2D case  $0 < J'/J < 1$ . At  $J'/J < 0.4$  Eqs. (13), (14), and (20) still yield unphysical behavior of magnetization and SRO parameters for  $T$  close to  $T_M$  (as shown in Figs. 1 and 2 for  $J'/J = 0.3$ ). At the same time, the approximation of single effective SRO parameter improves the behavior of magnetization for  $T$  close to  $T_M$  and provides a qualitatively correct description of thermodynamics at arbitrary temperatures. The price which we pay is an overesti-

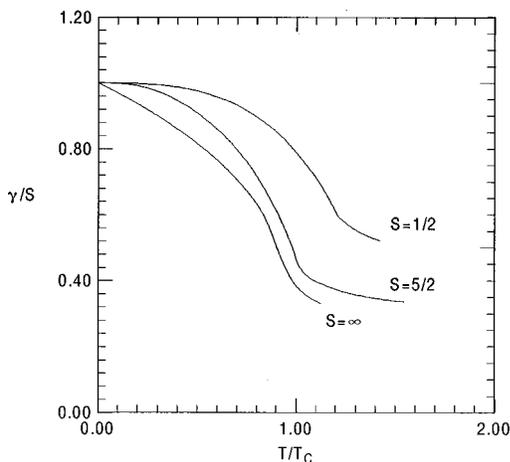


FIG. 3. Temperature dependence of the SRO parameters of quasi-2D ferromagnets for different spin values in the approximation of effective SRO parameter.

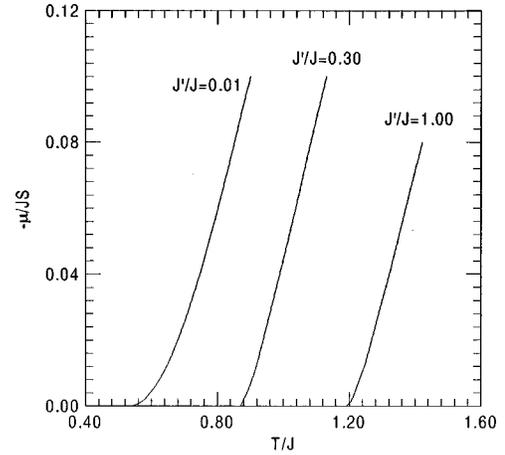


FIG. 4. Temperature dependence of the chemical potential of the boson-pseudofermion systems in quasi-2D ferromagnets in the approximation of effective SRO parameter.

mation of  $T_M$  even in comparison with the results of Eqs. (13), (14), and (20), since the temperature dependence of the ratio of effective inter- and intralayer couplings [which is  $J'/J$  for spectrum (29)] is absent in the approximation used. In particular, for  $J'/J \rightarrow 0$  the results obtained within approximation (28) are different from those of standard spin-wave theory only by quantum (ground-state) renormalization of  $\gamma$ . Note that according to Fig. 1 with decreasing  $J'/J$  the size of the region with noticeable SRO increases.

At small  $T - T_M$  we have  $-\mu \propto (T - T_M)^2$  (see Fig. 4 for a ferromagnetic case, the same situation takes place in the AFM case) so that, according to Eq. (22), the critical exponent for the correlation length is  $\nu = 1$ . Since the magnetization changes linearly near  $T_M$ , we have also  $\beta = 1$ . The influence of higher-order terms in  $1/S$  on these results is discussed in Sec. VI. Note that if we determine, following Ref. 32, the critical exponent  $\nu$  from a not too narrow temperature interval near  $T_M$ , this becomes closer to the experimental value.

At very low temperatures ( $T \ll |J'|S$ ) and arbitrary  $J'/J$  the calculation can be performed analytically. The corrections to magnetization of a ferromagnet are proportional to  $T^{3/2}$

$$\bar{S} = S - \frac{1}{8\pi^{3/2}} \sqrt{\frac{J}{J'}} \left( \frac{T}{JS} \right)^{3/2} \zeta(3/2), \quad (35)$$

where  $\zeta(3/2)$  is the Riemann zeta function. At the same time, SRO parameters have a more weak  $T^{5/2}$  dependence

$$\gamma = S - \frac{3}{32\pi^{3/2}} \sqrt{\frac{J}{J'}} \left( \frac{T}{JS} \right)^{5/2} \zeta(5/2), \quad (36)$$

$$\gamma' = S - \frac{3}{32\pi^{3/2}} \left( \frac{J}{J'} \right)^{3/2} \left( \frac{T}{JS} \right)^{5/2} \zeta(5/2). \quad (37)$$

For  $J' = J$  this result corresponds to that of the Dyson theory<sup>33</sup> to leading order in  $1/S$ . For an antiferromagnet we have

$$\bar{S} = \bar{S}_0 - \frac{T^2}{24c\sqrt{JJ'\gamma_0\gamma'_0}}, \quad (38)$$

where  $\gamma_0, \gamma'_0$  and  $\bar{S}_0$  are the zero-temperature values of corresponding parameters,  $c = \sqrt{4J\gamma_0(2J\gamma_0 + J'\gamma'_0)}$  is the spin-wave velocity. The corresponding temperature dependences of  $\gamma$  and  $\gamma'$  are given by

$$\gamma = \gamma_0 - \frac{\pi^2 T^4}{120c^3\sqrt{JJ'\gamma_0\gamma'_0}}, \quad (39)$$

$$\gamma' = \gamma'_0 - \frac{\pi^2 T^4}{120c^3} \sqrt{\frac{J\gamma_0}{(J'\gamma'_0)^3}}. \quad (40)$$

In the case of small interlayer couplings  $J'/J \ll 1$  and higher temperatures, logarithmic singularities occur, and we can pick out them from the integrals in Eqs. (13), (14), and (20) in the same way as discussed in Ref. 14. In the quantum regime which takes place at not too low temperatures, where

$$\begin{aligned} J'S \ll T \ll JS & \quad (\text{FM}), \\ (JJ')^{1/2}S \ll T \ll |J|S & \quad (\text{AFM}), \end{aligned} \quad (41)$$

we obtain

$$\bar{S} = S - \frac{T}{4\pi JS} \ln \frac{T}{J'S} \quad (\text{FM}), \quad (42a)$$

$$\bar{S} = \bar{S}_0 - \frac{T}{4\pi|J|\gamma} \ln \frac{T^2}{8JJ'\gamma\gamma'} \quad (\text{AFM}), \quad (42b)$$

with  $\gamma \approx \gamma_0$  [the 2D values (34) can be used for  $\gamma_0$  and  $\bar{S}_0$ ] and  $\gamma'$  being defined by the equation

$$\gamma' = S - \frac{T}{4\pi JS} \left( \ln \frac{T}{J'\gamma'} - 1 \right) \quad (\text{FM}), \quad (43a)$$

$$\gamma' = \bar{S}_0 - \frac{T}{4\pi|J|\gamma} \left( \ln \frac{T^2}{8JJ'\gamma\gamma'} - 1 \right) \quad (\text{AFM}) \quad (43b)$$

so that  $\gamma'_0 = \bar{S}_0$ . Note that in this case the infrared cutoff for the integrals over quasimomenta is

$$q_0 = \begin{cases} (T/JS)^{1/2} & (\text{FM}) \\ T/c & (\text{AFM}) \end{cases} \quad (44)$$

( $c = \sqrt{8|J|\gamma}$ ) rather than the boundary of the Brillouin zone. Since  $q_0 \ll 1$ , the continuum approximation for the excitation spectrum (and also interaction vertex) can be used in the quantum regime. Owing to the thermodynamic identity  $(\partial\bar{S}/\partial T)_S = (\partial\mathcal{S}/\partial h)_T$  (with  $\mathcal{S}$  being the entropy,  $h$  being the magnetic field) the presence of  $T \ln T$  terms in the magnetization of a ferromagnet may be of interest in connection with the adiabatic cooling (see, e.g., Ref. 34).

For the critical temperatures in the regime (41) we obtain from Eqs. (42) the results

$$T_C = \frac{4\pi JS^2}{\ln(T/J'\gamma'_c)}, \quad (45)$$

$$T_N = \frac{4\pi|J|\gamma_c\bar{S}_0}{\ln(T^2/8JJ'\gamma_c\gamma'_c)}$$

with  $\gamma_c = \gamma(T_M) \approx \gamma_0$  and  $\gamma'_c = \gamma'(T_M) = T_M/4\pi|J|\gamma$ . Comparing these results with the criteria of quantum regime (41) we obtain the condition of applicability of the results (45) as  $2\pi S \ll \ln(J/J')$ . It is important that  $\gamma'_c \ll \gamma'$  and the interlayer coupling is strongly renormalized with the temperature. At the same time, only ground-state (quantum) renormalizations are important for the intralayer coupling at  $|J'| \ll |J|$ .

In the case of large  $S$  (again supposing  $T \gg |J|S$ ) we obtain for both ferro- and antiferromagnet

$$\bar{S} = S - \frac{T}{4\pi|J|S} \ln \frac{32JS}{J'\gamma'} \quad (46)$$

with

$$\gamma' = S - \frac{T}{4\pi|J|S} \left( \ln \frac{32JS}{J'\gamma'} - 1 \right), \quad (47)$$

This leads to the expression for the critical temperature of a classical magnet with  $1 \ll \ln(J/J') \ll 2\pi S$

$$T_M = \frac{4\pi|J|S^2}{\ln(32JS/J'\gamma'_c)}, \quad (48)$$

where  $\gamma'_c = T_M/4\pi|J|S$ . As it should be, the critical temperature is the same for the classical ferro- and antiferromagnetic case. With the logarithmic accuracy we reproduce in this case the well-known results where  $\gamma'_c/S \rightarrow 1$  (see, e.g., Ref. 35). Note that the factor of 32 which is often neglected leads to significant lowering of  $T_M$  as well as above-considered temperature dependence of  $\gamma'$ .

#### D. Mean-field Schwinger-boson approach

Similar results can be obtained within the Schwinger-boson representation. This is performed in the same way as in Refs. 8, 9 and 13. The Heisenberg Hamiltonian is written down in the form

$$\begin{aligned} H = -\frac{1}{2} \sum_{ij} J_{ij} & \left[ \frac{1}{4} (s_{i\uparrow}^\dagger s_{i\uparrow} - s_{i\downarrow}^\dagger s_{i\downarrow}) (s_{j\uparrow}^\dagger s_{j\uparrow} - s_{j\downarrow}^\dagger s_{j\downarrow}) \right. \\ & \left. + s_{i\uparrow}^\dagger s_{i\downarrow} s_{j\downarrow}^\dagger s_{j\uparrow} \right] - \mu \sum_i (s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow}), \end{aligned} \quad (49)$$

where the chemical potential of bosons is introduced to take into account the constraint (8).

In the ferromagnetic case we subtract from the Hamiltonian (49) the term

$$H_c = \frac{1}{8} \sum_{ij} J_{ij} (s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow}) (s_{j\uparrow}^\dagger s_{j\uparrow} + s_{j\downarrow}^\dagger s_{j\downarrow}) \equiv \frac{J_0 S^2}{2} \quad (50)$$

to obtain

$$\tilde{H} = -\frac{1}{4} \sum_{\langle ij \rangle} J_{ij} : \mathcal{F}_{ij}^\dagger \mathcal{F}_{ij} : - \mu \sum_i (s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow}), \quad (51)$$

where  $\tilde{H} = H - H_c$ ,  $\mathcal{F}_{ij} = \sum_\sigma s_{i\sigma}^\dagger s_{j\sigma}$ , and  $: \dots :$  stands for the normal ordering. Further the tilde at the Hamiltonian  $H$  will be dropped. Introducing the averages of the Bose operators

$$\gamma_{ij} = \langle \mathcal{F}_{ij} \rangle = \langle \mathcal{F}_{ij}^\dagger \rangle, \quad (52)$$

we derive the mean-field Hamiltonian

$$H_{\text{MF}} = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \gamma_{ij} \mathcal{F}_{ij} - \mu \sum_i (s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow}). \quad (53)$$

Such a procedure can be justified if we generalize the Schwinger-boson representation to the  $SU(N)$  model with arbitrary  $N$  by introducing the operators  $s_{im}^\dagger$  ( $m = 1 \dots N$ ) and consider the limit  $N \rightarrow \infty$ .<sup>8</sup>

In the quasi-2D case there are only two independent values of  $\gamma_{ij}$ :

$$\gamma_{ij} = \begin{cases} \gamma & i, j \text{ within the same plane,} \\ \gamma' & \text{otherwise.} \end{cases} \quad (54)$$

Introducing  $\lambda = -\mu - \gamma J_0$  and passing to quasimomentum representation we obtain

$$H_{\text{MF}} = \sum_{\mathbf{q}\sigma} E_{\mathbf{q}} s_{\mathbf{q}\sigma}^\dagger s_{\mathbf{q}\sigma}, \quad (55)$$

where  $E_{\mathbf{q}} = \lambda - \Gamma_{\mathbf{q}}$ . Note that in the absence of external magnetic field the spectrum of bosons is doubly degenerate. The self-consistent equations have the form

$$\gamma = \sum_{\mathbf{k}\sigma} N_{\mathbf{k}\sigma} \cos k_x, \quad \gamma' = \sum_{\mathbf{k}\sigma} N_{\mathbf{k}\sigma} \cos k_z,$$

$$2S = \sum_{\mathbf{k}\sigma} N_{\mathbf{k}\sigma}. \quad (56)$$

As well as in Refs. 9 and 13, at low enough temperatures the Bose condensation takes place. Introducing external magnetic field (see Sec. V) removes the degeneracy of the boson spectrum, and only one of two bosons is condensed. Let  $N_{\mathbf{k}\uparrow}$  (but not  $N_{\mathbf{k}\downarrow}$ ) contain the condensate contribution at  $k \rightarrow 0$ :

$$N_{\mathbf{k}\uparrow} \rightarrow N_{\mathbf{k}} + 2n_B \delta_{\mathbf{k}0}, \quad (57)$$

where  $2n_B$  is the density of condensed bosons. Thus the self-consistent equations takes the same form as in the BKJ representation with  $\bar{S} \rightarrow n_B$ ,  $N(E_f) = 0$ .

In the antiferromagnetic case we subtract the term (50) from the Hamiltonian to obtain (cf. Refs. 8, 14, and 15)

$$\tilde{H} = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} : \mathcal{A}_{ij}^\dagger \mathcal{A}_{ij} : - \mu \sum_i (s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow}), \quad (58)$$

where  $\mathcal{A}_{ij} = s_{i\uparrow}^\dagger s_{j\downarrow}^\dagger$ . Passing to the mean-field approximation we have

$$H_{\text{MF}} = -\frac{1}{2} \sum_{\langle ij \rangle} \gamma_{ij} J_{ij} (\mathcal{A}_{ij} + \mathcal{A}_{ij}^\dagger) - \mu \sum_i (s_{i\uparrow}^\dagger s_{i\uparrow} + s_{i\downarrow}^\dagger s_{i\downarrow}), \quad (59)$$

where

$$\gamma_{ij} = \gamma_{ij} = \langle \mathcal{A}_{ij} \rangle = \langle \mathcal{A}_{ij}^\dagger \rangle. \quad (60)$$

Diagonalizing the Hamiltonian obtained one obtains

$$H_{\text{MF}} = \sum_{\mathbf{q}} E_{\mathbf{q}} (\alpha_{\mathbf{q}}^\dagger \alpha_{\mathbf{q}} + \beta_{\mathbf{q}}^\dagger \beta_{\mathbf{q}}), \quad (61)$$

where  $E_{\mathbf{q}} = (\lambda^2 - \Gamma_{\mathbf{q}}^2)^{1/2}$ . Thus the self-consistent equations take the form<sup>14,15</sup>

$$\gamma = \sum_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}}{2E_{\mathbf{k}}} \cos k_x (N_{\mathbf{k}\uparrow} + N_{\mathbf{k}\downarrow} + 1), \quad (62a)$$

$$\gamma' = \sum_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}}{2E_{\mathbf{k}}} \cos k_z (N_{\mathbf{k}\uparrow} + N_{\mathbf{k}\downarrow} + 1), \quad (62b)$$

$$2S = \sum_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}}{E_{\mathbf{k}}} (N_{\mathbf{k}\uparrow} + N_{\mathbf{k}\downarrow} + 1) - 1. \quad (62c)$$

As well as in the ferromagnetic case, only  $N_{\mathbf{k}\uparrow}$  contains the condensate contribution. Picking this out as

$$N_{\mathbf{k}\uparrow}/E_{\mathbf{k}\uparrow} \rightarrow N_{\mathbf{k}}/E_{\mathbf{k}} + n_B (\delta_{\mathbf{k}0} + \delta_{\mathbf{k}\mathbf{Q}}) \quad (63)$$

[ $\mathbf{Q} = (\pi, \pi, \pi)$  is the wave vector of the antiferromagnetic structure] we get the SSWT equations (32) with  $\coth(E_f/T) = 1$ ,  $\bar{S} \rightarrow n_B$ .

The corrections to above results can be obtained within the  $1/N$  expansion in a generalized Heisenberg  $SU(N)$  model (see, e.g., Refs. 8, 36–39). As argued in the introduction (see also Sec. VI), the same results can be more easily obtained by higher-order  $1/S$  expansion. Thus the BKJ approach turns out to be more practical than the Schwinger-boson one.

#### IV. SSWT OF THE EASY-AXIS 2D MAGNETS

Consider now the 2D magnets with the easy-axis anisotropy. Besides the spin-wave excitations, the topological excitations (domain walls) contribute to thermodynamic quantities (see, e.g., discussion in Ref. 40). Such excitations cannot be taken into account in the approach under consideration. However, in the limit of small anisotropy

$$D/|J| \ll 1, \eta \ll 1, \quad (64)$$

one can expect that the non-spin-wave excitations are important only in a narrow critical region. Outside this region thermodynamics can be described in terms of spin waves. Thus we restrict ourselves to the case where Eq. (64) is satisfied.

Consider first the ferromagnetic case. Decoupling four-fold terms in the Hamiltonian we obtain

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + E_f \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}, \quad (65)$$

where

$$E_{\mathbf{k}} = \lambda - \Gamma_{\mathbf{k}}, \quad E_f = (2S + 1)\lambda, \quad (66)$$

$$\lambda = J_0 (\gamma + \eta \bar{S}) + D [(2S - 1) - 4 \langle b_i^\dagger b_i \rangle] - \mu,$$

$$\Gamma_{\mathbf{k}} = J_{\mathbf{k}}[\gamma + \eta \langle b_i^\dagger b_{i+\delta} \rangle],$$

and

$$\gamma = \bar{S} + \langle b_i^\dagger b_{i+\delta} \rangle. \quad (67)$$

It should be noted that the expression for the excitation spectrum (66) is in fact the first-order  $1/S$  expansion result. In particular, the spectrum (66) violates the requirement of vanishing of the single-site anisotropy at  $S = 1/2$  (this situation is discussed in Ref. 7). To correct this inconsistency we perform two replacements in the spectrum (66), which can be justified by calculating higher-order terms in  $1/S$ :

$$(2S-1) - 4 \langle b_i^\dagger b_i \rangle \rightarrow (2S-1)[1 - 2 \langle b_i^\dagger b_i \rangle / S] \rightarrow (2S-1) \times (\bar{S}/S)^2, \quad (68)$$

$$\bar{S} - \langle b_i^\dagger b_{i+\delta} \rangle \rightarrow S[1 - 2 \langle b_i^\dagger b_i \rangle / S][1 + \langle b_i^\dagger b_i \rangle / S - \langle b_i^\dagger b_{i+\delta} \rangle / S] \rightarrow \bar{S}^2 / \gamma.$$

Then the boson spectrum takes the form

$$E_{\mathbf{k}} = \gamma(J_0 - J_{\mathbf{k}}) + JS\Delta - \mu, \quad (69)$$

where

$$\Delta(T) = [(2S-1)D/|JS| + (J_0S/J\gamma)\eta](\bar{S}/S)^2 \quad (70)$$

is the dimensionless energy gap renormalized by spin-wave interactions. The system of the self-consistent equations reads

$$\gamma = \bar{S} + \frac{1}{J_0} \sum_{\mathbf{k}} J_{\mathbf{k}} N_{\mathbf{k}}, \quad (71)$$

$$\bar{S} = S - \sum_{\mathbf{k}} N_{\mathbf{k}} + (2S+1)N(E_f).$$

In the antiferromagnetic case we obtain

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}}(\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}) + E_f \sum_{\mathbf{k}} (c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}}) \quad (72)$$

with the spectrum

$$E_{\mathbf{k}} = \sqrt{\lambda^2 - \Gamma_{\mathbf{k}}^2}, \quad E_f = (2S+1)\lambda, \quad (73)$$

$$\lambda = \gamma J_0 + |JS|\Delta - \mu, \quad \Gamma_{\mathbf{k}} = \gamma J_{\mathbf{k}},$$

and  $\Delta$  is the same as in Eq. (70). The system of the self-consistent equations takes the form

$$\gamma = \bar{S} + \sum_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}}{2E_{\mathbf{k}}} \cos k_x \coth \frac{E_{\mathbf{k}}}{2T}, \quad (74)$$

$$\bar{S} = \left(S + \frac{1}{2}\right) \coth \frac{E_f}{2T} - \sum_{\mathbf{k}} \frac{\lambda}{2E_{\mathbf{k}}} \coth \frac{E_{\mathbf{k}}}{2T}. \quad (75)$$

Note that the proportionality of the gap in the spin-wave spectrum to the squared sublattice magnetization was obtained earlier within the renormalized spin-wave theory,<sup>7,41</sup> which takes into account the influence of spin-wave interac-

tions on the spectrum in a non-self-consistent way, and it is in agreement with the experimental data.<sup>42</sup>

Using the smallness of the anisotropy and picking out the logarithmic singularities in the same way as in Sec. III C we obtain

$$\bar{S} = S - \frac{T}{4\pi JS} \ln \frac{T}{JS\Delta}, \quad (\text{FM}), \quad (76)$$

$$\bar{S} = \bar{S}_0 - \frac{T}{4\pi|J|\gamma} \ln \frac{T^2}{8(J\gamma)^2\Delta}, \quad (\text{AFM}).$$

Unlike the quasi-2D case, we have the unphysical result  $\Delta(T_M) = 0$  because of the proportionality of the gap to  $(\bar{S}/S)^2$  (in fact a finite value of the gap at  $T = T_M$  should be caused by topological effects which are not taken into account). Thus we are unable to describe the dependence  $\Delta(T)$  close to  $T_M$ . Denoting  $\Delta_c = \Delta(T_M)$  we have for the critical temperature at  $2\pi S \ll \ln(1/\Delta)$

$$T_C = \frac{4\pi JS^2}{\ln(T/JS\Delta_c)}, \quad (77)$$

$$T_N = \frac{4\pi|J|\bar{S}_0\gamma_c}{\ln[T^2/8(J\gamma_c)^2\Delta_c]}.$$

In the case of large  $S$  we obtain for both ferro- and antiferromagnets

$$\bar{S} = S - \frac{T}{4\pi|J|S} \ln \frac{32}{\Delta}. \quad (78)$$

This leads to the expression for the critical temperature of a classical magnet with  $1 \ll \ln(1/\Delta) \ll 2\pi S$

$$T_M = \frac{4\pi|J|S^2}{\ln(32/\Delta_c)}. \quad (79)$$

To leading logarithmic accuracy we can set  $\Delta_c = \Delta(0)$  in the above results. A more correct calculation of  $\Delta_c$ , as well as the corrections to the results (77) and (79) will be obtained in Sec. VI. Note also that in the approximation  $\Delta(T) = \Delta(0)$ , i.e., at neglecting the temperature dependence of the gap, we reproduce correctly the mean-field result in the Ising limit

$$\bar{S} = SB_S(J_0S\bar{S}/T), \quad (80)$$

where  $B_S(x)$  is the spin- $S$  Brillouin function.

## V. INFLUENCE OF THE EXTERNAL MAGNETIC FIELD AND THE MAGNETIC SUSCEPTIBILITY

In this section we consider the influence of a weak external magnetic field  $h$  in a ferromagnet. This is described by the additional term in the Hamiltonian

$$H_h = -h \sum_i S_i^z. \quad (81)$$

The magnetic field results in an increase of magnetization, so that the total magnetization can be represented as

$$\bar{S} = \bar{S}_{\text{sp}} + \bar{S}_{\text{ind}}, \quad (82)$$

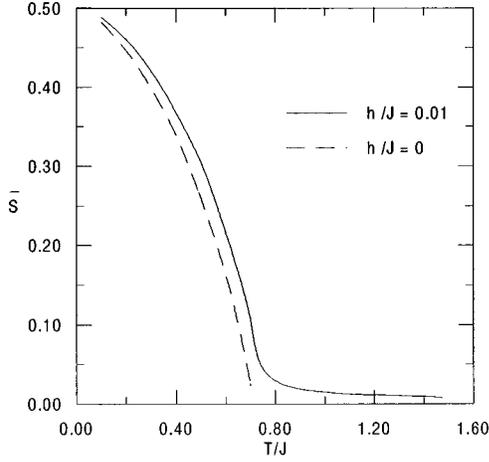


FIG. 5. Temperature dependence of the magnetization  $\bar{S}$  for a  $S=1/2$  quasi-2D ferromagnet with  $J'/J=0.1$  in the external magnetic field.

where  $\bar{S}_{\text{sp}} = \bar{S}(h=0)$  is the spontaneous magnetization,  $\bar{S}_{\text{ind}}$  is the field-induced part. Owing to the second term in Eq. (82) the temperature dependence  $\bar{S}(T)$  is changed: sharply decreasing in the vicinity of  $T_M$ ,  $\bar{S}$  nevertheless vanishes only in the limit  $T \rightarrow \infty$ . We consider a possible approach to the description of such a behavior in both versions of SSWT that are based on the Dyson-Maleev representation (or its generalization with the use of the BKJ representation) and Schwinger-boson representation.

First we use the BKJ representation. The calculations, which are similar to those described above, result in Eqs. (13) and (14) with the spectrum of spin waves

$$E_{\mathbf{k}} = \gamma(J_0 - J_{\mathbf{k}}) + h - \mu_0, \quad (83)$$

where  $\mu_0$  is the chemical potential in the absence of a magnetic field:  $\mu_0 = 0$  at  $T < T_C$  and  $\mu_0(T > T_C)$  is determined from the condition  $\bar{S}(T, h=0) = 0$ .

Formally, the spectrum (83) has the same form as in the case of an anisotropic magnet (69) (we can associate with the anisotropy the effective ‘‘magnetic field’’  $h_A = JS\Delta$ ). However, there is an important difference: in the case of the ‘‘true’’ magnetic field the chemical potential is taken at  $h = 0$ , so that the phase transition with vanishing  $\bar{S}$  is absent (see below), while in the case of anisotropic magnet it should be determined in the presence of anisotropy field  $h_A$ , and  $\bar{S}$  vanishes at  $T_C$ . However, at  $T \ll T_C$  this difference is not important ( $\mu = \mu_0 = 0$  in this region) and the magnetic anisotropy can be also described by introducing the temperature-dependent magnetic anisotropy field  $h_A$ .

The temperature dependence of magnetization obtained by the numerical solution of Eqs. (13) and (14) with the spectrum (83) is shown in Fig. 5. At low temperatures  $T \ll T_C$  we have  $\bar{S}_{\text{sp}} \gg \bar{S}_{\text{ind}}$  and the magnetization has mainly an exchange origin. On the other hand, at  $T > T_C$  magnetization is entirely caused by the influence of an external field and

$$\bar{S} \approx \chi_0^{zz} h, \quad T \gg T_C, \quad (84)$$

where

$$\chi_0^{zz} = \left( \frac{\partial \bar{S}}{\partial h} \right)_{h=0} = \frac{1}{4T} \sum_{\mathbf{q}} \frac{1}{\sinh^2(E_{\mathbf{q}}/2T)} - \frac{(S+1/2)^2}{T \sinh^2(E_f/2T)}. \quad (85)$$

The first term in Eq. (85) differs from the result of the spin-wave theory by the form of the spectrum only, and the last term describes the correction owing to the kinematical interaction. In a narrow region near  $T_C$  both contributions in Eq. (82) are of the same order, and magnetization considerably differs from its zero-field value.

It follows from Eq. (85) that  $\chi_0^{zz} \propto (T - T_M)^{-2}$  so that the critical exponent is  $\gamma = 2$ . Note that magnon-magnon interactions are taken into account in Eq. (85) only by renormalization of the single-particle spectrum. It is possible to improve result (85) by taking into account two-particle interactions in a RPA-type way, i.e., by considering the sum of the one-loop diagrams. This is performed in the next section.

Now we consider the influence of the external field in the Schwinger-boson representation. Carrying out calculations similar to these in Sec. III D we find for the boson spectrum

$$E_{\mathbf{k}\sigma} = \gamma_{\sigma}(J_0 - J_{\mathbf{k}}) - \frac{1}{2}h\sigma - \mu, \quad (86)$$

where  $\gamma_{\sigma} = \langle s_{i\sigma}^{\dagger} s_{i\sigma} \rangle$ . The expression for the magnetization has the form

$$\bar{S} = \frac{1}{2} \sum_{\mathbf{k}} (N_{\mathbf{k}\uparrow} - N_{\mathbf{k}\downarrow}) + n_B, \quad (87)$$

where we have taken into account the possibility of the condensation of bosons with up ‘‘spins.’’ There is also the condition of spin conservation at each site

$$S = \frac{1}{2} \sum_{\mathbf{k}} (N_{\mathbf{k}\uparrow} + N_{\mathbf{k}\downarrow}) + n_B. \quad (88)$$

At not too high temperatures  $T < T_h$ , where  $T_h$  is determined by the conditions

$$S = \frac{1}{2} \sum_{\mathbf{k}} (N_{\mathbf{k}\uparrow} + N_{\mathbf{k}\downarrow}), \quad \mu = -h/2, \quad (89)$$

the branch  $E_{\mathbf{k}\uparrow}$  is gapless and  $n_B > 0$ . At  $T > T_h$  both branches have a gap, and the condition (88) with  $n_B = 0$  determines the common chemical potential. Thus, the Schwinger-boson representation also allows us to describe the behavior of magnetization in the whole field interval, and expression (87) just describes magnetization as a sum of spontaneous and field-induced components.

Up to now we have considered the small magnetic-field values  $h \ll J$ . In the opposite limit one can neglect the dispersion of the boson spectrum (83) and derive by using the BKJ representation the standard result

$$\bar{S} = SB_S(Sh/T). \quad (90)$$

It should be noted that the correct result (90) is obtained only due to the presence of pseudofermions, the Bose field alone leading to the unphysical phase transition with the vanishing of magnetization at  $T \sim h$ .

A somewhat different situation takes place in the Schwinger boson representation. In the case  $h \gg J$ , we have  $n_B \equiv 0$  and the equation for  $x = \exp(-\mu/T)$  has the form

$$\frac{x \cosh(h/2T) - 1}{x^2 + 1 - 2x \cosh(h/2T)} = S. \quad (91)$$

The solution to this equation reads

$$x = \left(1 + \frac{1}{2S}\right) \cosh \frac{h}{2T} + \frac{1}{2S} \sqrt{(2S+1)^2 \cosh^2 \frac{h}{2T} - 4S(S+1)}. \quad (92)$$

With the use of Eq. (91) we obtain the expression for the magnetization

$$\bar{S} = S \frac{x \sinh(h/2T)}{x \cosh(h/2T) - 1} \approx S \tanh(h/2T) \equiv SB_{1/2}(h/2T). \quad (93)$$

Thus in the limit of large magnetic fields the Schwinger-boson approach reproduces the correct results only for  $S = 1/2$ .

## VI. FLUCTUATION CORRECTIONS TO SSWT FOR 2D AND QUASI-2D MAGNETS

As already discussed, SSWT overestimates the value of  $T_M$ . In particular, for the simple cubic lattice the SSWT result for  $S \rightarrow \infty$  is  $T_M/S^2 = 1.803|J|$ . At the same time, the result of the spherical model (see, e.g., Refs. 32 and 43) in this limit reads

$$\frac{S^2}{3T_M} = \sum_{\mathbf{k}} \frac{1}{J_0 - J_{\mathbf{k}}}, \quad (94)$$

which coincides with the corresponding result of the Tyablikov approximation.<sup>44</sup> One obtains from Eq. (94)  $T_M/S^2 = 1.319|J|$  which is close to the result of the high-temperature series expansion (see, e.g., Refs. 35 and 44). As pointed in Sec. III, for  $S = 1/2$  the value of  $T_M$  is overestimated by 1.2 times.

In the quasi-2D case, formulas (45) and (48) [and the corresponding results of the 2D case with the small easy-axis anisotropy (77) and (79)] coincide with the result of the Tyablikov approximation to logarithmic accuracy and thus seem to be correct. However, this accuracy is also insufficient to treat the experimental data (see the detailed discussion in Ref. 27) and the overestimation of  $T_M$  reaches 1.7–2.0 times for the quasi-2D case and nearly 1.5 times for the anisotropic 2D case (the reason for weaker overestimation of  $T_M$  in the anisotropic case will be explained below). Thus in the quasi-2D magnets and 2D magnets with small easy-axis anisotropy (in both cases  $T_M \ll |J|S^2$ ), the overestimation of  $T_M$  is even higher than in the 3D case.

The values of the critical exponents derived above ( $\beta = \nu = 1$  and  $\gamma = 2$ ) are also in drastic discrepancy with the molecular-field values ( $\nu = \beta = 1/2$ ,  $\gamma = 1$ ), experimental data ( $\nu = 0.7$ ,  $\beta = 0.33$ ,  $\gamma = 1.4$ ) for isotropic magnets, and exact values ( $\nu = 1$ ,  $\beta = 1/8$ ,  $\gamma = 7/4$ ) for easy-axis magnets,

which are known from the Onsager solution of the 2D Ising model. Thus, SSWT poorly describes the critical behavior.

At the same time, SSWT describes much better the local properties (e.g., the pair spin-correlation function at neighbor sites) than those determined by the scale of the correlation length. Indeed, at  $S = 1/2$  the Tyablikov approximation yields the unphysical result  $\Delta \mathcal{E}(T_C) = \mathcal{E}(T_C) - \mathcal{E}(0) < 0$ .<sup>45</sup> In the limit  $S \rightarrow \infty$  this approximation gives  $\Delta \mathcal{E}(T_C)/|\mathcal{E}(0)| = 0.6$  which is also lower than the value which can be derived from the calculations in Sec. III (0.84). Besides that, the Tyablikov approximation implies a not quite correct form of the excitation spectrum at low temperatures. In particular, the spin-wave stiffness demonstrates a  $T^{3/2}$  dependence at low temperatures, instead of a  $T^{5/2}$  one.

Generally speaking, the properties on the scales of order of the correlation length cannot be treated correctly within one-particle picture, and the Tyablikov approximation gives only a rough (but rather successful) description of these. A regular way of describing thermodynamics at not too low temperatures within spin-wave theory is to consider collective excitations rather than one-particle ones. For low-dimensional magnets with  $T_M \ll |J|S^2$ , where large logarithms occur (see Secs. III A and IV) and fluctuations have a 2D nature in a broad temperature region (except for the critical region), this can be performed analytically in a close analogy with the isotropic magnets of the dimensionality  $d = 2 + \varepsilon$  [where  $\beta = 1 + \mathcal{O}(\varepsilon)$ , see, e.g., Ref. 46].

In this section we take into account the interaction corrections to the SSWT results for the magnets with small inter-layer coupling and/or anisotropy. Consider first the 2D Heisenberg magnet with the easy-axis anisotropy. In the ferromagnetic case we have

$$H = \sum_{\mathbf{q}} E_{\mathbf{q}}^0 b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \frac{1}{4} \sum_{\mathbf{q}_1 \dots \mathbf{q}_4} \varphi(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}_3, \mathbf{q}_4) b_{\mathbf{q}_1}^{\dagger} b_{\mathbf{q}_2}^{\dagger} b_{\mathbf{q}_3} b_{\mathbf{q}_4} \delta_{\mathbf{q}_1 + \mathbf{q}_2, \mathbf{q}_3 + \mathbf{q}_4}, \quad (95)$$

where

$$E_{\mathbf{q}}^0 = S(J_0 - J_{\mathbf{q}}) + |J|Sf, \\ \varphi(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q}_3, \mathbf{q}_4) = J_{\mathbf{q}_3} + J_{\mathbf{q}_4} - J_{\mathbf{q}_1 - \mathbf{q}_3} - J_{\mathbf{q}_1 - \mathbf{q}_4} \\ \approx -2|J|(\mathbf{q}_1 \mathbf{q}_2 + f), \quad (96)$$

and

$$f = (2S - 1)D/|JS| + (J_0/J)\eta S \quad (97)$$

is the bare gap in the excitation spectrum. In the antiferromagnetic case, we use the operators  $B_{\mathbf{q}}$  which are the Fourier transformation of  $B_i$  of Eq. (17) and satisfy

$$a_{\mathbf{q}} = (B_{\mathbf{q}} + B_{\mathbf{q}+\mathbf{Q}})/2, \\ b_{-\mathbf{q}}^{\dagger} = (B_{\mathbf{q}} - B_{\mathbf{q}+\mathbf{Q}})/2, \quad (98)$$

where  $\mathbf{Q} = (\pi, \pi, \pi)$  is the wave vector of the AFM structure. Then, up to some unimportant constant, we have the Hamiltonian of the same form Eq. (95), but for the operators  $B_{\mathbf{q}}$ .

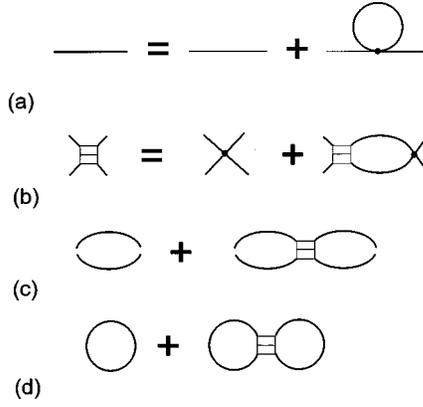


FIG. 6. Diagrams corresponding to the spin-wave interaction contribution to different quantities (a) one-particle Green function of SSWT (b) effective vertex in RPA (c) nonuniform RPA susceptibility (d) correction to (staggered) magnetization  $\delta\bar{S} = S - \bar{S}$ . Simple and bold lines denote the bare and renormalized one-particle Green functions, point stands for the bare vertex.

Note that in this case  $E_{\mathbf{q}}^0$  in Eq. (95) has not the meaning of an excitation spectrum because of non-Bose commutation relations for  $B_{\mathbf{q}}$ :

$$[B_{\mathbf{q}}, B_{\mathbf{p}}^{\dagger}] = \delta_{\mathbf{q}, \mathbf{p}} + \delta_{\mathbf{q}, \mathbf{p} + \mathbf{Q}}. \quad (99)$$

The diagrams which give the first-order renormalizations of  $E_{\mathbf{q}}$  and correspond to SSWT are shown in Fig. 6(a) (see, e.g., Ref. 25 for a detailed description of this diagram technique). Further on we suppose that all such renormalizations (which result in the replacements  $J \rightarrow J\gamma/S$  and  $f \rightarrow \Delta$  in  $E_{\mathbf{q}}^0$ ) are already performed and such diagrams can be omitted.

To obtain the corrections to SSWT, higher-order diagrams should be considered. They lead to renormalization of one-particle energy (and occurrence of the damping) and also to vertex corrections. As discussed above, SSWT treats the excitation spectrum satisfactorily (this spectrum is already renormalized by first-order diagrams). The calculations of damping of spin waves, which occurs only in the second order of perturbation theory, shows that it is small in a broad temperature region.<sup>47</sup> Thus only vertex corrections should be taken into account. At not too low temperatures ( $T \gg |J|S\Delta$ ) the RPA-type diagrams of Fig. 6(b) are most important since each loop contains a logarithmic divergence of the type  $\ln(1/\Delta)$ . The integral equation for the vertex reads

$$\begin{aligned} \Phi(\mathbf{k}, \mathbf{k} - \mathbf{q}; \mathbf{p} - \mathbf{q}, \mathbf{p}) &= \varphi(\mathbf{k}, \mathbf{k} - \mathbf{q}; \mathbf{p} - \mathbf{q}, \mathbf{p}) - \frac{T}{(J\gamma)^2} \\ &\times \sum_{\mathbf{s}} \frac{\varphi(\mathbf{k}, \mathbf{k} - \mathbf{q}; \mathbf{s} - \mathbf{q}, \mathbf{s})}{(s^2 + \Delta)[(s - \mathbf{q})^2 + \Delta]} \\ &\times \Phi(\mathbf{s}, \mathbf{s} - \mathbf{q}; \mathbf{p} - \mathbf{q}, \mathbf{p}). \end{aligned} \quad (100)$$

[We have retained only the contribution of the modes with the Matsubara frequency  $\omega_n = 0$ , which yields the logarithmic divergence, and dropped the terms with  $\omega_n \neq 0$  with simultaneously cutting the summation over quasimomenta at the wave vector  $q_0$ , which is determined by Eq. (44)]. As can be seen from Eq. (78), the account of logarithmically diver-

gent terms in the classical case can also be performed in the continuum approximation with  $q_0^2 = 32$  (in this case, the ‘lattice’ renormalizations are also present in model parameters; see Ref. 28). The result of the solution of Eq. (100) (see Appendix B) in the 2D case reads

$\Phi(\mathbf{k}, \mathbf{k} - \mathbf{q}; \mathbf{p} - \mathbf{q}, \mathbf{p})$

$$\begin{aligned} &= \frac{2|J|\gamma\mathbf{k}(\mathbf{q} - \mathbf{p})}{\bar{S}_0 - (T/2\pi|J|\gamma)\ln[q_0/\max(\Delta^{1/2}, q)]} \\ &- 2|J|f \left[ 1 - \frac{T}{\pi|J|\gamma^2} \frac{\mathbf{q}(\mathbf{q} + \mathbf{k} - \mathbf{p})}{q^2} \ln \frac{q}{\Delta^{1/2}} \right]. \end{aligned} \quad (101)$$

Note that the logarithmic corrections to the vertex in the isotropic case were obtained earlier in Ref. 48. For the static (staggered) nonuniform longitudinal susceptibility (for the AFM case the shift  $\mathbf{q} \rightarrow \mathbf{q} + \mathbf{Q}$  is to be performed), we obtain from the diagrams of Fig. 6(c) the result

$$\begin{aligned} \chi_{\mathbf{q}}^{zz} &= \frac{\chi_{\mathbf{q}0}^{zz}}{1 + (|J|\gamma/2\bar{S})q^2\chi_{\mathbf{q}0}^{zz}} \\ &= \frac{(\bar{S}/\bar{S}_0)\chi_{\mathbf{q}0}^{zz}}{1 - (T/2\pi|J|\gamma\bar{S}_0)\ln[q_0/\max(\Delta^{1/2}, q)]}, \end{aligned} \quad (102)$$

where

$$\begin{aligned} \chi_{\mathbf{q}0}^{zz} &= \frac{T}{(J\gamma)^2} \sum_{\mathbf{p}} \frac{1}{(p^2 + \Delta)[(\mathbf{p} - \mathbf{q})^2 + \Delta]} \\ &\approx \begin{cases} T/[2\pi(J\gamma q^2)^2] \ln(q^2/\Delta), & q^2 \gg \Delta \\ \chi_0 = T/[4\pi(J\gamma)^2\Delta], & q^2 \ll \Delta \end{cases} \end{aligned} \quad (103)$$

is the ‘bare’ longitudinal susceptibility. Thus, as well as in RPA for itinerant magnets,<sup>50</sup> the spin susceptibility is enhanced by the interaction. The first line of Eq. (102) was obtained earlier for 3D magnets in Ref. 49. It follows from Eq. (102) that the excitation spectrum has different forms at small and large enough momenta:

$$\chi_{\mathbf{q}}^{zz} \approx \begin{cases} \chi_{\mathbf{q}0}^{zz}, & |J|q^2\chi_{\mathbf{q}0}^{zz} \ll \bar{S}/S \\ 2\bar{S}/(|J|\gamma q^2), & |J|q^2\chi_{\mathbf{q}0}^{zz} \gg \bar{S}/S. \end{cases} \quad (104)$$

The first line corresponds to the standard spin-wave contribution [it is also subdivided in two cases as given by Eq. (103)]. The second line corresponds to the non-spin-wave regime: at  $q^2 \gg \Delta$  one can neglect the anisotropy and  $\chi_{\mathbf{q}}^{zz} \propto 1/q^2$  is given, in particular, by the spherical model,<sup>32</sup> which treats the spin excitations in essentially a non-spin-wave way. Depending on the temperature value, three cases are possible.

(i) Low temperatures,  $T \ll T_M \sim 2\pi|J|S^2/\ln(q_0^2/\Delta)$ . Then the second condition in Eq. (104) cannot be satisfied and thus the excitations in the whole Brillouin zone have a spin-wave nature.

(ii) Intermediate temperatures,  $(\bar{S}/S)/\ln(q_0^2/\Delta) \ll T/2\pi|J|S^2 \ll \bar{S}/S$  ( $T$  is of the same order as  $T_M$ ). Then at small enough  $q$  we still have  $\chi_{\mathbf{q}}^{zz} \approx \chi_{\mathbf{q}0}^{zz}$ , but the second condition in Eq. (104) holds for large enough  $q$  where  $\Delta \exp(2\pi|J|\gamma\bar{S}/T) \ll q^2 < q_0^2$ .

(iii) Critical region,  $T/2\pi|J|S^2 \gg \bar{S}/S$  ( $1 - T/T_M \ll 1$ ). In this regime the first condition in Eq. (104) is satisfied only for  $q^2 \ll \Delta$  (hydrodynamic region) whereas at all other  $q$  the condition in the second line of Eq. (104) is satisfied.

The corrections to relative (sublattice) magnetization  $\bar{\sigma} \equiv \bar{S}/\bar{S}_0$  [see diagrams of Fig. 6(d)] are given by

$$\bar{\sigma} = 1 - \frac{T}{|J|\gamma\bar{S}_0} \sum_{\mathbf{k}} \frac{1}{k^2 + \Delta} + \frac{T^2}{2(|J|\gamma)^3\bar{S}_0} \sum_{\mathbf{k}\mathbf{q}} \frac{\Phi(\mathbf{k}, \mathbf{k}-\mathbf{q}; \mathbf{k}-\mathbf{q}, \mathbf{k})}{(k^2 + \Delta)^2[(\mathbf{k}-\mathbf{q})^2 + \Delta]}. \quad (105)$$

Integration leads to the result

$$\bar{\sigma} = 1 - \frac{t}{2} \left[ \ln \frac{q_0^2}{\Delta_0} + 4 \ln \frac{1}{\max(\bar{\sigma}, t)} - 2(1 - \bar{\sigma}) + \Phi_a(t/\bar{\sigma}) \right], \quad (106)$$

where  $t = T/(2\pi|J|\bar{S}_0\gamma_0)$ . The function  $\Phi_a$  takes into account the (unknown) nonsingular contribution of non-RPA diagrams. Again, we have three temperature regions described above. In region (i) only the first term in the square brackets is to be taken into account and the magnetization demonstrates the spin-wave behavior (76) and (78) for quantum and classical cases, respectively. In region (ii) all the terms, except for the last, are important, which leads to a significant modification of the dependence  $\bar{S}(T)$ . The function  $\Phi_a$  in both regimes (i) and (ii) can be neglected and the result (106) completely describes the behavior of the magnetization in these two regimes. Finally, in region (iii) the contribution of  $\Phi_a$  is of the same order as the other terms in the square brackets. It should be noted that the factor of 4 before the second term in the square brackets is the sum of 2 which arises from the temperature renormalization of  $\Delta^{1/2}(T) \propto \Delta_0^{1/2} \max(\bar{\sigma}, t)$ , and also a contribution of 2 arises from the vertex renormalization. Thus one can see that in the case of small anisotropy (the same situation takes place for small interlayer coupling, see below), the contribution from the renormalization of the single-particle spectrum and interaction vertex are of the same order, so that SSWT is insufficient even outside the critical region.

For the Curie (Néel) temperatures we obtain the equations

$$T_C = 4\pi JS^2 \left[ \ln \frac{T_C}{JS\Delta_0} + 4 \ln \frac{4\pi JS^2}{T_C} + C_F \right]^{-1} \quad (\text{FM}), \quad (107a)$$

$$T_N = 4\pi J\bar{S}_0\gamma_0 \left[ \ln \frac{T_N^2}{c^2\Delta_0} + 4 \ln \frac{4\pi|J|\bar{S}_0\gamma_0}{T_N} + C_{AF} \right]^{-1} \quad (\text{AFM}), \quad (107b)$$

$$T_M = 4\pi JS^2 \left[ \ln \frac{32}{\Delta_0} + 4 \ln \frac{4\pi|J|S^2}{T_M} + C_{cl} \right]^{-1} \quad (\text{classical}) \quad (107c)$$

with the constants  $C_{F,AF,cl} = -2 - 4 \ln 2 + \Phi_a^{F,AF,cl}(\infty)$ , which are still not determined within our approach. However, it is

important that all the logarithmic terms are included in Eq. (107) and  $C$  gives only a small contribution to above results. The gap  $\Delta_c$  at the ordering temperature, which remained indeterminate in Sec. IV, can be now estimated as  $\Delta_c \propto t^2$ . The coefficient of the proportionality is of the order of unity and influences the constants  $C$  only.

In the isotropic quasi-2D case the infrared cutoff for integrals over the Brillouin zone is  $J'/J$  rather than  $\Delta$ . Then we obtain in the same way

$$\bar{\sigma} = 1 - \frac{t}{2} \left[ \ln \left( q_0^2 \frac{|J|\gamma_0}{|J'|\gamma'_0} \right) + 3 \ln \frac{1}{\max(\bar{\sigma}, t)} - 2(1 - \bar{\sigma}) + \Phi_{ic}(t/\bar{\sigma}) \right] \quad (108)$$

and

$$T_C = 4\pi JS^2 \left[ \ln \frac{T_C}{|J'|S} + 3 \ln \frac{4\pi JS^2}{T_C} + C'_F \right]^{-1} \quad (\text{FM}), \quad (109a)$$

$$T_N = 4\pi|J|S\bar{S}_0\gamma_0 \left[ \ln \frac{T_N^2}{8|J'|\gamma'_0\gamma_0} + 3 \ln \frac{4\pi|J|\bar{S}_0\gamma_0}{T_N} + C'_{AF} \right]^{-1} \quad (\text{AFM}) \quad (109b)$$

$$T_M = 4\pi JS^2 \left[ \ln \frac{32}{\Delta_0} + 3 \ln \frac{4\pi JS^2}{T_M} + C'_{cl} \right]^{-1} \quad (\text{classical}). \quad (109c)$$

In this case we have  $\gamma'(T) \propto \gamma'_0 \max(\bar{\sigma}, t)$  which leads to that the coefficient at the second term in the square brackets is 3 (instead of 4 in the anisotropic case). This is why the interaction corrections are weaker in the anisotropic case: within SSWT the above-mentioned coefficient is 1 in the quasi-2D case (which is three times smaller than the correct value) and 2 in the anisotropic case (only two times smaller than the correct value). Note that the results (108), (109) are valid for all four combinations of the signs of intra- and interplane exchange integrals (for mixed combinations, FM and AFM denote the type of the in-plane ordering).

The same results (106)–(109) were obtained within the RG approach in Ref. 28. (Note that the different sign at the third term of the square brackets of Eqs. (106) and (108) is the misprint of this paper). Derivation of general expressions for the case where both interlayer coupling and anisotropy are of the same order can be also found in Ref. 28.

With neglect of the functions  $\Phi_a(x)$  and  $\Phi_{ic}(x)$ , Eqs. (106) and (108) still yield unphysical behavior near  $T_M$ . The point  $T^*$ , where the derivative  $\partial\bar{S}/\partial T$  diverges, can be determined from the conditions

$$\bar{\sigma}(t^*)/t^* \approx \begin{cases} 3/2 & \text{quasi-2D,} \\ 2 & \text{easy-axis 2D,} \end{cases} \quad (110)$$

TABLE I. The experimental parameters and ordering temperatures of layered magnets and the corresponding calculated values of  $T_M$  in the standard spin-wave-theory (SWT), SSWT, and RPA (in brackets taking into account the constant  $C_{AF} = -0.7$ ).

Compound	$S$	$J$ (K)	$J'$ (K)	$\Delta_0$	$T_M^{\text{SWT}}$ (K)	$T_M^{\text{SSWT}}$ (K)	$T_M^{\text{RPA}}$ (K)	$T_M^{\text{exp}}$ (K)
$\text{La}_2\text{CuO}_4$	1/2	1600	0.8	$\approx 0$	672	537	343	325
$\text{K}_2\text{NiF}_4$	1	102	$\approx 0$	0.0088	160	125	90.0 (97.0)	97.1
$\text{Rb}_2\text{NiF}_4$	1	82	$\approx 0$	0.046	180	118	88.4 (95.0)	94.5
$\text{K}_2\text{MnF}_4$	5/2	8.4	$\approx 0$	0.015	74.8	52.1	42.7 (45.1)	42.1
$\text{CrBr}_3$	3/2	12.38	1.0	0.024	79.2	51.2	39.0	40.0

which should be used together with Eq. (106) or Eq. (108);  $t^*$  is the value of  $t$  corresponding to  $T^*$ . The condition (110) should be used together with Eqs. (106) or (108) to obtain the value of  $t_r^*$ .

The functions  $\Phi_a(x)$  and  $\Phi_{ic}(x)$  describe the crossover from an isotropic 2D Heisenberg to 2D Ising and 3D Heisenberg behavior, respectively. As discussed above, these functions give considerable contributions in the crossover region between regimes (ii) and (iii) and in the critical regime (iii), where essentially non-spin-wave excitations should be taken into account. An account of these functions results in slightly decreasing the temperature  $T^*$  in comparison with that given by Eq. (110), and  $T^*$  becomes the temperature of a rapid decrease of  $\bar{S}$  (in fact, the characteristic temperature of a crossover). For a quantum antiferromagnet, the calculation of  $\Phi_{ic}(x)$  can be performed within the  $1/N$  expansion in the  $O(N)$  model.<sup>27</sup> For an arbitrary  $x = t/\bar{\sigma}$ , the result of this calculation is very cumbersome. In the critical region ( $x \gg 1$ ) it provides the correct critical behavior<sup>27</sup>

$$\bar{\sigma}^2 = \left[ \frac{T_{\text{Neel}}}{4\pi|J|\bar{S}_0\gamma_0} \right]^{1-\beta_3} \left[ \frac{1}{1-A_0} \left( 1 - \frac{T}{T_{\text{Neel}}} \right) \right]^{2\beta_3} \quad (111)$$

with  $A_0 \approx 0.9635$  and  $\beta_3 = (1 - 8/\pi^2 N)/2 \approx 0.36$ . The value of  $C'_{AF}$  obtained by this expansion is very small,  $C'_{AF} = -0.0660$ . Other critical exponents can also be calculated within the  $1/N$  expansion in the  $O(N)$  model (see, e.g., Ref. 51):

$$\nu_3 = 1 - 32/3\pi^2 N \approx 0.64, \quad \gamma_3 = 2(1 - 12/\pi^2 N) \approx 1.21$$

(note that the scaling relations are slightly violated because of approximate character of this expansion for  $N=3$ ). Thus the results of the spherical model for the critical exponents above  $T_M$  (see, e.g., Ref. 32) become radically improved. In particular, the fluctuations correct the critical behavior of the magnetic susceptibility.

For practical purposes, it is useful to have simple interpolation expressions for the functions  $\Phi(x)$ , which enable one to describe the crossover temperature region. Taking into account the closeness of  $T^*$  to  $T_M$  which is given by Eqs.

(107) and (109) and using Eq. (110), we can write down the simplest expressions for  $\Phi(x)$  in the form:

$$\Phi_a^{\text{F,AF,cl}}(x) = \frac{x}{\sqrt{x^2+1}} (C_{\text{F,AF,cl}} - 2 + 8 \ln 2),$$

$$\Phi_{ic}^{\text{F,AF,cl}}(x) = \frac{x}{\sqrt{x^2+1}} (C'_{\text{F,AF,cl}} - 1 + 3 \ln 3) \quad (112)$$

( $x < 1$ ). The constants  $C_{\text{F,AF,cl}}$  and  $C'_{\text{F,cl}}$  can be, in principle, obtained from numerical calculations or by comparing with experimental data (see below). However, one should expect that they are small enough and can be neglected.

## VII. COMPARISON WITH EXPERIMENTAL DATA

To discuss the experimental situation, we consider first the compounds with layered perovskite structure. The parameters used are given by Table I. The experimental values of transition temperatures are also given and compared with the theoretical one (for experimental data see Ref. 35 and references therein, and Ref. 2 for  $\text{La}_2\text{CuO}_4$ ). The values of  $J'$  and  $\Delta_0 = \Delta(0)$  are obtained from the low-temperature behavior of the sublattice magnetization. This procedure gives the possibility of determining correctly the parameters since the results obtained in Secs. III C and IV work well at low temperatures (in particular they give correct results for ground-state renormalizations). Note that for the anisotropic perovskites the parameters obtained are also in agreement with the experimental data on the spin-wave spectrum.<sup>35</sup> It should be stressed that the experimentally observable gap in the spin-wave spectrum is  $\Delta(T)$  whereas  $D, \eta$  plays the role of the bare parameters. The same situation takes place in the quasi-2D case where  $J\gamma/S$  and  $J'\gamma'/S$  are experimentally observable rather than the bare parameters  $J$  and  $J'$ . Since in the systems under consideration the parameters  $\gamma'$  and  $\Delta$  have strong temperature dependence (see Secs. III C and IV), it is important to take into account this dependence when treating the experimental data.

One can see from Table I that for all the systems the estimated values of transition temperatures are close to the experimental results (for  $\text{La}_2\text{CuO}_4$  the experimental data on  $J'$  are contradictory; one of the possibilities of improving the agreement with experimental data is introducing a small easy-axis anisotropy<sup>28</sup>). At the same time, using SSWT with-

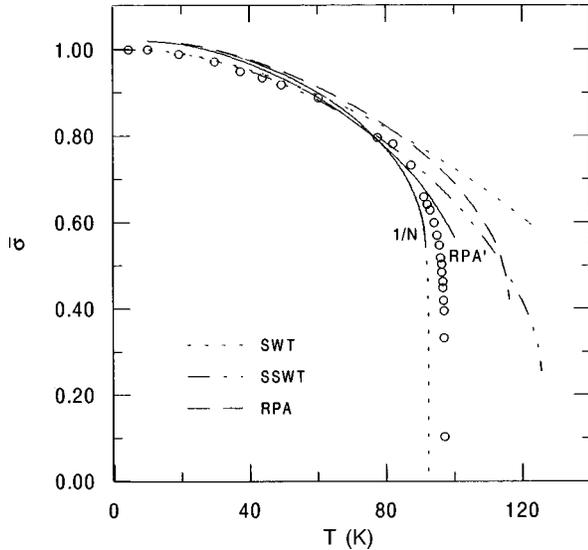


FIG. 7. Temperature dependence of the relative sublattice magnetization  $\bar{\sigma}(T)$  of  $\text{K}_2\text{NiF}_4$  in the SWT, SSWT, RPA approaches and  $1/N$  expansion for the  $O(N)$  model as compared with the experimental data (circles). The RPA' curve corresponds to the inclusion of the function  $\Phi_a^{\text{AF}}(t/\bar{\sigma})$  given by Eq. (112). The short-dashed line is the extrapolation of the result of the  $1/N$  expansion to the critical region (see Ref. 29).

out fluctuation corrections overestimates  $T_N$  by about 1.7 times, although improves somewhat the results of standard spin-wave theory. For the anisotropic compounds  $T_N$  is slightly underestimated. This may be due to two reasons: a nonzero value of  $C_{\text{AF}}$  in this case ( $C_{\text{AF}} \approx -0.7$  is obtained by best fit to the experimental data) and (less important) a small interlayer coupling which also increases the transition temperature.

The temperature dependence of the sublattice magnetization for  $\text{K}_2\text{NiF}_4$  is shown and compared with different theoretical results in Fig. 7. Regimes (i) and (ii) correspond to  $T < 80$  K where the RPA (RG) result is in good agreement with the experimental data. It can be seen also that the account of the function  $\Phi_a^{\text{AF}}(t/\bar{\sigma})$  given by Eq. (112) improves considerably the agreement in the crossover temperature region. The  $1/N$  expansion in the  $O(N)$  model<sup>27</sup> also gives a satisfactory description of this region, but does not describe correctly low enough temperatures, since, as discussed in the Introduction, it implies an essentially non-spin-wave picture of the excitation spectrum.

The parameter values and Curie temperature for the ferromagnetic compound  $\text{CrBr}_3$  (see Ref. 52 for experimental data) are also presented in Table I. Here both interplane coupling and anisotropy are important, and we obtain (see also Ref. 28)

$$T_M = 4\pi |J| \bar{S}_0 \gamma_0 \left\{ \ln \left[ \frac{2q_0^2}{\Delta_c + 2\alpha_c + \sqrt{\Delta_c^2 + 4\alpha_c \Delta_c}} \right] + 2 \ln \frac{4\pi |J| \bar{S}_0 \gamma_0}{T_M} + C \left( \frac{\Delta}{\alpha} \right) \right\}^{-1}, \quad (113)$$

where

$$\alpha_c = J' \gamma_c' / (J \gamma_c) = T_M |J'| / [4\pi (J \gamma_0)^2],$$

$$\Delta_c = \Delta_0 [T_M / (4\pi J \bar{S}_0 \gamma_0)]^2. \quad (114)$$

The (unknown) function  $C(\Delta/\alpha)$  satisfies  $C(0) = C'$  and  $C(\infty) = C$  where  $C$  and  $C'$  are defined above. Since the in-plane lattice structure is nonsquare, we have used the effective value of the in-plane exchange integral determined in the continuum limit from the excitation spectrum as  $E_{\mathbf{q}} \approx \gamma J_{\text{ef}}(q_x^2 + q_y^2) + O(J', J\Delta)$ . One can see that the agreement with experimental  $T_C$  is excellent.

## VIII. CONCLUSIONS

In the present paper we have investigated in detail the capabilities of the self-consistent spin-wave theory, which is based on boson representations for spin operators, for a description of layered magnets. To improve the SSWT at not too low temperatures, we have introduced a pseudofermion field. For magnets with a low transition point,  $T_M \ll |J|S^2$ , analytical results were obtained. These results have different forms in quantum ( $T \ll |J|S$ ) and classical ( $T \gg |J|S$ ) regimes. In the quantum case the magnetization demonstrates in some temperature region the  $T \ln T$  behavior. The proposed version of SSWT gives a qualitative (and at not too high temperatures—quantitative) description of the thermodynamics of layered magnets. An important advantage of SSWT (in comparison with the methods that are based on investigation of continuum models, e.g., nonlinear  $\sigma$  model) is the possibility of describing the short-range order above the transition point.

At the same time, even in the case of layered magnets SSWT is unable to treat quantitatively the transition points and thermodynamics at high enough temperatures ( $T > 0.8T_M$ ). We have performed a systematic treatment of corrections to SSWT in the case  $T_M \ll |J|S^2$ , which is based on summation of the higher-order  $1/S$  terms. The inclusion of the RPA corrections (which permits us to take into account next-leading logarithmic singularities) yields an excellent description of the behavior of (sublattice) magnetization at arbitrary  $T < T_M$  except for a narrow critical region, where an account of non-spin-wave excitations is required. The approach used is somewhat reminiscent of the theory of itinerant magnets.<sup>50</sup> As well as in the latter case, the fluctuation corrections within the RPA approximation lead to significant lowering of the transition temperature and improve radically the agreement with experimental data. The simple analytical results obtained give a quantitative description of the magnetization behavior practically up to  $T_M$ . At the same time, the consideration of the critical region (e.g., correct calculation of critical exponents) requires an account of essentially non-spin-wave excitations. For quasi-2D isotropic magnets this can be performed within the  $1/N$  expansion in the  $O(N)$  model.<sup>27</sup> A description of the critical region for magnets with the easy-axis anisotropy, where the topological (domain-wall) excitations are present, is still an open problem.

A regular calculation of higher-order corrections in the 3D case, where the kinematical spin-wave interaction should be also taken into account, but the logarithmic terms are

absent, is also a matter for further investigations. The same is valid for magnets with the essential role of topological excitations (easy-plane systems, antiferromagnetic half-integer spin chains, etc.).

### APPENDIX A: VARIATIONAL PRINCIPLE IN THE HEISENBERG MODEL

In this appendix we consider a variational approach to SSWT. This is a generalization of approaches of Refs. 6 and 7 to the quasi-2D case, which provides the possibility of improving the behavior of the magnetization at not too small  $J'/J$ .

We apply the Feynman-Peierls-Bogoliubov variation principle for the free energy  $F = -\ln \text{Sp}(e^{-\beta H})$  (see, e.g., Refs. 44,53)

$$F < F_0 + \langle H - H_0 \rangle_0, \quad (\text{A1})$$

where  $H_0$  is the trial Hamiltonian,  $F_0$  is the free energy corresponding to  $H_0$ , and  $\langle \dots \rangle_0$  stands for the average with  $H_0$ .

Consider first the case of a ferromagnet. Assuming the spin-wave character of spin dynamics, we choose  $H_0$  as the Hamiltonian of noninteracting bosons and fermions

$$H_0 = -\frac{1}{2}J_0\gamma S + \gamma \sum_{\mathbf{k}} (J_0 - J_{\mathbf{k}}) b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + (2S+1)\gamma J_0 \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - \mu \sum_{\mathbf{k}} [b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + (2S+1)c_{\mathbf{k}}^\dagger c_{\mathbf{k}}]. \quad (\text{A2})$$

This expression differs from the Hamiltonian of the standard spin-wave theory by the factor  $\gamma$  which is a variational parameter describing the renormalization of the spin-wave spectrum, and by the presence of the Fermi operators taking into account the kinematical interaction between spin waves. Then we obtain

$$F_0 = T \sum_{\mathbf{q}} \ln \frac{1 - \exp(-E_{\mathbf{q}}/T)}{1 - \exp(-E_f/T)} \quad (\text{A3})$$

and

$$\langle H \rangle_0 = -\frac{1}{2}J_0\bar{S}^2 - \bar{S} \sum_{\mathbf{q}} J_{\mathbf{q}} N_{\mathbf{q}} - \frac{1}{2} \sum_{\mathbf{p}\mathbf{q}} J_{\mathbf{q}-\mathbf{p}} N_{\mathbf{q}} N_{\mathbf{p}} - \mu \sum_{\mathbf{q}} [N_{\mathbf{q}} + (2S+1)N_f],$$

$$\langle H_0 \rangle_0 = \gamma J_0 (S - \bar{S}) - \gamma \sum_{\mathbf{q}} J_{\mathbf{q}} N_{\mathbf{q}} - \mu \sum_{\mathbf{q}} [N_{\mathbf{q}} + (2S+1)N_f], \quad (\text{A4})$$

where the magnetization reads

$$\bar{S} = \left( S + \frac{1}{2} \right) \coth \frac{E_f}{T} - \frac{1}{2} - \sum_{\mathbf{q}} N_{\mathbf{q}} \quad (\text{A5})$$

and  $E_f = \gamma J_0 - \mu$ . The equation for  $\gamma$  is determined from the condition  $\partial F / \partial \gamma = 0$  and has the form

$$(\gamma - \bar{S}) \left[ \sum_{\mathbf{q}} J_{\mathbf{q}} \frac{\partial N_{\mathbf{q}}}{\partial \gamma} + J_0 \frac{\partial \bar{S}}{\partial \gamma} \right] = \sum_{\mathbf{p}\mathbf{q}} J_{\mathbf{p}-\mathbf{q}} N_{\mathbf{p}} \frac{\partial N_{\mathbf{q}}}{\partial \gamma} + \sum_{\mathbf{q}} J_{\mathbf{q}} N_{\mathbf{q}} \frac{\partial \bar{S}}{\partial \gamma}. \quad (\text{A6})$$

In the antiferromagnetic case we use the trial Hamiltonian

$$H_0 = -\frac{1}{2}J_0\gamma S + \frac{1}{2}\gamma \sum_{\mathbf{k}} [J_0(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}) - J_{\mathbf{k}}(a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} b_{-\mathbf{k}})] + (2S+1)\gamma J_0 \sum_{\mathbf{k}} (c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}}) - \mu \sum_{\mathbf{k}} [a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + (2S+1)(c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + d_{\mathbf{k}}^\dagger d_{\mathbf{k}})] \quad (\text{A7})$$

to obtain

$$(\gamma - \bar{S}) \left[ \sum_{\mathbf{q}} J_{\mathbf{q}} \frac{\partial L_{\mathbf{q}}}{\partial \gamma} + J_0 \frac{\partial \bar{S}}{\partial \gamma} \right] = \sum_{\mathbf{p}\mathbf{q}} J_{\mathbf{p}-\mathbf{q}} L_{\mathbf{p}} \frac{\partial L_{\mathbf{q}}}{\partial \gamma} + \sum_{\mathbf{q}} J_{\mathbf{q}} L_{\mathbf{q}} \frac{\partial \bar{S}}{\partial \gamma}, \quad (\text{A8})$$

where

$$E_{\mathbf{q}} = \sqrt{(\gamma J_0 - \mu)^2 - (\gamma J_{\mathbf{q}})^2}, \quad L_{\mathbf{q}} = \frac{\gamma J_{\mathbf{q}}}{E_{\mathbf{q}}} \left( N_{\mathbf{q}} + \frac{1}{2} \right), \quad (\text{A9})$$

and

$$\bar{S} = \left( S + \frac{1}{2} \right) \coth \frac{E_f}{T} - \sum_{\mathbf{q}} \frac{J_0 \gamma - \mu}{E_{\mathbf{q}}} \left( N_{\mathbf{q}} + \frac{1}{2} \right). \quad (\text{A10})$$

In the 2D case ( $J' = 0$ ) we have

$$\sum_{\mathbf{p}\mathbf{q}} J_{\mathbf{p}-\mathbf{q}} N_{\mathbf{p}} \frac{\partial N_{\mathbf{q}}}{\partial \gamma} = \frac{1}{J_0} \left( \sum_{\mathbf{q}} J_{\mathbf{q}} N_{\mathbf{q}} \right) \left( \sum_{\mathbf{p}} J_{\mathbf{p}} \frac{\partial N_{\mathbf{p}}}{\partial \gamma} \right) \quad (\text{A11})$$

and a similar result with the replacement  $N_{\mathbf{q}} \rightarrow L_{\mathbf{q}}$ . Then Eqs. (A6) and (A8) reduce to

$$\gamma - \bar{S} = \frac{1}{J_0} \sum_{\mathbf{q}} J_{\mathbf{q}} N_{\mathbf{q}} \quad (\text{FM}),$$

$$\gamma - \bar{S} = \frac{1}{J_0} \sum_{\mathbf{q}} J_{\mathbf{q}} L_{\mathbf{q}} \quad (\text{AFM}). \quad (\text{A12})$$

These equations coincide with those of Sec. III A. At small  $J'/J$  the values of integrals over the Brillouin zone are determined by the region of small quasimomenta  $q_x^2, q_y^2 < J'/J$ . Then it is possible to set

$$J_{\mathbf{p}-\mathbf{q}} \approx J_0, \quad J_{\mathbf{q}} \approx J_0 \quad (\text{A13})$$

in this case, which again leads to Eqs. (A12). If  $J'/J$  is not small enough, the approximation (A13) becomes invalid and it is necessary to use Eq. (A6) or (A8) up to the limit of the cubic crystal,  $J' = J$ , where equality (A11) is again satisfied and passing to Eq. (A12) becomes justified. The same situation is realized for hypercubic lattices of any dimensionality in the nearest-neighbor approximation.

### APPENDIX B: THE SOLUTION OF INTEGRAL EQUATION FOR THE RENORMALIZED VERTEX OF SPIN-WAVE INTERACTION

The equation for the vertex (100) has a degenerate kernel. We search for a solution in the form

$$\Phi(\mathbf{k}, \mathbf{k}-\mathbf{q}; \mathbf{p}-\mathbf{q}, \mathbf{p}) = J(A\mathbf{q} - B\mathbf{p})\mathbf{k} - 2J\tilde{\Delta}(\mathbf{p}, \mathbf{q}). \quad (\text{B1})$$

Then we obtain after some algebraic manipulations

$$A = \frac{2}{\bar{S}_0/\gamma - R + M_q} [1 + 2\mathbf{q}(\mathbf{p}-\mathbf{q})(\Gamma_q - M_q/q^2) + 2\Delta(J\chi_{q_0}^{zz} - \Gamma_q)],$$

$$B = \frac{2}{\bar{S}_0/\gamma - R + M_q},$$

$$\tilde{\Delta}(\mathbf{p}, \mathbf{q}) = \Delta[1 - \Gamma_q(A\mathbf{p}\mathbf{q} + Bq^2)], \quad (\text{B2})$$

where we have introduced the correction to the magnetization  $R = (\bar{S}_0 - \bar{S})/\gamma$  and the nonuniform susceptibility  $\chi_{q_0}^{zz}$

$$R = \frac{T}{|J|\gamma^2} \int_{s < q_0} \frac{d^2\mathbf{s}}{(2\pi)^2} \frac{1}{s^2 + \Delta},$$

$$\chi_{q_0}^{zz} = \frac{T}{(J\gamma)^2} \int \frac{d^2\mathbf{s}}{(2\pi)^2} \frac{1}{(s^2 + \Delta)[(\mathbf{s}-\mathbf{q})^2 + \Delta]}, \quad (\text{B3})$$

and  $\Gamma_q, M_q$  are defined by

$$\frac{T}{|J|\gamma^2} \int \frac{d^2\mathbf{s}}{(2\pi)^2} \frac{\mathbf{s}}{(s^2 + \Delta)[(\mathbf{s}-\mathbf{q})^2 + \Delta]} = \mathbf{q}\Gamma_q,$$

$$\frac{T}{|J|\gamma^2} \int_{s < q_0} \frac{d^2\mathbf{s}}{(2\pi)^2} \frac{s_i s_j}{(s^2 + \Delta)[(\mathbf{s}-\mathbf{q})^2 + \Delta]} = \frac{1}{2}R\delta_{ij} - M_q \left( \frac{\delta_{ij}}{2} - \frac{q_i q_j}{q^2} \right). \quad (\text{B4})$$

Calculating the integrals in Eq. (B4) and retaining only terms which are logarithmically divergent at  $\Delta \rightarrow 0$  yields

$$\Gamma_q = M_q/q^2 = \frac{1}{2}|J|\chi_{q_0}^{zz}, \quad (\text{B5})$$

where  $\chi_{q_0}^{zz}$  is given by Eq. (103), and finally we get

$$R = \frac{T}{2\pi|J|\gamma^2} \ln \frac{q_0}{\Delta^{1/2}}. \quad (\text{B6})$$

Combining the above formulas we obtain the result (101) of the main text.

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