Thermodynamics of a two-dimensional Heisenberg ferromagnet with dipolar interaction

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Thermodynamics of quantum and classical two-dimensional (2D) Heisenberg models with long-range dipole–dipole interaction has been investigated using various forms of self-consistent spin-wave theory (SSWT). It has been found that SSWT gives a much lower transition temperature T_c than the free-magnon (spin-wave) theory. For the classical spin, the T_c from SSWT lies within 9% of the Monte Carlo value, making SSWT the best approximation among those considered. It is proven that the random phase approximation vertex corrections to SSWT are rather small. The results depend strongly on the value of the spin, emphasizing the importance of using the quantum and not the classical 2D Heisenberg model even for large spins such as $S=7/2$.

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INTRODUCTION

Ultrathin magnetic films and multilayers became a very active field of research in the last two decades.[1] These two-dimensional (2D) magnetic systems demonstrate unique physical properties, such as oscillating interlayer exchange coupling and giant magnetoresistance.[2,3] They also have numerous technological applications, for example, in spintronics[4,5] and magnetic data recording. Theoretically, 2D magnetic systems are often approximated by a quantum or classical Heisenberg model. Therefore, a good understanding of this model is very important in order to predict the dynamics and thermodynamics of 2D magnetic systems, in particular to calculate the magnetization curve $M(T)$ and the Curie temperature T_c.

There is one important difference between magnetism in three-dimensional and two-dimensional systems. The 3D Heisenberg model always has long-range magnetic order at sufficiently low temperatures, with a transition temperature of the order of JS^2, where J is a typical value of the exchange integral. On the other hand, the 2D Heisenberg model has no long-range order at $T>0$, according to the Mermin–Wagner theorem,[6] provided that only an isotropic, short-range exchange interaction is included. Experiment shows, however, that even 2D magnetic systems have finite transition temperatures. The reason for this is the presence of additional small interactions (magnetocrystalline anisotropy, dipole-dipole interaction, or interlayer exchange in quasi-2D systems), and also the finite horizontal size of the sample. Each of these factors breaks the conditions of the Mermin–Wagner theorem (for a review, see, e.g., Ref. 7 and references therein), resulting in a finite $T_c \ll JS^2$. At the same time, the short-range order (SRO) is retained up to $T \sim JS^2$ (Ref. 8) in 2D and quasi-2D systems.

There are various theoretical approaches to the quantum 2D Heisenberg model (both with and without long-range order at $T>0$). Free-magnon [spin-wave (SW)] theory is only a very rough starting point that normally overestimates T_c by a factor of 2-4. Quantum Monte Carlo results have been reported.[9–12] The pure quantum self-consistent harmonic approximation[13,14] gives a quantitative solution of the *quantum* Heisenberg model with a computational effort that is similar to that of a *classical* Monte Carlo calculation. Note that the Weiss mean-field theory is pretty useless for low-dimensional systems since it does not reproduce the Mermin–Wagner theorem, but predicts a T_c of the order of JS^2.

Self-consistent spin-wave theory (SSWT) was first formulated for the Mermin–Wagner situation,[15–18] but it was later generalized to systems with long-range order.[7,19] SSWT can be formulated as the best possible one-magnon theory,[7,17] the zeroth-order term in the $1/N$ expansion of the SU(N) theory,[18,20] or as the mean-field magnon theory.[7] Note that here and in the following the words "mean field" are applied to *magnon occupation number operators* and have nothing to do with the Weiss mean field for *spin operators*. The SSWT expression can be further improved by renormalizing the magnon-magnon vertex[7] [this approximation is often called the random phase approximation (RPA)], often providing quantitative agreement with the experiment everywhere except the narrow critical region. The known weak point of SSWT is the erroneous critical behavior: it gives either a spin-wave transition with $\beta=1$ [β is the critical exponent in the magnetization vs temperature dependence: $M(T) \sim (T_c-T)^\beta$ when $T \to T_c-0$], or a first-order transition ($\beta=0$). However, SSWT describes perfectly the short-range order above T_c.

Unfortunately, all these approaches in their present forms do not include the dipole–dipole interaction. This is a serious drawback, since this interaction is very important for realistic systems, especially ferromagnetic materials (see Refs. 21 and 22 for a review). This interaction is sometimes treated as an effective easy-plane anisotropy; however, in contrast to the latter, it does break the conditions of the Mermin–Wagner theorem, resulting in a finite T_c.[23] While the easy-axis anisotropy creates a gap in the magnon spectrum, the dipolar interaction results in a more complicated dispersion law, roughly $\epsilon_k \sim k^{1/2}$ for small k.[23–25]

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This interaction has a strong effect on spin waves in thin films.[22,26] The competition between perpendicular anisotropy and dipolar interaction often results in what is called a reorientation transition.[27] Although the thermodynamics of the 2D classical Heisenberg model with the dipolar interaction has been studied rather extensively,[21,28–36] the quantum results are scarce. To the best of our knowledge, the only approaches applied in the quantum case are spin-wave theory[23–25] (free magnons) and the Tyablikov approximation.[37,38]

The classical Heisenberg model is very helpful for 3D systems, since in this case any large spin ($S \gg 1$) can be treated as a classical one. However, this is not true for the 2D systems. To understand why it is so, one needs to recall the arguments given by Bloch,[39] who first hinted that 2D magnetic systems should have no long-range order. Consider a 2D Heisenberg ferromagnet (FM). Its spin-wave dispersion relation is $E_{\mathbf{k}} = JSk^2$ for small k. Free-magnon theory gives the following expression for the magnetization:

$$\langle S_z \rangle = S - \frac{1}{V_{BZ}} \int_{BZ} \frac{d\mathbf{k}}{\exp(E_{\mathbf{k}}/T) - 1}. \tag{1}$$

From now on we measure temperature in energy units ($k_B \equiv 1$), and choose the lattice constant a as the unit of length. For small k

$$\frac{d\mathbf{k}}{\exp(E_{\mathbf{k}}/T) - 1} \approx 2\pi k\, dk \frac{T}{JSk^2}. \tag{2}$$

The integral (1) diverges at the lower limit and long-range order cannot exist at $T > 0$.

In terms of Eq. (1) any additional small interaction (anisotropy, interplanar exchange, dipolar forces) introduces a low-energy cutoff $\Delta \ll 1$ (see, e.g., Ref. 7) and the magnetization is given by (for a 2D square lattice)

$$S - \langle S_z \rangle \approx \frac{T}{4\pi JS} \int_{JS\Delta}^{T} \frac{dE}{E} = \frac{T}{4\pi JS} \ln\left(\frac{T}{JS\Delta}\right), \tag{3}$$

giving a spin-wave expression for T_c:

$$T_c \approx \frac{4\pi JS^2}{\ln(T_c/JS\Delta)} \ll 4\pi JS^2. \tag{4}$$

Thus T_c in the 2D case is much smaller than in the 3D case. The classical description is appropriate when the Curie temperature is much larger than any spin-wave frequency, namely, when $T_c \gg JS$. For the 3D Heisenberg model $T_c \sim JS^2$, and this criterion takes the well-known form $S \gg 1$. However, for the 2D Heisenberg model $T_c \ll JS^2$, and the classical description is only valid if $S \gg \ln(1/\Delta) \gg 1$ (see Ref. 7). The latter situation seems quite unrealistic; therefore the quantum effects are never negligible for 2D magnetic systems.

The goal of this paper is to construct a SSWT formalism for the 2D quantum Heisenberg model with dipolar interaction (and no magnetocrystalline anisotropy for the moment) and to investigate whether SSWT can be improved by RPA vertex corrections. The paper is organized as follows. In Sec. I we present the Heisenberg Hamiltonian, introduce magnons, and also write down the free-magnon expressions for the spin-wave spectrum and magnetization.[23,24] In Sec. II we develop the SSWT formalism. Section III describes our numerical SSWT implementation followed by SSWT results in Sec. IV. The RPA formalism is presented in Sec. V, and the last section offers our conclusions.

I. HAMILTONIAN AND FREE MAGNONS

We start with the spin Hamiltonian

$$H = -\frac{1}{2} \sum_{i \neq j} (J_{ij}\delta_{\alpha\beta} + Q_{ij}^{\alpha\beta}) S_i^{\alpha} S_j^{\beta}, \tag{5}$$

where

$$Q_{ij}^{\alpha\beta} = J_d (3R_{ij}^{\alpha} R_{ij}^{\beta} - \delta_{\alpha\beta} R_{ij}^2) R_{ij}^{-5}, \tag{6}$$

$\mathbf{R}_i$ are the sites of a simple square lattice in the xz plane, and $\mathbf{R}_{ij} \equiv \mathbf{R}_i - \mathbf{R}_j$. The dipolar interaction constant J_d is equal to $4\mu_B^2/a^3$, where μ_B is the Bohr magneton and a is the lattice constant. If J_d is sufficiently small, the ground state is ferromagnetic with an xz easy plane, and we take the z-axis direction for the ground-state magnetization. With the usual notation

$$S_i^{\pm} = S_i^x \pm iS_i^y, \tag{7}$$

we formally introduce magnons by the Holstein–Primakoff transformation

$$S_i^{+} = \sqrt{2S}(1 - a_i^{\dagger} a_i / 2S)^{1/2} a_i, \tag{8}$$

$$S_i^{-} = \sqrt{2S} a_i^{\dagger} (1 - a_i^{\dagger} a_i / 2S)^{1/2}, \tag{9}$$

$$S_i^{z} = S - a_i^{\dagger} a_i, \tag{10}$$

make a Fourier transform from site index $\mathbf{R}_i$ to the crystal momentum $\mathbf{k}$, and expand the Hamiltonian (5) into a series of $S^{-1/2}$ (see Refs. 23 and 24 for details):

$$H = S^2 N_0 + S^1 N_2(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) + S^{1/2} N_3(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) + S^0 N_4(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) + S^{-1/2} N_5(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) + \cdots, \tag{11}$$

where $N_n(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}})$ means a certain nth-order polynomial of the Bose operators $a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}$ in the normal form (creation operators to the left).

The free-magnon Hamiltonian is

$$H_0 \equiv S^1 N_2(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) - \mu \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} = \sum_{\mathbf{k}} \left\{ A_{\mathbf{k}}^0 a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} B_{\mathbf{k}}^0 a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} + \frac{1}{2} B_{\mathbf{k}}^0 a_{\mathbf{k}} a_{-\mathbf{k}} \right\}, \tag{12}$$

where

$$A_{\mathbf{k}}^0 = S(J_0 - J_{\mathbf{k}}) - \frac{1}{2} J_d S \left[S_1(\mathbf{k}) - \frac{3}{2} S_3 \right] - \mu, \tag{13}$$

$$B_{\mathbf{k}}^0 = -\frac{3}{2} J_d S \left[S_2(\mathbf{k}) + \frac{1}{2} S_3 \right], \tag{14}$$

and three lattice sums have been introduced:

$$S_3 \equiv \sum_{\mathbf{R}_i \neq \mathbf{0}} R_i^{-3} \approx 9.034, \tag{15}$$

$$S_1(\mathbf{k}) \equiv \sum_{\mathbf{R}_i \neq \mathbf{0}} (e^{i\mathbf{k}\cdot\mathbf{R}_i} - 1) R_i^{-3} \left[1 - 3\frac{Z_i^2}{R_i^2} \right], \tag{16}$$

$$S_2(\mathbf{k}) \equiv \sum_{\mathbf{R}_i \neq \mathbf{0}} (e^{i\mathbf{k}\cdot\mathbf{R}_i} - 1) \frac{X_i^2}{R_i^5}, \tag{17}$$

where $J_\mathbf{k}$ is equal to $2J\cos k_x + 2J\cos k_z$ for nearest neighbor exchange. For small k the lattice sums (16),(17) have the asymptotical form

$$S_1(\mathbf{k}) \approx 2\pi\frac{k_z^2}{k}, \quad S_2(\mathbf{k}) \approx -\frac{2}{3}\frac{\pi}{k}(2k_z^2 + k_x^2). \tag{18}$$

The "chemical potential" μ is a Lagrange multiplier used in spin-wave theory and SSWT to enforce the condition $\langle S_z \rangle \equiv \overline{S} = 0$ in the paramagnetic phase (in the ferromagnetic phase one has $\mu = 0$). The next step is eliminate the "anomalous" terms $a_\mathbf{k}^\dagger a_{-\mathbf{k}}^\dagger$ and $a_\mathbf{k} a_{-\mathbf{k}}$ by the Bogoliubov transformation

$$\begin{aligned} a_\mathbf{k} &= \cosh(\xi_\mathbf{k}) b_\mathbf{k} - \sinh(\xi_\mathbf{k}) b_{-\mathbf{k}}^\dagger, \\ a_\mathbf{k}^\dagger &= \cosh(\xi_\mathbf{k}) b_\mathbf{k}^\dagger - \sinh(\xi_\mathbf{k}) b_{-\mathbf{k}} \end{aligned} \tag{19}$$

with

$$\tanh(2\xi_\mathbf{k}) = \frac{B_\mathbf{k}^0}{A_\mathbf{k}^0}. \tag{20}$$

The Hamiltonian in the new magnon operators $b_\mathbf{k}^\dagger, b_\mathbf{k}$ becomes

$$H_0 = \text{const} + \sum_\mathbf{k} \epsilon_\mathbf{k}^0 b_\mathbf{k}^\dagger b_\mathbf{k}, \quad \epsilon_\mathbf{k}^0 = \sqrt{(A_\mathbf{k}^0)^2 - |B_\mathbf{k}^0|^2}, \tag{21}$$

and the expectation values are

$$\langle b_\mathbf{k}^\dagger b_\mathbf{k} \rangle = N_\mathbf{k} \equiv [\exp(\epsilon_\mathbf{k}^0/T) - 1]^{-1}, \tag{22}$$

$$\langle a_\mathbf{k}^\dagger a_\mathbf{k} \rangle = \frac{A_\mathbf{k}^0}{\epsilon_\mathbf{k}^0}\left(\langle b_\mathbf{k}^\dagger b_\mathbf{k} \rangle + \frac{1}{2} \right) - \frac{1}{2}, \tag{23}$$

$$\langle a_\mathbf{k}^\dagger a_{-\mathbf{k}}^\dagger \rangle = \langle a_\mathbf{k} a_{-\mathbf{k}} \rangle = -\frac{B_\mathbf{k}^0}{\epsilon_\mathbf{k}^0}\left(\langle b_\mathbf{k}^\dagger b_\mathbf{k} \rangle + \frac{1}{2} \right). \tag{24}$$

Alternatively, the expectation value (23) can be obtained from the free-magnon Matsubara Green's function[23]

$$G_\mathbf{k}^0(i\omega_n) = \frac{i\omega_n + A_\mathbf{k}^0}{(i\omega_n)^2 - (\epsilon_\mathbf{k}^0)^2}, \quad \omega_n \equiv 2\pi n T, \tag{25}$$

through the frequency summation

$$\langle a_\mathbf{k}^\dagger a_\mathbf{k} \rangle = \lim_{\tau \to +0} T \sum_{i\omega_n} e^{i\omega_n \tau} G_\mathbf{k}^0(i\omega_n). \tag{26}$$

The magnetization is

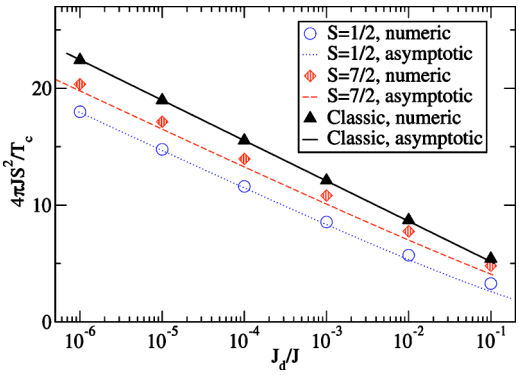

FIG. 1. (Color online) The free-magnon (SW) transition temperature T_c vs dipolar interaction J_d. The symbols are numerical results, while the curves are the asymptotical formulas (31) and (34).

$$\langle S_z \rangle \equiv \overline{S} = S - \frac{1}{N}\sum_\mathbf{k} \langle a_\mathbf{k}^\dagger a_\mathbf{k} \rangle = S - \frac{1}{N}\sum_\mathbf{k} \left[\frac{A_\mathbf{k}^0}{\epsilon_\mathbf{k}^0}\left(N_\mathbf{k} + \frac{1}{2} \right) - \frac{1}{2} \right]. \tag{27}$$

Let us define

$$j_d \equiv J_d/J. \tag{28}$$

For the case $j_d \ll 1$ and in the quantum regime ($JSj_d^{3/2} \ll T \ll JS$) the free-magnon (SW) magnetization is approximately equal to[23]

$$\overline{S} = S - \frac{T}{4\pi JS}\ln\left[\frac{2T}{\pi JS\sqrt{4\pi f}} j_d^{-3/2} \right], \tag{29}$$

where $f \equiv (3/8\pi)S_3 \approx 1.078$, and our notation corresponds to that of Ref. 23 as

$$D = JS, \quad \Omega_0 = 2\pi S J_d, \quad \alpha = 2f = (3/4\pi)S_3. \tag{30}$$

It gives the equation for the free-magnon T_c as

$$\frac{4\pi JS^2}{T_c} = \ln\left[\frac{4S}{\sqrt{\pi f}} j_d^{-3/2} \right] + \ln\left[\frac{T_c}{4\pi JS^2} \right]. \tag{31}$$

For the classical case the Bose function is replaced by

$$N_\mathbf{k} \to \frac{T}{\epsilon_\mathbf{k}}. \tag{32}$$

The analytical expressions for $\overline{S}$ and T_c are obtained by replacing $T/JS \to 32$ under the logarithm in Eqs. (29) and (31), yielding the classical spin-wave expressions

$$\overline{S} = S - \frac{T}{4\pi JS}\ln\left[\frac{32}{\pi\sqrt{\pi f}} j_d^{-3/2} \right], \tag{33}$$

$$\frac{4\pi JS^2}{T_c} = \ln\left[\frac{32}{\pi\sqrt{\pi f}} j_d^{-3/2} \right]. \tag{34}$$

On Fig. 1 the free-magnon transition temperature is presented as a function of j_d for three values of spin: $S = 1/2$, $S = 7/2$, and the classical spin. One can immediately see that the quantum asymptotic (31) works very well for small j_d

and small S (but not for $S=7/2$). The classical asymptotic (34) is also very good at small j_d. It can also be observed that even for such a large spin as $S=7/2$, the transition temperature still differs by about 10% from its classical value.

II. SELF-CONSISTENT SPIN-WAVE THEORY

Self-consistent spin-wave theory can be most easily formulated using the Feynman–Peierls–Bogoliubov variational principle.[40] For any Hamiltonian H and any trial Hamiltonian H_t, the free energy $F=-\ln \mathrm{Tr}(e^{-\beta H})$ satisfies the inequality

$$F < F' \equiv F_t + \langle H - H_t \rangle_t, \tag{35}$$

where F_t and the expectation value are calculated using H_t. SSWT is defined as the best possible one-magnon theory (according to this variational principle); namely, we take H_t to have the generalized free-magnon form

$$H_t = \sum_{\mathbf{k}} \left\{ A_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} B_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} + \frac{1}{2} B_{\mathbf{k}}^{*} a_{\mathbf{k}} a_{-\mathbf{k}} \right\}, \tag{36}$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are variational functions. They are found from the conditions

$$\frac{\delta F'}{\delta A_{\mathbf{k}}} = 0, \quad \frac{\delta F'}{\delta B_{\mathbf{k}}^{*}} = 0. \tag{37}$$

This variational procedure can be shown to be equivalent to the mean-field (MF) procedure, $H_t \equiv H_{MF}$.

In the following, we include only the three- and four-operator terms in the magnon–magnon interaction: $H \equiv H + V$, where $V \equiv S^{1/2} N_3(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) + S^0 N_4(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}})$ (and the N_3 term does not give any contribution). Such truncation of the Hamiltonian can be justified by comparison with the case of SSWT with no dipolar interaction, where the truncated Holstein–Primakoff Hamiltonian is equivalent to the Dyson–Maleev Hamiltonian. For the dipolar case, the Dyson–Maleev representation is not suitable due to the essentially non-Hermitian form of the Hamiltonian derived, and we use the truncated Holstein–Primakoff Hamiltonian instead.

The mean-field Hamiltonian takes the form (36) with $A_{\mathbf{k}} = A_{\mathbf{k}}^{MF}$, $B_{\mathbf{k}} = (B_{\mathbf{k}})^{*} = B_{\mathbf{k}}^{MF}$, and $A_{\mathbf{k}}^{MF}, B_{\mathbf{k}}^{MF}$ being certain functionals of $\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle$ and $\langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle$. This Hamiltonian is meaningful provided that $|B_{\mathbf{k}}^{MF}| \leqslant |A_{\mathbf{k}}^{MF}|$ in the whole Brillouin zone. It can be diagonalized by the Bogoliubov transformation (19)–(24), with $A_{\mathbf{k}}^{MF}, B_{\mathbf{k}}^{MF}$ instead of the free-magnon ones. The system of equations (22)–(24) should then be solved in a self-consistent cycle. Unfortunately, our numerical implementation (see below for details) shows that this system of MF equations has no physically reasonable solutions (except for rather high T). This is not surprising, since the MF approach does not work for anisotropic FMs either,[7] although it works fine for quasi-2D FMs.

There are two possible ways to overcome this difficulty. In the first one (we call it the $\gamma\delta$ model) we apply the constrained variational approach. Instead of using arbitrary functions $A_{\mathbf{k}}^{t}, B_{\mathbf{k}}^{t}$ in Eq. (36), we take the free-magnon expressions (13),(14) with exchange and dipolar interactions renormalized by parameters γ and δ, respectively:

$$J \to \gamma J, \quad J_d \to \delta J_d. \tag{38}$$

This yields

$$H_t = \sum_{\mathbf{k}} \left\{ A_{\mathbf{k}}^{t} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} B_{\mathbf{k}}^{t} a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} + \frac{1}{2} B_{\mathbf{k}}^{t} a_{\mathbf{k}} a_{-\mathbf{k}} \right\}, \tag{39}$$

$$A_{\mathbf{k}}^{t} = \gamma S(J_0 - J_{\mathbf{k}}) - \frac{1}{2} \delta J_d S \left[S_1(\mathbf{k}) - \frac{3}{2} S_3 \right] - \mu, \tag{40}$$

$$B_{\mathbf{k}}^{t} = -\frac{3}{2} \delta J_d S \left[S_2(\mathbf{k}) + \frac{1}{2} S_3 \right]. \tag{41}$$

Since γ renormalizes the short-range exchange interaction, it has the physical meaning of a short-range order parameter. In the absence of the dipolar interaction, the nearest-neighbor spin correlation function is equal to[7]

$$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \rangle = \gamma^2. \tag{42}$$

For $0 < j_d \ll 1$ the equality (42) is no longer exact, but it still holds to a high degree of accuracy. The parameter δ renormalizes the long-range dipolar interaction and has the meaning of some long-range order parameter, different from $\overline{S}/S$.

The Bogoliubov transformation (19)–(24) should now employ $A_{\mathbf{k}}^{t}, B_{\mathbf{k}}^{t}$ from Eqs. (40),(41). The variational procedure now consists of minimizing the trial free energy F' defined by (35) with respect to two parameters γ and δ. The variational equations are

$$0 = \frac{\partial F'}{\partial \gamma} = \sum_{\mathbf{k}} \left\{ A_{\mathbf{k}}^{MF} \frac{\partial \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle}{\partial \gamma} + B_{\mathbf{k}}^{MF} \frac{\partial \langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle}{\partial \gamma} - \epsilon_{\mathbf{k}}^{t} \frac{\partial N_{\mathbf{k}}^{t}}{\partial \gamma} \right\}, \tag{43}$$

$$0 = \frac{\partial F'}{\partial \delta} = \sum_{\mathbf{k}} \left\{ A_{\mathbf{k}}^{MF} \frac{\partial \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle}{\partial \delta} + B_{\mathbf{k}}^{MF} \frac{\partial \langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle}{\partial \delta} - \epsilon_{\mathbf{k}}^{t} \frac{\partial N_{\mathbf{k}}^{t}}{\partial \delta} \right\}. \tag{44}$$

The equations (43),(44), should be solved self-consistently together with Eqs. (22)–(24).

However, for reasons stated below, we are going to concentrate on the second approach to SSWT, which we call the $\gamma\overline{s^2}$ model. In this approach we give up attempts to obtain δ from the SSWT equations. Instead, we renormalize the dipolar interaction with a phenomenological multiplier $\overline{s^2} \equiv (\overline{S}/S)^2$:

$$J_d \to J_d \overline{s^2} \tag{45}$$

in the original Hamiltonian and ignore the dipolar contribution to the magnon–magnon interaction $N_3(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}) + S^0 N_4(a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}})$.

Let us examine the physical reasons for this approximation. The effective dipolar interaction can, generally speaking, have different temperature dependence for different distances $\mathbf{R}_{ij}$. Since the systematic attempt to build an $\mathbf{R}_{ij}$-dependent renormalization (magnon mean-field theory) does not seem to work, a more simple approximation is required. In particular, for $j_d \ll 1$ one can neglect the specific

character of the short-range dipolar interactions, since they are negligible compared to the short-range exchange interaction, and construct a renormalization which is valid in the $R_{ij}\to\infty$ limit. In the latter limit, the macroscopic theory can be applied, and therefore the effective dipolar interaction is proportional to the square of magnetization, i.e., Eq. (45). According to this approximation the effective dipolar interaction vanishes in the paramagnetic phase. In reality it does not vanish, but it becomes a short-range one (due to the finite correlation length), and can be neglected compared to the exchange interaction if $j_d \ll 1$. The approximation (45) is very similar to the way the anisotropy is treated in Ref. 7.

The initial Hamiltonian of the $\gamma\overline{s^2}$ model is therefore

$$H=\sum_{\mathbf{k}}\left\{\tilde{A}^0_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+\frac{1}{2}\tilde{B}^0_{\mathbf{k}}a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}+\frac{1}{2}\tilde{B}^0_{\mathbf{k}}a_{\mathbf{k}}a_{-\mathbf{k}}\right\}+\tilde{V}, \quad (46)$$

$$\tilde{A}^0_{\mathbf{k}}=S(J_0-J_{\mathbf{k}})-\frac{1}{2}\overline{s^2}J_dS\left[S_1(\mathbf{k})-\frac{3}{2}S_3\right]-\mu, \quad (47)$$

$$\tilde{B}^0_{\mathbf{k}}=-\frac{3}{2}\overline{s^2}J_dS\left[S_2(\mathbf{k})+\frac{1}{2}S_3\right], \quad (48)$$

$$\tilde{V}=\sum_{q,k_1,k_2}\frac{J_{\mathbf{q}}}{2N}\left\{\frac{1}{2}a^\dagger_{\mathbf{q}}a^\dagger_{\mathbf{k}_1}a_{\mathbf{k}_2}a_{\mathbf{q}+\mathbf{k}_1-\mathbf{k}_2}+\frac{1}{2}a^\dagger_{\mathbf{k}_1}a^\dagger_{\mathbf{k}_2}a_{\mathbf{q}+\mathbf{k}_1+\mathbf{k}_2}a_{-\mathbf{q}}-a^\dagger_{\mathbf{k}_1}a^\dagger_{\mathbf{k}_2}a_{\mathbf{k}_1+\mathbf{q}}a_{\mathbf{k}_2-\mathbf{q}}\right\}. \quad (49)$$

The renormalized exchange interaction $J\to\gamma J$ is now given by the constrained variational approach with just one parameter γ and

$$\tilde{A}^t_{\mathbf{k}}=\gamma S(J_0-J_{\mathbf{k}})-\frac{1}{2}\overline{s^2}J_dS\left[S_1(\mathbf{k})-\frac{3}{2}S_3\right]-\mu, \quad (50)$$

$$\tilde{B}^t_{\mathbf{k}}=\tilde{B}^0_{\mathbf{k}}=-\frac{3}{2}\overline{s^2}J_dS\left[S_2(\mathbf{k})+\frac{1}{2}S_3\right]. \quad (51)$$

The variational equation is

$$0=\frac{\partial F'}{\partial\gamma}=\sum_{\mathbf{k}}\left\{\tilde{A}^{MF}_{\mathbf{k}}\frac{\partial\langle a^\dagger_{\mathbf{k}}a_{\mathbf{k}}\rangle}{\partial\gamma}+\tilde{B}^{MF}_{\mathbf{k}}\frac{\partial\langle a_{\mathbf{k}}a_{-\mathbf{k}}\rangle}{\partial\gamma}-\tilde{\epsilon}^t_{\mathbf{k}}\frac{\partial N^t_{\mathbf{k}}}{\partial\gamma}\right\}, \quad (52)$$

$$\tilde{A}^{MF}_{\mathbf{k}}=S(J_0-J_{\mathbf{k}})-\frac{1}{2}\overline{s^2}J_dS\left[S_1(\mathbf{k})-\frac{3}{2}S_3\right]-\mu+\sum_{\mathbf{q}}\langle a^\dagger_{\mathbf{q}}a_{\mathbf{q}}\rangle[J_{\mathbf{q}}+J_{\mathbf{k}}-J_0-J_{\mathbf{q}-\mathbf{k}}], \quad (53)$$

$$\tilde{B}^{MF}_{\mathbf{k}}=-\frac{3}{2}\overline{s^2}J_dS\left[S_2(\mathbf{k})-\frac{1}{2}S_3\right]+\sum_{\mathbf{q}}\langle a_{\mathbf{q}}a_{-\mathbf{q}}\rangle\left[\frac{J_{\mathbf{k}}}{2}+\frac{J_{\mathbf{q}}}{2}-J_{\mathbf{q}-\mathbf{k}}\right]. \quad (54)$$

Equation (52) should be solved self-consistently in order to obtain γ and $\overline{s}$. In the next sections, we will present our numerical SSWT implementation followed by SSWT results.

III. NUMERICAL IMPLEMENTATION

In order to solve the SSWT (and SW) equations numerically, we have developed an *ad hoc* code. The most essential technical details are briefly listed below.

The lattice sums $S_1(\mathbf{k})$, $S_2(\mathbf{k})$, and S_3 have been calculated using the Ewald method, in a way similar to the one in Ref. 21, although different in technical details. First note the identity

$$R^{-n}=\frac{2}{\Gamma(n/2)}\int_0^\infty d\rho\, e^{-\rho^2R^2}\rho^{n-1}=\frac{2}{\Gamma(n/2)}\left\{\int_0^\eta d\rho\, e^{-\rho^2R^2)}\rho^{n-1}+\int_\eta^\infty d\rho\, e^{-\rho^2R^2}\rho^{n-1}\right\}, \quad (55)$$

where η is an arbitrary parameter of the order of unity. It can be applied to the sum $(n>2)$

$$\sum_{\mathbf{R}_i\neq\mathbf{0}}\frac{e^{i\mathbf{k}\cdot\mathbf{R}_i}}{R_i^n}=\frac{2}{\Gamma(n/2)}\left\{\int_0^\eta d\rho\,\rho^{n-1}\sum_{\mathbf{R}_i\neq\mathbf{0}}e^{i\mathbf{k}\cdot\mathbf{R}_i-\rho^2R_i^2}+\int_\eta^\infty d\rho\,\rho^{n-1}\sum_{\mathbf{R}_i\neq\mathbf{0}}e^{i\mathbf{k}\cdot\mathbf{R}_i-\rho^2R_i^2}\right\}. \quad (56)$$

The second term in this expression includes a rapidly convergent sum, but the first term should be made rapidly convergent using the Fourier transform with respect to the variable $\mathbf{R}_i$. The final expression for the sum (56) is

$$\sum_{\mathbf{R}_i\neq\mathbf{0}}\frac{e^{i\mathbf{k}\cdot\mathbf{R}_i}}{R_i^n}=\frac{2}{\Gamma(n/2)}\left\{\pi\int_0^\eta\frac{d\rho}{\rho^{3-n}}\sum_{\mathbf{G}}\exp\left[-\frac{(\mathbf{k}-\mathbf{G})^2}{4\rho^2}\right]-\frac{\eta^n}{n}+\int_\eta^\infty d\rho\,\rho^{n-1}\sum_{\mathbf{R}_i\neq\mathbf{0}}\exp(i\mathbf{k}\cdot\mathbf{R}_i-\rho^2R_i^2)\right\}, \quad (57)$$

where $\mathbf{G}$ are the reciprocal lattice vectors. In Eq. (57) both sums converge rapidly and are suitable for direct numerical evaluation with subsequent integration. The sums S_1, S_2, and S_3 are directly related to the sum (57), for example,

$$\tilde{S}_2(\mathbf{k})\equiv\sum_{\mathbf{R}_i\neq\mathbf{0}}e^{i\mathbf{k}\cdot\mathbf{R}_i}\frac{X_i^2}{R_i^5}=-\frac{\partial^2}{\partial k_x^2}\sum_{\mathbf{R}_i\neq\mathbf{0}}\exp(i\mathbf{k}\cdot\mathbf{R}_i)R_i^{-5} \quad (58)$$

and

$$S_2(\mathbf{k})=\tilde{S}_2(\mathbf{k})-\tilde{S}_2(0). \quad (59)$$

This technique gives the value of $S_3=9.033\,621\,78$ (cf. Ref. 34). For the sake of numerical efficiency, the lattice sums $S_1(\mathbf{k})$ and $S_2(\mathbf{k})$ have been parametrized over the whole Brillouin zone (BZ). Our expressions have the correct asymptotical form for $\mathbf{k}\to\mathbf{0}$ (up to the k^2 terms) and a 1% accuracy over the whole BZ.

The variational parameters of the MF theory are $\langle a^\dagger_{\mathbf{k}}a_{\mathbf{k}}\rangle$ and $\langle a_{\mathbf{k}}a_{-\mathbf{k}}\rangle$, or, actually, their Fourier transforms for a few

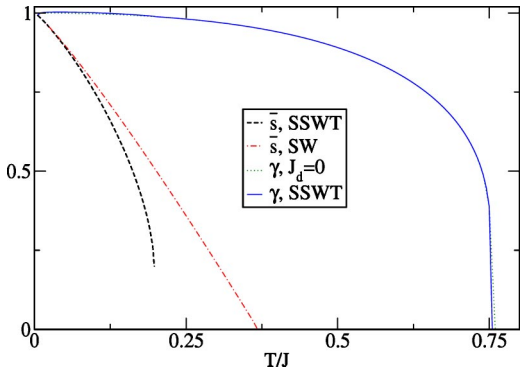

FIG. 2. (Color online) SSWT relative magnetization $\bar{s}$ and short-range order parameter γ vs temperature for $S=1/2$ and $j_d=10^{-3}$. For comparison, SW magnetization for $j_d=10^{-3}$, and γ from SSWT for $j_d=0$ (Mermin–Wagner situation) are also shown.

nearest-neighbor shells. $\gamma\bar{s}^2$ and $\gamma\delta$ models have just one and two parameters, respectively. Our own elaborate minimization schemes were used to find the values of the variational parameters which give a minimum of F'. In all cases, the chemical potential μ has been calculated on each iteration to ensure $\bar{S}=0$ in the paramagnetic region.

The numerical integration over the 2D BZ has been performed by the adaptive sevent-point Newton–Cotes method recursively, first for the x axis, then for the z axis. It is very important that the BZ integration is done by an adaptive method, since the main contributions to most integrals come from the region of very small k. The lower limit of integration k_{low} is a parameter which must be chosen small enough to achieve good convergence of the results. $k_{low}=10^{-12}$ has been found to be sufficient for all our calculations.

Special care has to be taken for very small k to achieve the stability of the code in spite of inevitable numerical errors. For example, $1-\cos k_{x,z}$ must be replaced by $k_{x,z}^2/2$. Also the Bose function must be replaced by $T/\epsilon_{\mathbf{k}}$ for $\epsilon_{\mathbf{k}} \ll T$ and by $\exp(-\epsilon_{\mathbf{k}}/T)$ for $\epsilon_{\mathbf{k}} \gg T$. The results appear to be rather insensitive to the particular cutoff values used. We used a k cutoff equal to 10^{-3} for $1-\cos k_{x,z}$. The lower cutoff for $\epsilon_{\mathbf{k}}/T$ in the Bose function was equal to 10^{-3}, and the upper cutoff was taken to be 20.

The double $\mathbf{k},\mathbf{q}$ integrals over the Brillouin zone were calculated in real space, with Fourier coefficients calculated by the Newton–Cotes method as described above. For the MF and $\gamma\delta$ models the inclusion of $n_x,n_z=-5,\ldots,+5$ neighbors has been found to be sufficient, while for the RPA correction to magnetization (Sec. V below), we have taken $n_x,n_z=-6,\ldots,+6$ neighbors. For the $\gamma\bar{s}^2$ model only the exchange interaction and not the dipolar one enters the double BZ integral; thus only the nearest-neighbor terms are present in the real-space sum.

IV. SSWT RESULTS

In Fig. 2 we present the relative magnetization $\bar{s}\equiv\bar{S}/S$ and the SRO parameter γ as a function of T from $\gamma\bar{s}^2$-SSWT for $S=1/2$ and $j_d=10^{-3}$. The SW magnetization curve is also shown for comparison. The two magnetization curves are rather different. SW theory gives an almost linear $\bar{S}(T)$ dependence and a spin-wave phase transition (second-order phase transition with $\beta=1$). On the contrary, SSWT gives a first-order phase transition (formally $\beta=0$). This means that the magnetization reaches a finite minimal value $\bar{s}_{min}\approx 0.199$ at $T_c/J\approx 0.1976$. After that point the ferromagnetic solution to the SSWT equations ceases to exist abruptly and the system goes to the paramagnetic state.

Both kinds of critical behavior are completely nonphysical. However, outside the narrow critical region, SSWT is definitely superior to SW theory, and the SSWT T_c is much smaller than the obviously overestimated SW T_c. In particular, all realistic (experimental and Monte Carlo) magnetization curves have a sharp fall at $T\to T_c$ and resemble much more the SSWT curve with a step than the linear SW curve. The SRO parameter γ is close to unity in a wide range of temperatures, until it finally falls to zero at $T_{SRO}/J\approx 0.75$. Thus SSWT describes correctly the experimentally confirmed[8] wide region with considerable short-range order above T_c. Two $\gamma(T)$ curves for $j_d=10^{-3}$ and $j_d=0$ (Mermin–Wagner situation) practically coincide; hence SRO is rather insensitive to the strength of the dipolar interaction and to the presence or absence of long-range order.

For $S=1/2, j_d=10^{-3}$ we have $\gamma(T_c)\approx 0.989$; therefore we can say that practically $\gamma=1$ up to T_c. However, for classical and large spins $\gamma(T_c)$ takes values of the order of $0.7-0.9$, depending on j_d. In the latter cases, SSWT renormalization of the exchange interaction (i.e. γ) and not only of the dipolar interaction ($\bar{s}^2$) is important. The same trend has been observed earlier for quasi-2D magnets; see Fig. 3 of Ref. 7, which shows stronger $\gamma(T)$ dependence for larger values of S.

For $j_d \ll 1$ and small S the $\gamma\bar{s}^2$ model takes a particularly simple form. In that case we can put $\gamma=1$ and the SSWT magnetization is given by Maleev's formula (29) with $J_d \to J_d\bar{s}^2$:

$$\bar{S}=S-\frac{T}{4\pi JS}\ln\left[\frac{2T}{\pi JS\sqrt{4\pi f}}j_d^{-3/2}\bar{s}^{-3}\right]. \tag{60}$$

Equation (60) does not allow for arbitrary $\bar{s}$, but only for $\bar{s}$ larger than $\bar{s}_{min}$ which minimizes the function

$$\bar{s}-\frac{3T}{4\pi JS^2}\ln(\bar{s}),\ \text{namely},\ \bar{s}_{min}=\frac{3T_c}{4\pi JS^2}, \tag{61}$$

with the equation for the SSWT T_c:

$$\frac{4\pi JS^2}{T_c}=\ln\left[\frac{4S}{\sqrt{\pi f}}j_d^{-3/2}\right]-2\ln\left[\frac{T_c}{4\pi JS^2}\right]+3(1-\ln 3). \tag{62}$$

There is no solutions of Eq. (60) for $T>T_c$; therefore the first-order character of the SSWT phase transition is fully contained in a simple equation (60).

For the classical case, one uses Eq. (33) with $J_d\to J_d\bar{s}^2$ and obtains the equation for classical SSWT T_c:

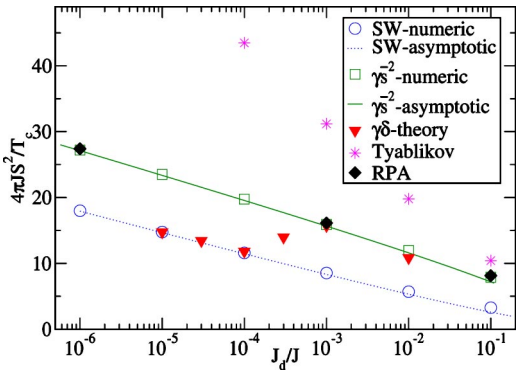

FIG. 3. (Color online) The transition temperature T_c vs dipolar interaction J_d from different approaches for $S=1/2$. The symbols are numerical results and the curves are the asymptotical formulae (31),(62).

$$\frac{4\pi JS^2}{T_c} = \ln\left[\frac{32}{\pi\sqrt{\pi f}} j_d^{-3/2}\right] - 3\ln\left[\frac{T_c}{4\pi JS^2}\right] + 3(1-\ln 3). \tag{63}$$

Note that the coefficient before the $\ln(T_c/4\pi JS^2)$ term has changed its value from +1 to −2 as compared to the free-magnon theory in the quantum case, and from 0 to −3 in the classical case (cf. Ref. 7). Similar equations in the case of layered magnets with small interlayer coupling and/or easy-axis anisotropy were obtained by the renormalization group method,[41] the magnetic ordering temperature being obtained as a crossover temperature.

The transition temperature as a function of j_d is shown in Fig. 3 for $S=1/2$. Several different approximations are presented. The $\gamma\bar{s}^2$-SSWT and SW curves are qualitatively similar, with the SSWT T_c being 1.5−2.5 times lower than the SW one. The asymptotical formulas (31),(62) work very well for $S=1/2$. The result of the $\gamma\delta$-SSWT, however, is quite different. The latter theory predicts rather different behavior for small and large j_d.

For $j_d \lesssim 10^{-4}$, the $\gamma\delta$-SSWT essentially reproduces SW behavior. Both γ and δ are close to unity in a wide range of temperatures, and they both go to zero at $T_{SRO}\approx 0.75$ (for $S=1/2$). This essentially implies that there is long-range order ($\delta\neq 0$) in the paramagnetic phase, which is inconsistent with observations. The magnetization curves and T_c in this region are very close to the free-magnon ones.

For $j_d \gtrsim 10^{-3}$ $\gamma\delta$-SSWT gives a first-order phase transition like that in the $\gamma\bar{s}^2$-SSWT, and δ goes to zero for $T\to T_c-0$, the value for T_c being also close to the $\gamma\bar{s}^2$-SSWT value. To summarize, the $\gamma\delta$-SSWT $T_c(j_d)$ curve has two regions: free-magnon-like and $\gamma\bar{s}^2$-SSWT-like with a crossover between them and a nonmonotonic $T_c(j_d)$ behavior. We find these results also completely nonphysical and conclude that $\gamma\delta$-SSWT is a bad approximation. Therefore we abandon it in favor of the $\gamma\bar{s}^2$-SSWT.

The Tyablikov approximation ($J\to\bar{s}J, J_d\to\bar{s}J_d$) result is also presented in Fig. 3. This approximation gives good T_c for 3D systems and also for anisotropic 2D systems.[12] The situation seems to be different for the system under consideration (2D ferromagnet with dipolar interaction and no anisotropy). T_c from the Tyablikov approximation is much smaller than the SSWT one, especially for small values of j_d. This approximation predicts a first-order phase transition with an enormous step of $\bar{s}_{min}\approx 1/2$ at T_c [which immediately follows from Eq. (29) upon the substitution $J\to\bar{s}J, J_d\to\bar{s}J_d$]. Also, by definition, it does not account for the short-range order above T_c.

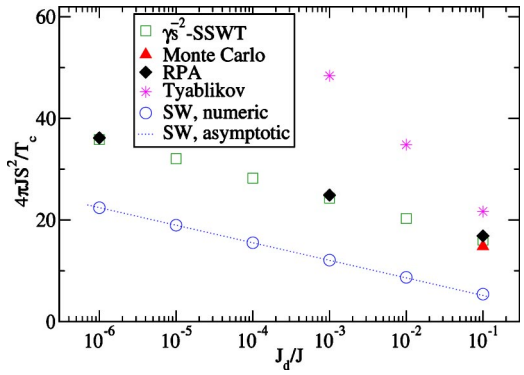

FIG. 4. (Color online) The transition temperature T_c vs dipolar interaction J_d from different approaches for classical spin. The symbols are numerical results and the curve is the free-magnon asymptotical formula (34). The Monte Carlo result for $J_d/J=0.1$ is taken from Ref. 30.

In Fig. 4 the T_c values from various approximations are compared again, this time for classical spins. A classical Monte Carlo (MC) result[30] for $j_d=0.1$ ($T_c/JS^2\approx 0.85$) is also presented in Fig. 4 for comparison. One can see that the SSWT value for T_c lies within 9% of the MC result, which is a good agreement for such a relatively simple and parameter-free approximation as SSWT. In contrast, the free-magnon and Tyablikov approximations are much less accurate. Because of this, and the factors mentioned above, the usefulness of the Tyablikov approximation for the 2D systems with dipolar interaction can be questioned. Note that the present discussion refers to the original Tyablikov decoupling, while more elaborate Green's function approaches[38,42,43] can give much better results, especially in the low-temperature region.

Figure 5 summarizes the spin dependence of the SSWT Curie temperature. As for the SW theory (Fig. 1), the quantum effects cannot be ignored, even for such a large spin as $S=7/2$. The formulas (62),(63), which work fine for small spins, fail for the large and classical ones, mainly due to the $\gamma=1$ approximation. In the latter case, the complete (numerical) form of $\gamma\bar{s}^2$-SSWT must be used.

V. RPA VERTEX CORRECTIONS

For the anisotropic or quasi-2D FM with $\Delta\ll 1$, SSWT results can be systematically improved by including a RPA-like correction to the magnon–magnon vertex.[7] Here we apply the same approximation to the FM with the dipolar interaction to investigate whether the RPA corrections are important also in this case. The approach outlined below is not exactly the standard RPA theory; however, for brevity, it will be called the "RPA approximation." The best justifica-

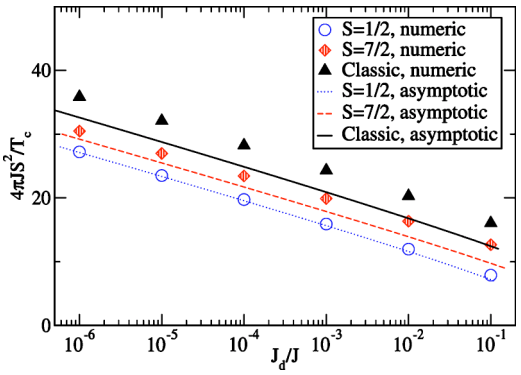

FIG. 5. (Color online) The $\gamma\bar{s}^2$-SSWT transition temperature T_c as a function of dipolar interaction J_d for different values of spin. The symbols are numerical results, while the curves are the asymptotical formulas (62),(63).

tion for such a procedure is a comparison with experiment, which has been done in Refs. 7, 20, and 41 for the cases of anisotropic and quasi-2D FMs.

The idea of the approximation is to renormalize the magnon–magnon vertex (49) in the RPA way, as shown in Fig. 6(a). The magnon Green's function of the $\gamma\bar{s}^2$-SSWT

$$G^t_{\mathbf{k}}(i\omega_n) = \frac{i\omega_n + \tilde{A}^t_{\mathbf{k}}}{(i\omega_n)^2 - (\tilde{\varepsilon}^t_{\mathbf{k}})^2}, \quad \omega_n \equiv 2\pi nT, \tag{64}$$

plays the role of the free-magnon Green's function (single lines in Fig. 6); namely, the exchange interaction is renormalized as $\tilde{J}=\gamma J$ (which is only important for large and classical spins), and the dipolar interaction is renormalized as $\tilde{J}_d=\bar{s}^2 J_d$; and we define $\tilde{j}_d \equiv \tilde{J}_d/\tilde{J}=\bar{s}^2 j_d/\gamma$.

The bare vertex (49) is first renormalized by the SSWT parameter γ:

$$\tilde{V} = \frac{1}{4N}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4} \phi(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_3,\mathbf{k}_4) a^\dagger_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a_{\mathbf{k}_3} a_{\mathbf{k}_4} \times \delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4), \tag{65}$$

where

$$\phi(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_3,\mathbf{k}_4) = \tilde{J}_{\mathbf{k}_3} + \tilde{J}_{\mathbf{k}_4} - \tilde{J}_{\mathbf{k}_1-\mathbf{k}_3} - \tilde{J}_{\mathbf{k}_1-\mathbf{k}_4}. \tag{66}$$

Provided that $k_1,\ldots,k_4 \ll 1$, ϕ becomes

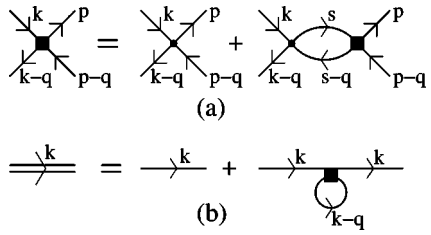

FIG. 6. The diagrams corresponding to the RPA renormalization of (a) magnon–magnon vertex and (b) magnon Green's function.

$$\phi(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_3,\mathbf{k}_4) \approx -2\tilde{J}\mathbf{k}_1\mathbf{k}_2. \tag{67}$$

This lowest-order expression would not suffice for SSWT, but we expect it to be good enough for calculating RPA vertex corrections.

The diagram in Fig. 6(a) corresponds to the integral equation for the renormalized vertex $\Phi(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_3,\mathbf{k}_4;i\omega_n)$:

$$\Phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p};i\omega_n) = \phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p}) - T\sum_{i\omega_n'}\sum_{\mathbf{s}} \phi(\mathbf{k},\mathbf{s}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{s}) \times G^t_{\mathbf{s}}(i\omega_n') G^t_{\mathbf{s}-\mathbf{q}}(i\omega_n'-i\omega_n)\Phi(\mathbf{s},\mathbf{p}-\mathbf{q};\mathbf{s}-\mathbf{q},\mathbf{p};i\omega_n). \tag{68}$$

Since the SSWT vertex ϕ does not depend on any Matsubara frequencies, the renormalized vertex Φ depends on one frequency $i\omega_n$ only. Below, when we are going to calculate the vertex correction to magnetization, the $i\omega_n=0$ term dominates, since it leads to logarithmic divergences. Therefore, we can neglect the frequency dependence of Φ and put $i\omega_n$ to zero in Eq. (68). Although the frequency sum

$$T\sum_{i\omega_n'} G^t_{\mathbf{s}}(i\omega_n') G^t_{\mathbf{s}-\mathbf{q}}(i\omega_n') \tag{69}$$

could be performed exactly, for $j_d \ll 1$ it can be replaced with its classical value $TG^t_{\mathbf{s}}(0)G^t_{\mathbf{s}-\mathbf{q}}(0)$ if the upper integration cutoff q_0^2 (equal to $T/\tilde{J}S$ and 32 for the quantum and classical cases, respectively) is simultaneously introduced. Equation (68) then becomes

$$\Phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p}) = \phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p}) - T\sum_{s<q_0} \phi(\mathbf{k},\mathbf{s}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{s}) \times G^t_{\mathbf{s}}(0) G^t_{\mathbf{s}-\mathbf{q}}(0)\Phi(\mathbf{s},\mathbf{p}-\mathbf{q};\mathbf{s}-\mathbf{q},\mathbf{p}). \tag{70}$$

We use the expression (67) for $\phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p})$ and seek the solution of Eq. (70) for given $\mathbf{p}$ and $\mathbf{q}$ in the form

$$\Phi(\mathbf{k}) \equiv \Phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p}) = \tilde{J}\mathbf{k}(A\mathbf{q}-B\mathbf{p}), \tag{71}$$

where A and B are yet unknown constants. Equation (70) becomes

$$\Phi(\mathbf{k}) = -2\tilde{J}\mathbf{k}\cdot(\mathbf{p}-\mathbf{q}) + \frac{2T}{S^2}\sum_{\alpha,\beta=x,z} k_\alpha (A_{q_\beta} - B_{p_\beta})\Lambda_{\alpha\beta}, \tag{72}$$

where

$$\Lambda_{\alpha\beta} = (\tilde{J}S)^2 \sum_{s<q_0} (s_\alpha - q_\alpha) s_\beta G^t_{\mathbf{s}}(0) G^t_{\mathbf{s}-\mathbf{q}}(0). \tag{73}$$

$\Lambda_{\alpha\beta}$ can be evaluated approximately with only logarithmically large terms being included. For $q^2 \gg \tilde{j}_d^{5/4}$ it is easy to show that

$$(\tilde{J}S)^2 \sum_{s<q_0} s_\beta G^t_{\mathbf{s}}(0) G^t_{\mathbf{s}-\mathbf{q}}(0) = \frac{q_\beta}{4\pi}\ln\left(\frac{q^2}{\tilde{j}_d^{3/2}}\right), \tag{74}$$

$$(\tilde{J}S)^2 \sum_{s<q_0} s_\alpha s_\beta G_{\mathbf{s}}^t(0) G_{\mathbf{s}-\mathbf{q}}^t(0) = \frac{q_\alpha q_\beta}{4\pi} \ln\left(\frac{q^2}{\tilde{j}_d^{3/2}}\right) + \frac{\delta_{\alpha\beta}}{8\pi} \ln\left(\frac{q_0^2}{q^2}\right) \tag{75}$$

and

$$\Lambda_{\alpha\beta} = \frac{\delta_{\alpha\beta}}{8\pi} \ln\left(\frac{q_0^2}{q^2}\right), \quad q^2 \gg \tilde{j}_d^{5/4}. \tag{76}$$

In the opposite limit we can put $\mathbf{q}=\mathbf{0}$ and

$$\Lambda_{\alpha\beta} = (\tilde{J}S)^2 \sum_{s<q_0} s_\alpha s_\beta [G_s^t(0)]^2 = \Lambda \delta_{\alpha\beta}, \tag{77}$$

where

$$\Lambda = \frac{1}{(2\pi)^2} \int_0^{q_0} k^3 dk \frac{(k^2 + 2\pi f \tilde{j}_d)^2}{(k^2 + 4\pi f \tilde{j}_d)^2} \times \int_0^{2\pi} d\varphi \frac{\cos^2\varphi}{(k^2 + 2\pi \tilde{j}_d k \sin^2\varphi)^2}, \tag{78}$$

where $f \approx 1.078$. As for the case of the integral in Eq. (27), the φ integral must be performed exactly before the k integral can be calculated. The result (again to logarithmic accuracy) is

$$\Lambda_{\alpha\beta} = \frac{\delta_{\alpha\beta}}{8\pi} \ln\left(\frac{q_0^2}{\tilde{j}_d^{5/4}}\right), \quad q^2 \ll \tilde{j}_d^{5/4}. \tag{79}$$

Equations (76) and (79) can be combined as

$$\Lambda_{\alpha\beta} = \Lambda \delta_{\alpha\beta}, \quad \Lambda = \frac{1}{8\pi} \ln\left[\frac{q_0^2}{\max(q^2, \tilde{j}_d^{5/4})}\right]. \tag{80}$$

This immediately gives the solution of Eq. (72):

$$A = B = \frac{2}{1 - (2T/\tilde{J}S^2)\Lambda} \tag{81}$$

and

$$\Phi(\mathbf{k},\mathbf{p}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{p}) = -\frac{2\tilde{J}\mathbf{k}\cdot(\mathbf{p}-\mathbf{q})}{1 - t \ln[q_0^2/\max(q^2, \tilde{j}_d^{5/4})]}, \tag{82}$$

where

$$t \equiv \frac{T}{4\pi \tilde{J} S^2}. \tag{83}$$

The renormalized vertex (82) is equal to the SSWT vertex (67) renormalized by a **q**-dependent denominator. For the anisotropic FM (Ref. 7) this denominator is essentially equal to the SSWT magnetization, but for the dipolar interaction this is no longer true.

The vertex-renormalized Green's function is given by the diagram in Fig. 6(b):

$$G_{\mathbf{k}}(i\omega_n) = G_{\mathbf{k}}^t(i\omega_n) - T G_{\mathbf{k}}^t(i\omega_n)^2 \times \sum_{i\omega_n'} \sum_{\mathbf{q}} \Phi(\mathbf{k},\mathbf{k}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{k}) G_{\mathbf{k}-\mathbf{q}}^t(i\omega_n'), \tag{84}$$

and the magnetization is

$$\begin{aligned} \overline{S} &= S + T \sum_{\mathbf{k}} \sum_{i\omega_n} G_{\mathbf{k}}(i\omega_n) \\ &= S + T \sum_{\mathbf{k}} \sum_{i\omega_n} G_{\mathbf{k}}^t(i\omega_n) - T^2 \sum_{\mathbf{k},\mathbf{q}} \sum_{i\omega_n, i\omega_n'} G_{\mathbf{k}}^t(i\omega_n)^2 G_{\mathbf{k}-\mathbf{q}}^t(i\omega_n') \\ &\quad \times \Phi(\mathbf{k},\mathbf{k}-\mathbf{q};\mathbf{k}-\mathbf{q},\mathbf{k}). \end{aligned} \tag{85}$$

The frequency sums are equal to

$$T \sum_{i\omega_n} G_{\mathbf{k}}^t(i\omega_n) = -\left[\frac{\tilde{A}_{\mathbf{k}}^t}{\tilde{\epsilon}_{\mathbf{k}}^t}\left(N(\tilde{\epsilon}_{\mathbf{k}}^t) + \frac{1}{2}\right) - \frac{1}{2}\right] \equiv -P_{\mathbf{k}}, \tag{86}$$

where $N(\epsilon) \equiv [\exp(\epsilon/T) - 1]^{-1}$ [cf. Eq. (23)]; and

$$T \sum_{i\omega_n} G_{\mathbf{k}}^t(i\omega_n)^2 = \frac{N'(\tilde{\epsilon}_{\mathbf{k}}^t)}{2(\tilde{\epsilon}_{\mathbf{k}}^t)^2}\left[2(\tilde{A}_{\mathbf{k}}^t)^2 - (\tilde{B}_{\mathbf{k}}^t)^2\right] + \frac{2N(\tilde{\epsilon}_{\mathbf{k}}^t) + 1}{4(\tilde{\epsilon}_{\mathbf{k}}^t)^2}(\tilde{B}_{\mathbf{k}}^t)^2 \equiv K_{\mathbf{k}}, \tag{87}$$

respectively. The classical limits of these two expressions are

$$P_{\mathbf{k}} \to \frac{T\tilde{A}_{\mathbf{k}}^t}{(\tilde{\epsilon}_{\mathbf{k}}^t)^2}, \quad K_{\mathbf{k}} \to \frac{T(\tilde{A}_{\mathbf{k}}^t)^2}{(\tilde{\epsilon}_{\mathbf{k}}^t)^4}. \tag{88}$$

The final expression for the magnetization is

$$\overline{S} = S - \sum_{\mathbf{k}} P_k - \sum_{\mathbf{k}\mathbf{p}} \frac{2\tilde{J}(\mathbf{k}\cdot\mathbf{p}) K_{\mathbf{k}} P_{\mathbf{p}}}{1 - t \ln[q_0^2/\max(|\mathbf{k}-\mathbf{p}|^2, \tilde{j}_d^{5/4})]}. \tag{89}$$

This equation should be solved self-consistently with Eq. (52) for γ and $\overline{S}$. As usual, we perform the double $\mathbf{k},\mathbf{p}$ integration in real space. The RPA values for T_c are presented in Figs. 3 and 4 for $S=1/2$ and classical spins, respectively. For spin 1/2 the RPA corrections to SSWT are negligible. For classical spins the RPA value for T_c is 1–5 % lower than the SSWT one, which is still a surprisingly small difference compared to the anisotropic FM.[7] Since the SSWT T_c is already lower than the Monte Carlo T_c for $j_d=0.1$, the RPA apparently does not improve the SSWT result.

CONCLUSION

In this paper we have investigated the thermodynamics of 2D quantum and classical Heisenberg ferromagnets with dipole-dipole interaction, mostly focusing on the Curie temperature. We have applied noninteracting spin-wave theory and various interacting spin-wave theories (SSWT, RPA, Tyablikov approximation). We have developed several forms of self-consistent spin-wave theory: mean-field SSWT, variational $\gamma\delta$-SSWT, and finally $\gamma\overline{s^2}$-SSWT. All these theories can be derived from the Feynman–Peierls–Bogoliubov variational principle with different constraints.

The idea of $\gamma\overline{s^2}$-SSWT is to renormalize the exchange interaction with a variational parameter γ and dipolar inter-

action with a phenomenological parameter $\overline{s^2}$. We have found that only this form of SSWT is able to provide physically meaningful results everywhere except in the narrow critical region. This situation is very similar to the case of an anisotropic magnet,[7] where a similar phenomenological coefficient is also necessary in order to build the SSWT formalism.

We have shown that the SSWT Curie temperature depends strongly on the spin S. Even for spin $S=7/2$ we found that T_c still differs from the classical one, namely, it is about 10% lower. This is an expected result, since the criterion for the classical regime ($T_c/JS \gg 1$) no longer implies $S \gg 1$, as for 3D systems, but rather $S \gg \ln(J/J_d)$. The parameter γ also shows strong spin dependence: for $S=1/2$ the value of γ at $T=T_c$ is almost exactly unity (no renormalization of exchange), while in the opposite limit of classical spins, $\gamma(T_c)$ is of the order of 0.7-0.9, depending on j_d.

For the classical spin and $J_d/J=0.1$ we have compared our results to a Monte Carlo calculation.[30] It turns out that the SSWT value for T_c is quite good (namely, it is 9% lower than the MC result), while the free-magnon and Tyablikov approximations give very bad estimates of T_c. The RPA corrections are negligible for $S=1/2$, while for the classical spin they reduce T_c by a few percent, worsening the agreement with the MC data. The dipolar case is thus considerably different from the anisotropic and quasi-2D FM cases,[7] where the SSWT T_c is always overestimated, while the RPA corrections reduce it significantly, improving the agreement with the experiment.

It is difficult to make a direct comparison of the present model with experiment, since realistic thin films usually have strong anisotropy and consist of more than one monolayer. However, the near-linear dependence of $1/T_c$ on $\ln(j_d)$ has been demonstrated in a Monte Carlo calculation.[29] This is a typical dependence for nearly-Mermin–Wagner systems, and a similar one has been previously established for anisotropic 2D ferromagnets.[44] The experiments[45,46] on thin films with in-plane magnetization show that T_c of the film is much lower than the bulk T_c, with thinner films having lower T_c. Application of SSWT to systems that possess both dipolar interaction and anisotropy and consist of more than one atomic layer is the topic of further investigation. In particular, phenomena such as reorientation transition and striped phases, which have been previously studied within the classical Heisenberg model,[21,31,34–36] should be considered.

Our conclusion is that SSWT is a relatively simple, computationally cheap, and reliable theory for studying two-dimensional spin systems with dipole-dipole interaction, with the ability to treat quantum spins being its strongest point.

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