# Critical behavior and the Néel temperature of quantum quasi-two-dimensional Heisenberg antiferromagnets

V. Yu. Irkhin\* and A. A. Katanin Institute of Metal Physics, Ekaterinburg 620219, Russia (Received 15 November 1996)

The nonlinear- $\sigma$  model and its generalization on *N*-component spins, the O(N) model, are considered to describe thermodynamics of a quantum quasi-two-dimensional (quasi-2D) Heisenberg antiferromagnet. A comparison with standard spin-wave approaches is performed. The sublattice magnetization, Néel temperature, and spin-correlation function are calculated to first order of the 1/N expansion. A description of crossover from a 2D-like to 3D regime of sublattice magnetization temperature dependence is obtained. The values of the critical exponents derived are  $\beta = 0.36$ ,  $\eta = 0.09$ . An account of the corrections to the standard logarithmic term of the spin-wave theory modifies considerably the value of the Néel temperature. The thermodynamic quantities calculated are universal functions of the renormalized interlayer coupling parameter. The renormalization of the interlayer coupling parameter turns out to be considerably temperature dependent. A good agreement with experimental data on La<sub>2</sub>CuO<sub>4</sub> is obtained. The application of the approach used to the case of a ferromagnet is discussed. [S0163-1829(97)02018-3]

#### I. INTRODUCTION

Great interest has been paid to properties of quasi-twodimensional (quasi-2D) antiferromagnets in connection with the investigations of layered perovskites<sup>1</sup> and copper-oxide systems, including high- $T_c$  superconductors. In particular, La<sub>2</sub>CuO<sub>4</sub> gives one of the best known examples of a quasi-2D system with small magnetic anisotropy. Unlike 2D systems, quasi-2D ones have finite values of magnetic ordering temperature. At small interlayer couplings J' the value of magnetic transition temperature is small in comparison with the intraplane exchange parameter J. There are a number of approximations which enable us to describe the thermodynamics of such systems. The standard spin-wave theory (SWT) takes into account only the spin-wave excitations which exist for quasi-2D systems in a wide temperature range up to about J (Refs. 2,3). SWT does not take into account the dynamic and kinematic interaction between spin waves, which are important at temperatures near magnetic phase transition point. By this reason, SWT gives too high values of the magnetic transition temperature. Recently, the self-consistent spin-wave theory<sup>2-4</sup> (SSWT) has been proposed which takes into account partially the interaction between spin waves. However, the value of the Néel temperature in SSWT is still too high in comparison with experiment, and the critical behavior is described quite incorrectly.

To describe the magnetic phase transition we have to take into consideration fluctuation (non-spin-wave) corrections to thermodynamic quantities. It is difficult to take into account such corrections in the standard technique of the Green's functions because of essentially nonlinear character of equations of motion. There exists the interpolation approximation by Tyablikov<sup>5</sup> which is based on the random-phase decoupling of equations of motion for the transverse spin Green's function. This approach often yields results which are roughly satisfactory from the experimental point of view. At the same time, it is difficult to justify and improve such approximations.

To develop a perturbation theory which correctly describes the critical behavior, we have to introduce a formal large parameter in the Heisenberg model. Thus the Heisenberg model can be treated as a model with a large degeneracy within the 1/N expansion. This expansion may be introduced in two different ways. The first way<sup>6-9</sup> treats the Heisenberg model as a particular case (M=2) of the SU(M) model (i.e., of the model with M states per spin degree of freedom at each site). Since the  $M \rightarrow \infty$  limit corresponds to SSWT (see, e.g., Ref. 4), at finite M thermodynamics is described in terms of the spin-wave picture of excitation spectrum. The second way 10,12 is to consider the Heisenberg model as a particular case (N=3) of the O(N)model (i.e., of the model with N-component spins). The limit  $N \rightarrow \infty$  gives the quantum spherical model and the large-N case corresponds to the fluctuation (non-spin-wave) picture. The advantage of the 1/N (or 1/M) expansions over, say, the quasiclassical 1/S expansion is their applicability near the phase transition temperature.

Since N=3 and M=2 are in fact not large, the convergence of such expansions must be investigated separately. For low-dimensional magnets with d=2 (see Ref. 7) and  $d=2+\varepsilon$  (Ref. 9) the results in the SU(M) model coincide in the zeroth order in 1/M with those of the one-loop renormalization-group (RG) analysis, and in the first order in 1/M with the results of the two-loop RG analysis. In these cases the 1/M corrections to thermodynamic quantities are small. However, quasi-2D systems belong to 3D symmetry group so that corresponding 1/M corrections are not small (see discussion in Ref. 9) and the series in 1/M is poorly convergent. Unlike the 1/M expansion in the SU(M) model, the first-order 1/N corrections in the O(N) model, which were considered in the quantum 2D case<sup>12</sup> and in the classical case at an arbitrary dimensionality  $2 \le d \le 4$  (see, e.g., Ref. 13), lead to results which are close to those obtained by

12 318

other methods. The applicability of the 1/N expansion at arbitrary dimensionality  $2 \le d \le 4$  is important for the investigation of quasi-2D systems since they demonstrate the dimensional crossover from 2D to 3D behavior (see, e.g., Ref. 1). On the other hand, the renormalization-group  $\varepsilon$  expansion is not appliciable for d=2 and d=3 simultaneously: for  $\varepsilon = d-2$  it cannot describe satisfactorily the case d=3 and vice versa, for  $\varepsilon = 4 - d$  the behavior at  $d \rightarrow 2$  is poor.

Thus, instead of direct calculation of corrections to SSWT, we start in this paper from the quantum spherical model,  $O(\infty)$  and then find the 1/N corrections. Although the results in the  $O(\infty)$  and SU( $\infty$ ) models are different, it will be shown that already in the first order in 1/N at low enough temperatures the results in the O(N) model are identical to those in SU( $\infty$ ) (i.e., in SSWT). At higher temperatures the results of SSWT are modified due to fluctuation corrections.

The plan of the paper is as follows. In Sec. II we review various approximations in the theory of quasi-2D systems, which are based on the spin-wave picture of excitation spectrum, and analyze the corresponding expressions for the Néel temperature. In Sec. III we formulate the O(N) model for the quasi-2D case and the technique of the 1/N expansion, which is a generalization of that by Chubukov *et al.*<sup>12</sup> for the 2D case. In Sec. IV we calculate the magnetization, Néel temerature, and spin-correlation function to first order in 1/N. In Sec. V we discuss our results and compare them with experimental data on La<sub>2</sub>CuO<sub>4</sub>.

#### II. SPIN-WAVE APPROXIMATIONS IN THE THEORY OF QUASI-2D ANTIFERROMAGNETS

We start from the Heisenberg Hamiltonian of a quasi-2D antiferromagnet

$$H = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j \tag{1}$$

with the exchange interactions  $J_{i,i+\delta} = J$  for  $\delta$  in a plane and  $J_{i,i+\delta} = J'$  for  $\delta$  perpendicular to the planes.

At small values of interlayer coupling J' it is possible to derive analytical results for the Néel temperature. First we consider the standard spin-wave theory. The spectrum of spin waves has the form

$$E_{\mathbf{q}}^{\rm SWT} = S(J_0^2 - J_{\mathbf{q}}^2)^{1/2}, \qquad (2)$$

where  $J_q$  is the Fourier transforms of the exchange parameter

$$I_{\mathbf{q}} = 2J(\cos q_x + \cos q_y) + 2J' \cos q_z. \tag{3}$$

The sublattice magnetization is determined by

$$\overline{S} = S + \frac{1}{2} - \sum_{\mathbf{q}} \frac{J_0 S}{2E_{\mathbf{q}}} \operatorname{coth} \frac{E_{\mathbf{q}}}{2T}.$$
(4)

For small values of J'/J SWT yields different analytical expressions for the Néel temperature in the quantum regime  $(T_{\text{Néel}} \ll JS)$  and classical regime  $(T_{\text{Néel}} \gg JS)$ . We have

$$T_{\text{N\'eel}}^{\text{SWT}} = 4 \,\pi J S^2 \times \begin{cases} 1/\ln(T_{\text{N\'eel}}^2/8JJ'S^2) & \ln(J/J') \ge 2 \,\pi S \\ 1/\ln(Jq_0^2/J') & 1 \ll \ln(J/J') \ll 2 \,\pi S. \end{cases}$$
(5)

Here  $q_0 \approx \pi$  is a cutoff parameter determined by the boundary of the Brillouin zone. Note that for the quantum case the main contribution to integrals over the wave vector comes from the region with  $q \leq T$ , while in the classical case the value of  $T_{\text{Néel}}$  is determined by the whole Brillouin zone.

The spin-wave spectrum in SSWT and the Tyablikov approach is renormalized in different ways. SSWT (Refs. 2–4) takes into account the interaction between spin waves in the simplest self-consistent Born approximation. There exist several generalizations of SSWT on quasi-2D systems.<sup>14–16</sup> We will follow the approach of Refs. 14,16 which gives more satisfactory results at small J'/J. The spin-wave spectrum in SSWT has the form

$$E_{\mathbf{q}}^{\rm SSWT} = S(\gamma_0^2 - \gamma_{\mathbf{q}}^2)^{1/2}, \tag{6}$$

$$\gamma_{\mathbf{q}} = 2 \gamma (\cos q_x + \cos q_y) + 2 \gamma' \cos q_z$$

where  $\gamma$  and  $\gamma'$  are the renormalized exchange parameters which are determined from the self-consistent equations

$$\gamma/J = \sum_{\mathbf{q}} \frac{\gamma_{\mathbf{q}}S}{E_{\mathbf{q}}} \cos q_x \coth \frac{E_{\mathbf{q}}}{2T} + 2\overline{S}(T), \tag{7}$$

$$\gamma'/J' = \sum_{\mathbf{q}} \frac{\gamma_{\mathbf{q}}S}{E_{\mathbf{q}}} \cos q_z \coth \frac{E_{\mathbf{q}}}{2T} + 2\overline{S}(T).$$
(8)

The sublattice magnetization is given by

$$\overline{S} = S + \frac{1}{2} - \sum_{\mathbf{q}} \frac{\gamma_0 S}{2E_{\mathbf{q}}} \operatorname{coth} \frac{E_{\mathbf{q}}}{2T}.$$
(9)

At small values of J'/J we have

$$\overline{S} = \overline{S}_0 - \frac{T}{4\pi\gamma S} \times \begin{cases} \ln(T^2/8\gamma\gamma'S^2) & S(JJ')^{1/2} \ll T \ll JS \\ \ln(\gamma q_0^2/\gamma') & JS \ll T \ll JS^2, \end{cases}$$
(10)

where  $\overline{S}_0$  is the sublattice magnetization in the ground state. The quantity  $\gamma$  varies slowly with temperature in the whole region  $T < T_{\text{N\acute{e}l}}$  and may be replaced by its zero-temperature value  $\gamma(0)$ . According to Refs. 2 and 3 we have

$$\gamma(0) = 1.1571J, \quad \overline{S}_0 = 0.3034$$
 (11)

for S = 1/2 and  $\gamma(0) = J$ ,  $\overline{S}_0 = S$  for  $S \to \infty$ . The second case in Eq. (10) may be realized only in the classical limit  $S \ge 1$ . One can see from Eq. (10) that the value of the critical exponent for the magnetization is  $\beta_{SW}=1$ . The same critical behavior takes place at an arbitrary d > 2. This result is correct only at  $d=2+\varepsilon$  to leading order in  $\varepsilon$  ( $\beta=1-2\varepsilon$ , see, e.g., Refs. 10,9), and for higher dimensionalities  $\beta < 1$ .

As follows from Eq. (10), the Néel temperature is determined by (see Ref. 14; note that some coefficients in this paper are incorrect)

$$T_{\text{N\acute{e}el}}^{\text{SSWT}} = 4 \pi \gamma_c S \overline{S}_0 \\ \times \begin{cases} 1/\ln(T_{\text{N\acute{e}el}}^2/8 \gamma_c \gamma_c' S^2) & \ln(J/J') \ge 2 \pi S \\ 1/\ln(q_0^2 \gamma_c / \gamma_c') & 1 \le \ln(J/J') \le 2 \pi S. \end{cases}$$

$$(12)$$

Here  $\gamma_c \approx \gamma(0)$  and  $\gamma'_c$  are the renormalized exchange parameters at  $T = T_{\text{N\acute{e}el}}$ , The value of  $\gamma'_c$  determined from Eq. (8) is

$$\gamma_c' = (T_{\text{N\'eel}}/4\pi\gamma_c S^2)J' \tag{13}$$

in both the quantum and classical regimes. Note that the renormalization of the interlayer coupling in Eq. (12) plays a crucial role in lowering the Néel temperature in comparison with its SWT value (5) since  $\gamma_c \gamma'_c / JJ' = T_{\text{Néel}} / 4\pi JS^2 \ll 1$ .

In the Tyablikov theory<sup>5</sup> (TT) the excitation spectrum has the form

$$E_{\mathbf{q}}^{\mathrm{TT}} = \overline{S}(J_0^2 - J_{\mathbf{q}}^2)^{1/2}.$$
 (14)

As well as in a ferromagnet, the proportionality of the spectrum to  $\overline{S}$  is not quite correct at low temperatures: in the antiferromagnet the spin-wave frequency varies as  $T^4$ , while the sublattice magnetization as  $T^2$  (see, e.g., Ref. 17). The equation for  $\overline{S}$  at S = 1/2 reads

$$1/\overline{S} = \sum_{\mathbf{q}} \frac{J_0 \overline{S}}{E_{\mathbf{q}}} \tanh \frac{E_{\mathbf{q}}}{2T}$$
(15)

and has a more complicated form for higher spins.<sup>5</sup> Near the Néel temperature TT yields at arbitrary *S* and any space dimensionality d>2

$$\overline{S} = \left[ \frac{2\Gamma_S T_{\text{N\'eel}}^{\text{TT}}}{SJ_0} \left( 1 - \frac{T}{T_{\text{N\'eel}}^{\text{TT}}} \right) \right]^{1/2}, \quad (16)$$

where  $\Gamma_S$  is some function of *S*,  $\Gamma_{1/2}=3$ . Thus, unlike SSWT, the critical exponent for the magnetization has the standard mean-field value,  $\beta_{TT}=1/2$ . For small J'/J, TT yields

$$T_{\text{N\acute{e}el}}^{\text{TT}} \approx \frac{4 \, \pi J S^2}{\ln(J q_0^2 / J')}.$$
(17)

The result (17) is lower than the SSWT value (12) and closed to experimental data (see Sec. V). On the other hand, the result (17) coincides with that of the spherical model [which is adequate only in the classical limit  $S \rightarrow \infty$  (Refs. 18,19)] and with the result of the spin-wave approximation (5) in the classical regime  $T_{\text{N\acute{e}el}} \gg JS$ . The Tyablikov approximation gives the same result (17) (with the replacement  $J \rightarrow -J, J' \rightarrow -J'$ ) for the Curie temperature of a ferromagnet (J, J' < 0). This demonstrates that near the critical temperature TT does not take into account quantum fluctuations which are important for small values of *S*. Thus we may conclude that TT is satisfactory from the practical, but not from theoretical point of view.

To leading logarithmic accuracy, all the discussed approaches give the same value of the Néel temperature. However, this accuracy is insufficient to treat experimental data. In particular, the factor of  $q_0^2 \sim 10$  in the classical regime is often not taken into account (see, e.g., Ref. 1), although this factor gives an essential contribution to  $T_{\text{Néel}}$ .

To improve the description of the critical region and obtain a better appoximation for the Néel temperature in the quantum case, it is necessary to take into account fluctuation corrections to the spin-wave theory result for  $T_{\text{Néel}}$  Eq. (5) more correctly than in SSWT and TT. To this end we use in the next sections the 1/N expansion in the O(N) model.

### III. THE QUANTUM NONLINEAR- $\sigma$ MODEL AND O(N) MODEL FOR QUASI-2D QUANTUM ANTIFERROMAGNETS

To describe thermodynamics of quantum antiferromagnets we consider the nonlinear- $\sigma$  model which was proposed for the one-dimensional Heisenberg model in Ref. 20. In the 2D case this model was applied in Refs. 11,12. The large value of the correlation length  $\xi \gg a$  (*a* is the lattice parameter in the plane) plays a crucial role in the Haldane's mapping of an antiferromagnetic Heisenberg model (1) to the quantum nonlinear- $\sigma$  model (see, e.g., Ref. 4). This gives a possibility to separate and integrate out the "fast" modes with space scale  $l \leq \Lambda^{-1}$  ( $\Lambda$  satisfies to  $\xi^{-1} \ll \Lambda \ll a^{-1}$ ) retaining "slow" modes with  $l > \Lambda^{-1}$ .

In the quasi-2D case we have  $\xi(T \le T_{\text{N\acute{e}el}}) = \infty$ . However, at small q we have

$$J_0 - J_q \simeq J(aq)^2 + 2J'(1 - \cos q_z).$$
(18)

Thus besides the "true" correlation length  $\xi$ , there exists also another variable with scaling dimensionality of length

$$\xi_{J'} = 1/\alpha^{1/2} \gg a, \tag{19}$$

where  $\alpha = 2J'/Ja^2$  is the interlayer coupling parameter; in this paper we consider only the case where  $\alpha \ll 1$ . On the scale of order of  $\xi_{J'}$  the regime of fluctuations changes from 2D to 3D. Thus we may use the scale  $\xi_{J'}$  to separate fast and slow modes in the Haldane's mapping. Depending on the value of the imaginary time slab thickness

$$L_{\tau} = c/T \tag{20}$$

 $(c \sim JSa$  is the fully renormalized spin-wave velocity), three regimes are possible: (i)  $L_{\tau} \sim \xi_{J'}$ , or, equivalently,  $T \sim \alpha^{1/2}c \sim (JJ')^{1/2}$ . This is an analog of the quantum critical regime  $L_{\tau} \sim \xi$  in the 2D case,<sup>11,12</sup> (ii)  $a \ll L_{\tau} \ll \xi_{J'}$ , i.e.  $\alpha^{1/2}c \ll T \ll c$  which is an analog of the renormalized classical regime  $a \ll L_{\tau} \ll \xi$  in the 2D case, and (iii) the classical regime  $L_{\tau} \ll a$  (i.e.,  $JS \ll T$ ).

Since regime (i) is well described by the standard spinwave theory (or by SSWT), we do not treat the thermodynamics at temperatures of order of  $(JJ')^{1/2}$ . From Eqs. (5) and (12) one can see that  $T_{\text{N\acute{e}el}} \ge (JJ')^{1/2}$ . In regimes (ii) and (iii) implementation of principles of finite-size scaling gives

$$T_{\text{N\'eel}} = \rho_s \Phi(\xi_{J'} / L_\tau, \xi_{J'} / a),$$

where  $\rho_s \sim JS^2$  is the fully renormalized spin stiffness,  $\Phi(x,y)$  is a scaling function with  $\Phi(\infty,\infty)=0$ . In regime (ii) we have  $\xi_{J'}/L_{\tau} \ll \xi_{J'}/a$ , so that

$$T_{\text{N\acute{e}el}} = \rho_s \Phi(\xi_{J'}/L_{\tau}, \infty) = \rho_s \Phi_q(T_{\text{N\acute{e}el}}/\alpha^{1/2}c), \quad (21)$$

while in regime (iii)  $\xi_{J'}/L_{\tau} \gg \xi_{J'}/a$  and

$$T_{\text{N\'eel}} = \rho_s \Phi(\infty, \xi_{J'}/a) = \rho_s \Phi_{\text{cl}}(1/\alpha^{1/2}a).$$
(22)

Note that the results of SWT Eq. (5) and SSWT Eq. (12) for the Néel temperature agree with Eq. (21) for the quantum regime and with Eq. (22) for the classical regime. At the same time, the result of the Tyablikov approximation (17) satisfies the classical regime scaling form (22) for all spin values, which confirms the absence of quantum fluctuations at the critical temperature in this approximation. As follows from Eq. (22), the value of the Néel temperature in the classical regime depends on fluctuations on a scale of order of the lattice constant, i.e., is nonuniversal. Therefore in this regime we cannot eliminate fast modes by Haldane's mapping. Further we will assume that the "renormalized classical" regime (ii) takes place.

We use the same procedure as used by  $Haldane^{20}$  (see full discussion in Ref. 4) to integrate out fast modes. Thus the partition function has in terms of a path integral the form

$$Z = \int D\boldsymbol{\sigma}_{i}(\tau) \exp\left\{-\frac{\chi_{0}}{2} \int_{0}^{1/T} d\tau \sum_{i} (\partial_{\tau}\boldsymbol{\sigma}_{i})^{2} - \frac{1}{2} S^{2} \int_{0}^{1/T} d\tau \sum_{ij} J_{ij}(\boldsymbol{\sigma}_{i} - \boldsymbol{\sigma}_{j})^{2}\right\} \prod_{i} \delta(\boldsymbol{\sigma}_{i}^{2} - 1),$$
(23)

where  $\boldsymbol{\sigma}$  is a three-component unit-length vector field, *i* is the index of a site,  $\chi_0$  is the uniform magnetic susceptibility. In the continual limit we reproduce the standard threedimensional quantum nonlinear- $\boldsymbol{\sigma}$  model. However, in the quasi-2D case the large value of  $\xi_{J'}$  gives a possibility to pass to the continual limit only within the layers:  $\boldsymbol{\sigma}_i(\tau) \rightarrow \boldsymbol{\sigma}_{i_z}(\mathbf{r}, \tau)$  where **r** is a 2D vector,  $i_z$  is the index of a layer. The partition function takes the form

$$Z = \int D\boldsymbol{\sigma}_{i_{z}}(r,\tau) \exp\left\{-\frac{\rho_{s}^{0}}{2} \int_{0}^{1/T} d\tau \int d^{2}\mathbf{r} \sum_{i_{z}} \left[\frac{1}{c_{0}^{2}} (\partial_{\tau}\boldsymbol{\sigma}_{i_{z}})^{2} + (\boldsymbol{\nabla}\boldsymbol{\sigma}_{i_{z}})^{2} + \frac{\alpha}{2} (\boldsymbol{\sigma}_{i_{z}+1} - \boldsymbol{\sigma}_{i_{z}})^{2}\right]\right\} \delta(\boldsymbol{\sigma}_{i_{z}}^{2} - 1), \qquad (24)$$

where  $\rho_s^0 = JS^2$  is the bare spin stiffness,  $c_0 = (\rho_s^0/\chi_0)^{1/2}$  is the bare value of the spin-wave velocity. Here and hereafter we use the system of units where a = 1.

To pass to the O(N) model we replace the threecomponent field  $\sigma_{i_z}(\mathbf{r}, \tau)$  with the *N*-component one  $\sigma_{i_z}^m(\mathbf{r}, \tau), m=1...N$ . The constraint condition  $\sigma^2=1$  may be taken into account by introducing the slave field  $\lambda_{i_z}(\mathbf{r}, \tau)$ . To calculate the dynamic susceptibility we also introduce the external nonuniform time-dependent magnetic field  $h_{i_z}^m(\mathbf{r}, \tau)$ . Then we obtain the partition function of the O(N) model in the form

$$Z[h] = \int D\sigma D\lambda \exp\left\{-\frac{1}{2g} \int_{0}^{1/T} d\tau \int d^{2}\mathbf{r} \sum_{i_{z}} \left[\frac{1}{c_{0}^{2}} (\partial_{\tau}\sigma_{i_{z}})^{2} + (\nabla \sigma_{i_{z}})^{2} + \frac{\alpha}{2} (\sigma_{i_{z}+1} - \sigma_{i_{z}})^{2} + i\lambda (\sigma_{i_{z}}^{2} - 1) - 2gh_{i_{z}} (\sigma_{i_{z}} - \overline{\sigma})\right]\right\},$$
(25)

where  $g = N/\rho_s^0$  is the coupling constant,  $\overline{\sigma}^m = \langle \sigma_{i_z}^m(\mathbf{r}, \tau) \rangle$  is the average part of the field  $\sigma$ , which is supposed to be static and uniform. After integrating over  $\overline{\sigma} = \sigma - \overline{\sigma}$  the partition function takes the form

$$Z[h] = \int D\lambda \exp(NS_{\text{eff}}[\lambda, h]), \qquad (26)$$

$$S_{\text{eff}}[\lambda,h] = \frac{1}{2} \operatorname{Indet} \hat{G}_0 + \frac{1}{2g} (1 - \overline{\sigma}^2) \operatorname{Sp}(i\lambda) + \frac{1}{2g} \operatorname{Sp}[(i\lambda\overline{\sigma} - h/\rho_s^0) \hat{G}_0(i\lambda\overline{\sigma} - h/\rho_s^0)],$$
(27)

where

$$\hat{G}_0 = \left[ \partial_{\tau}^2 / c_0^2 + \nabla^2 + \alpha \Delta_z \right]^{-1},$$

$$\Delta_z \sigma_{i_z}(\mathbf{r}, \tau) = \sigma_{i_z+1}(\mathbf{r}, \tau) - \sigma_{i_z}(\mathbf{r}, \tau).$$
(28)

Since *N* enters Eq. (26) only as a prefactor in the exponent, expanding near the saddle point generates a series in 1/N. At  $T < T_{\text{N\acute{e}el}}$  we have the saddle-point value  $i\lambda = 0$  and  $\overline{\sigma}^2 \neq 0$ . The Green's function of the field  $\overline{\sigma}$  is defined by

$$G^{mn}(\mathbf{q}, q_z, \omega_n) = \frac{\rho_s^0}{Z[0]} \int \frac{d^2 \mathbf{p}}{(2\pi)^2} \int \frac{dp_z}{2\pi} \sum_{\omega_l} \times \frac{\partial^2 Z[h]}{\partial h^m(p, p_z, \omega_l) \partial h^n(\mathbf{q} - \mathbf{p}, q_z - p_z, \omega_{l-n})} \bigg|_{h=0},$$
(29)

where  $h(\mathbf{p}, p_z, \omega)$  is the Fourier transform of  $h_{i_z}(\mathbf{r}, \tau)$ . Note that only diagonal elements  $G^{mm}$  are nonzero, and they are proportional to the nonuniform dynamic spin susceptibility:

$$G^{mn}(\mathbf{q},q_z,\omega) = \frac{\rho_s^0}{S^2} \chi^{mm}(\mathbf{q}+\mathbf{Q},q_z+\pi,\omega)\,\delta_{mn}\,,\qquad(30)$$

where  $\mathbf{Q} = (\pi, \pi)$  is the wave vector of antiferromagnetic structure in the plane; for N=3

$$\chi^{\alpha\beta}(\mathbf{q}, q_z, \omega) = \sum_i e^{i(\mathbf{q}\mathbf{R}_i + q_z R_i^z)} \langle \langle S_0^{\alpha} | S_i^{\beta} \rangle \rangle_{\omega}, \qquad (31)$$

where  $S_i^{\alpha}$  are spin operators,  $\alpha, \beta = x, y, z$ . Since the partition function Z[0] is invariant under rotations in the spin space, further we will assume  $\overline{\sigma}^m = \overline{\sigma} \delta_{mN}$  where  $\overline{\sigma}$  plays the role of the relative sublattice magnetization  $\overline{S}/S$ . Then  $G^{NN}$  corresponds to the longitudinal Green's function,  $G_l$ , while other diagonal components (wich are all equal) to the transverse Green's function,  $G_t$ . At  $T < T_{\text{Néel}}$ , the value of  $\overline{\sigma}$  is determined by the constraint  $\langle \sigma^2 \rangle = 1$  which takes the form

$$1 - \overline{\sigma}^2 = \frac{T}{\rho_s^0} \sum_{\omega_n} \sum_m \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \int \frac{dk_z}{2\pi} G^{mm}(k, k_z, \omega_n).$$
(32)

We use the relativistic (hard) cutoff  $\omega_n^2 + k^2 < \Lambda^2$  of frequency summations and momentum integrations; in this regularization scheme the value of the bare spin-wave velocity  $c_0$  is replaced by the fully renormalized one, c, which will be putted to be equal to unity except for the final results.

In the limit  $N \rightarrow \infty$  we may replace in Eq. (27)  $\lambda$  by its saddle-point value to obtain the "free" Green's function (which is the same for transverse and longitudinal components)

$$G_0(k,k_z,\omega_n) = [\omega_n^2 + k^2 + \alpha(1 - \cos k_z)]^{-1}.$$
 (33)

After evaluation of the integrals and frequency summation in Eq. (32) we obtain the Néel temperature in the limit  $N \rightarrow \infty$ 

$$T_{\text{N\acute{e}el}}^{0} = \frac{4 \pi \rho_s^{N=\infty}}{N \ln(2T_{\text{N\acute{e}el}}^{2}/\alpha)},$$
(34)

where  $\rho_s^{N=\infty} = N(1/g - 1/g_c)$  is the renormalized spin stiffness in zeroth order in 1/N,  $g_c = 2\pi^2/\Lambda$ . To compare the result (34) with the result of the SSWT we note that the value of spin stiffness in SSWT is  $\rho_s^{\text{SSWT}} = \gamma S \overline{S_0}$  (for S = 1/2 this equals 0.176J which is somewhat lower than the result of two-loop RG analysis<sup>21</sup> and numerical calculations,<sup>22</sup>  $\rho_s = 0.181J$ ) and the value of the spin-wave velocity is  $c^{\text{SSWT}} = \sqrt{8} \gamma S$ . Thus we see that the value (34) is N times smaller than the corresponding SSWT value (12) (besides that, in SSWT  $\alpha$  is replaced by its renormalized value,  $\alpha_c^{\text{SSWT}} = 2\gamma'_c/\gamma_c < \alpha$ ). Further we will show that, as well as in the calculation<sup>12</sup> of the correlation length in the 2D case in the first order in 1/N, (i) the factor of N in the denominator of Eq. (34) is to be replaced by N-2, (ii)  $\rho_s^{N=\infty}$ and  $\alpha$  in Eq. (34) are to be replaced by their renormalized values,  $\rho_s$  and  $\alpha_c$ , (iii) terms of order of  $\ln \ln(2T^2/\alpha)$  and unity, which do not enter the SSWT result for  $T_{\text{Néel}}$ , occur in the denominator of Eq. (34).

The exact Green's function may be expressed as

$$G^{mm}(k,k_{z},\omega_{n}) = [\omega_{n}^{2} + k^{2} + \alpha(1 - \cos k_{z}) + \Sigma(k,k_{z},\omega_{n})]^{-1} - C(k,k_{z},\omega_{n})\delta_{mN}.$$
(35)

To first order in 1/N the self-energy  $\Sigma(k,k_z,\omega_n)$  and the function  $C(k,k_z,\omega_n)$ , which describes renormalizations owing to the long-range order, are given by<sup>12</sup>

$$\begin{split} \Sigma(k,k_z,\omega_n) \\ &= \frac{2T}{N} \sum_{\omega_m} \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{dq_z}{2\pi} \\ &\times \frac{G_0(\mathbf{k} + \mathbf{q},k_z + q_z,\omega_n + \omega_m) - G_0(q,q_z,\omega_m)}{\widetilde{\Pi}(q,q_z,\omega_m)}, \end{split}$$

(36)

$$C(k,k_z,\omega_n) = \frac{2\,\overline{\sigma}^2}{g} \frac{1}{\widetilde{\Pi}(k,k_z,\omega_n)},\tag{37}$$

 $\widetilde{\Pi}(q,q_z,\omega_n) = \Pi(q,q_z,\omega_n) + \frac{2}{g}\overline{\sigma}^2 G_0(q,q_z,\omega_n), \quad (38)$ 

$$\Pi(q,q_z,\omega_n) = T \sum_{\omega_l} \int \frac{d^2 \mathbf{p}}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{dp_z}{2\pi} \times G_0(\mathbf{p}+\mathbf{q},p_z+q_z,\omega_l+\omega_n) G_0(p,p_z,\omega_l).$$
(39)

Note that the quantity *C* in Eq. (37) has in fact the zeroth order in 1/N, but the corresponding contribution to the constraint is of order of 1/N. The polarization operator  $\Pi(q,q_z,\omega_n)$  determines the longitudinal Green's function in the zeroth order in 1/N

$$G_l^{N=\infty}(q,q_z,\omega_n) = \frac{\prod(q,q_z,\omega_n)}{q^2 \prod(q,q_z,\omega_n) + 2\,\overline{\sigma}^2/g}.$$
 (40)

To first order in 1/N the constraint (32) takes the form

$$1 - \overline{\sigma}^{2} = gT \sum_{\omega_{m}} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} \int \frac{dk_{z}}{2\pi} G_{0}(k,k_{z},\omega_{m})$$
$$-gT \sum_{\omega_{m}} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} \int \frac{dk_{z}}{2\pi} G_{0}^{2}(k,k_{z},\omega_{m}) \Sigma(k,k_{z},\omega_{m})$$
$$-\frac{2\overline{\sigma}^{2}T}{N} \sum_{\omega_{m}} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} \int \frac{dk_{z}}{2\pi} \frac{G_{0}^{2}(k,k_{z},\omega_{m})}{\widetilde{\Pi}(k,k_{z},\omega_{m})}.$$
(41)

Following Ref. 12 we introduce the function

$$I(k,k_{z},\omega_{m}) = T \sum_{\omega_{n}} \int \frac{d^{2}\mathbf{q}}{(2\pi)^{2}} \int \frac{dq_{z}}{2\pi} G_{0}^{2}(q,q_{z},\omega_{n})$$
$$\times [G_{0}(\mathbf{k}+\mathbf{q},k_{z}+q_{z},\omega_{m}+\omega_{n})$$
$$-G_{0}(k,k_{z},\omega_{m})]$$
(42)

and represent Eq. (41) in the following convenient form:

$$1 = gT \sum_{\omega_m} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \int \frac{dk_z}{2\pi} G_0(k, k_z, \omega_m) - gR(T, x_{\overline{\sigma}}) + \overline{\sigma}^2 [1 - F(T, x_{\overline{\sigma}})], \qquad (43)$$

where

$$R(T, x_{\overline{\sigma}}) = \frac{2T}{N} \sum_{\omega_m} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \int \frac{dk_z}{2\pi} \frac{I(k, k_z, \omega_m)}{\widetilde{\Pi}(k, k_z, \omega_m)}, \quad (44)$$

$$F(T, x_{\overline{\sigma}}) = \frac{2T}{N} \sum_{\omega_m} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \int \frac{dk_z}{2\pi} \frac{G_0^2(k, k_z, \omega_m)}{\widetilde{\Pi}(k, k_z, \omega_m)}, \quad (45)$$

and

$$x_{\overline{\sigma}} = 4\pi \overline{\sigma}^2 / gT. \tag{46}$$

The calculation of functions I,  $\Pi$  for the quasi-2D case is presented in Appendix A.

Thus the functions R and F determine the 1/N corrections to the constraint. Expressions (43)–(45) enable one to investigate the magnetization and to calculate the Néel temperature for a quantum quasi-2D antiferromagnet.

where

## IV. THE SUBLATTICE MAGNETIZATION, NÉEL TEMPERATURE, AND CORRELATION FUNCTIONS

As discussed in the beginning of the previous section, we consider the quantum case with  $\alpha$  being small enough to satisfy the condition  $\ln(2T_{\text{N\'eel}}^2/\alpha c^2) \ge 1$ . The calculation of the functions *R* and *F* at  $T \ge \alpha^{1/2}$  [i.e.,  $T \ge (JJ')^{1/2}$ ] is discussed in Appendix B. Neglecting the terms of order of  $1/\ln(2T_{\text{N\'eel}}^2/\alpha c^2)$  we have

$$R(T, x_{\overline{\sigma}}) = \frac{T}{2\pi N} \ln \frac{2T^2}{\alpha} - \frac{(3+2x_{\overline{\sigma}})T}{4\pi N} \ln \frac{4\pi\rho_s}{NTx_{\overline{\sigma}}} + \frac{T}{2\pi N} \frac{\ln(2T^2/\alpha)}{\ln(2T^2/\alpha) + x_{\overline{\sigma}}} + \frac{8T}{3\pi^3 N} \ln \frac{2T^2}{\alpha} \ln \frac{N\Lambda}{16\rho_s} - \frac{2T}{3\pi^3 N} \ln \frac{N\Lambda}{16\rho_s} + \frac{T}{4\pi} I_1(x_{\overline{\sigma}})$$
(47)

and

$$F(T, x_{\overline{\sigma}}) = \frac{1}{N} \ln \frac{4\pi\rho_s}{NTx_{\overline{\sigma}}} + \frac{8}{\pi^2 N} \ln \frac{N\Lambda}{16\rho_s} + I_2(x_{\overline{\sigma}}), \quad (48)$$

where the functions  $I_1(x_{\overline{\sigma}})$ ,  $I_2(x_{\overline{\sigma}})$  are defined in Appendix B. After substituting Eqs. (47) and (48) into the constraint equation (43) and using the results of Ref. 12 for the quantum-renormalized ground-state sublattice magnetization  $\overline{\sigma}_0 = \overline{\sigma}(T=0) = \overline{S}_0/S$  and the spin stiffness  $\rho_s$  of a quantum 2D antiferromagnet,

$$\frac{\overline{\sigma}_0^2}{\rho_s} = \frac{g}{N} \bigg( 1 - \frac{8}{3\pi^2 N} \ln \frac{N\Lambda}{16\rho_s} \bigg), \tag{49}$$

$$\rho_s = \rho_s^{N=\infty} \left( 1 + \frac{32}{3\pi^2 N} \ln \frac{N\Lambda}{16\rho_s} \right), \tag{50}$$

one can see that the sublattice magnetization, being expressed in terms of  $\rho_s$  and  $\overline{\sigma}_0$ , still depends on  $\Lambda$ , i.e., is nonuniversal. To make the sublattice magnetization completely universal we have to introduce the quantum-renormalized parameter of the interlayer coupling

$$\alpha_r = \alpha \left[ 1 - \frac{8}{3 \pi^2 N} \ln \frac{N \Lambda}{16 \rho_s} \right]. \tag{51}$$

We shall demonstrate below that at low enough temperatures any regular (nondivergent) terms in the renormalized interlayer coupling parameter are absent, so that this is renormalized only due to temperature fluctuations at higher T. Being rewritten through the renormalized parameters, the constraint equation (43) reads

$$1 - \frac{NT}{4\pi\rho_{s}} \left[ \left( 1 - \frac{2}{N} \right) \ln \frac{2T^{2}}{\alpha_{r}} + \frac{3}{N} \ln \frac{4\pi\rho_{s}}{NTx_{\bar{\sigma}}} - \frac{2}{N} \frac{\ln(2T^{2}/\alpha_{r})}{\ln(2T^{2}/\alpha_{r}) + x_{\bar{\sigma}}} - I_{1}(x_{\bar{\sigma}}) \right]$$
$$= \frac{\bar{\sigma}^{2}}{\bar{\sigma}_{0}^{2}} \left[ 1 + \frac{1}{N} \ln \frac{4\pi\rho_{s}}{NTx_{\bar{\sigma}}} - I_{2}(x_{\bar{\sigma}}) \right].$$
(52)

Note that we have simply replaced  $\alpha$  by  $\alpha_r$  in the terms of order of 1/N in Eq. (52) since this yields an error of order of  $1/N^2$ .

First we consider the case  $x_{\overline{\sigma}} \gg 1$ , or, equivalently,

$$NT/4\pi\rho_s \ll \overline{\sigma}^2/\overline{\sigma}_0^2. \tag{53}$$

Since  $x_{\overline{\sigma}}$  is the decreasing function of temperature, this inequality is satified at low enough temperatures. In this case the integrals  $I_1(x_{\overline{\sigma}})$  and  $I_2(x_{\overline{\sigma}})$  are of order of  $1/x_{\overline{\sigma}}$ , i.e., are small. Thus to leading (zeroth) order in  $1/x_{\sigma}$  the constraint equation (52) coincides with that in the case of space dimensionality  $d=2+\varepsilon$  (Appendix C) with the replacement  $1/\varepsilon \rightarrow \ln(2/\alpha)$ , which corresponds to the limit  $\varepsilon \rightarrow 0$  with simultaneous cutting of the integrals over quasimomentum on the scale  $1/\xi_{J'}$ . Similar to the  $d=2+\varepsilon$  case (Appendix C) we transform the logarithmic term in the right-hand side of Eq. (52) into power and replace  $N \rightarrow N-2$ . Then we have

$$(\overline{\sigma}/\overline{\sigma}_{0})^{1/\beta_{2}}[1-I_{2}(x_{\overline{\sigma}})]$$

$$=1-\frac{NT}{4\pi\rho_{s}}\left[\left(1-\frac{2}{N}\right)\ln\frac{2T^{2}}{\alpha_{r}}+\frac{3}{N}\ln\frac{\overline{\sigma}_{0}^{2}}{\overline{\sigma}^{2}}\right]$$

$$-\frac{2}{N}\frac{\ln(2T^{2}/\alpha_{r})}{\ln(2T^{2}/\alpha_{r})+x_{\overline{\sigma}}}-I_{1}(x_{\overline{\sigma}})\right],$$
(54)

where, being expressed through the renormalized parameters,

$$x_{\overline{\sigma}} = \frac{4\pi\rho_s}{(N-2)T} \frac{\overline{\sigma}^2}{\overline{\sigma}_0^2}.$$
(55)

The "critical exponent"  $\beta_2$ , which is the limit of  $\beta_{2+\varepsilon}$  at  $\varepsilon \rightarrow 0$ , is given by

$$\beta_2 = \frac{1}{2} \frac{N-1}{N-2}.$$
 (56)

As well as in the  $d=2+\varepsilon$  case, two regimes are possible under the condition (53). Consider first the low-temperature (spin-wave) region where

$$T(N-2)\ln(2T^2/\alpha)/4\pi\rho_s \ll \overline{\sigma}^2/\overline{\sigma}_0^2.$$
(57)

In this region

$$\overline{\sigma} = \overline{\sigma}_0 \bigg[ 1 - \frac{T(N-1)}{8 \pi \rho_s} \ln \frac{2T^2}{\alpha_r c^2} \bigg].$$
(58)

At N=3 we reproduce the result of SSWT (10) with  $2\gamma'/\gamma$  being replaced by  $\alpha_r$ . The factor N-1 in Eq. (58) has a simple physical meaning: this is the number of gapless (Goldstone) modes. We can conclude that in the temperature interval (57) spin-wave excitations give the main contribution to the dependence  $\overline{\sigma}(T)$ . Note that the spin-wave result (58) can be obtained also from the untransformed constraint equation (52).

To demonstrate that in the interval (57) the experimentally observed interlayer exchange parameter coincides with  $\alpha_r$  we calculate the self-energy  $\Sigma(k,k_z,0)$ . By using Eq. (36) we get

$$\Sigma(k,k_z,0) = \frac{8k^2}{3\pi^2 N} \ln \frac{N\Lambda}{16\rho_s}$$
(59)

irrespective of  $k_z$ . Thus we have

$$G_t^{-1}(k,k_z,0) = k^2 \left[ 1 + \frac{8}{3\pi^2 N} \ln \frac{N\Lambda}{16\rho_s} \right] + \alpha (1 - \cos k_z)$$
  
=  $Z^{-1} [k^2 + \alpha_r (1 - \cos q_z)].$  (60)

We see that the renormalized Green's function differs from the bare one by the renormalization factor Z and by replacement  $\alpha \rightarrow \alpha_r$  only. Thus the experimentally observed (fully renormalized) interlayer coupling is just  $\alpha_r$ . At higher temperatures the temperature renormalization of the interlayer coupling, which will be calculated below, becomes important.

At intermediate temperatures where

$$(N-2)T/4\pi\rho_s \ll \overline{\sigma}^2/\overline{\sigma}_0^2 \ll (N-2)T\ln(2T^2/\alpha)/4\pi\rho_s,$$
(61)

we have a 2D-like critical behavior of the sublattice magnetization,

$$(\overline{\sigma}/\overline{\sigma}_{0})^{1/\beta_{2}} = 1 - \frac{T}{4\pi\rho_{s}} \left[ (N-2)\ln\frac{2T^{2}}{\alpha_{r}} + 3\ln\frac{\overline{\sigma}_{0}^{2}}{\overline{\sigma}^{2}} - 2 \right].$$
(62)

For N=3 we have  $\beta_2=1$ , which coincides with the critical exponent of SWT and SSWT. However, the term with  $\ln(\overline{\sigma^2}/\overline{\sigma_0^2})$ , which is present in Eq. (62), leads to a significant modification of the dependence  $\overline{\sigma}(T)$  in the temperature region under consideration in comparison with SSWT and leads to a considerable lowering of the Néel temperature. With further approaching the transition point the behavior of the order parameter changes to 3D.

Consider the temperatures which are very close to  $T_{\text{N\acute{e}el}}$ , so that  $\overline{\sigma}$  is small enough to satisfy the inequality  $x_{\overline{\sigma}} \ll 1$ , i.e.,

$$\overline{\sigma}^2/\overline{\sigma}_0^2 \ll (N-2)T/4\pi\rho_s. \tag{63}$$

After expanding Eq. (52) near  $T=T_{\text{N\acute{e}el}}$ ,  $x_{\overline{\sigma}}=0$ , picking out the logarithmically divergent parts of  $I_1(x_{\overline{\sigma}})$  and  $I_2(x_{\overline{\sigma}})$  at small  $x_{\overline{\sigma}}$  analytically, and evaluating numerically the integrals, we have

$$1 - \frac{T}{T_{\text{N\acute{e}el}}} = \frac{\overline{\sigma}^2}{\overline{\sigma}_0^2} \bigg[ 1 + \frac{1}{N} \ln \frac{4 \pi \rho_s}{(N-2) T_{\text{N\acute{e}el}}} + \frac{8}{\pi^2 N} \ln x_{\overline{\sigma}} - A_0 \bigg],$$
(64)

where  $A_0 = 2.8906/N$ . The equation for  $T_{\text{N\acute{e}l}}$  reads

$$T_{\text{N\acute{e}el}} = 4 \pi \rho_s \bigg[ (N-2) \ln \frac{2T_{\text{N\acute{e}el}}^2}{\alpha_r c^2} + 3 \ln \frac{4 \pi \rho_s}{(N-2)T_{\text{N\acute{e}el}}} - 0.0660 \bigg]^{-1}.$$
 (65)

As will be clear below, the second term in the denominator, which is of order of  $lnln(2T_{N\acute{e}el}^2/\alpha)$ , leads to a significant lowering of Néel temperature in comparison with SSWT (where only the first term is taken into account). To calculate  $\overline{\sigma}$  in the region (63), we collect separately the logarithmic terms in Eq. (64) which comes from the quasimomenta  $q \ge \alpha^{1/2}$  (2D regime) and  $q \le \alpha^{1/2}$  (3D regime):

$$1 - \frac{T}{T_{\text{N\acute{e}el}}} = \frac{\overline{\sigma}^2}{\overline{\sigma}_0^2} (1 - A_0) \left[ 1 + \frac{1}{N} \ln \frac{4 \pi \rho_s}{(N - 2) T_{\text{N\acute{e}el}}} \right] \\ \times \left[ 1 + \frac{8}{\pi^2 N} \ln x_{\overline{\sigma}} \right].$$
(66)

Unlike the "2D-like" regime, the coefficients at the logarithms are different. Transforming the logarithmic terms into powers we obtain

$$\frac{\overline{\sigma}^2}{\overline{\sigma}_0^2} = \left[\frac{4\pi\rho_s}{(N-2)T_{\text{N\acute{e}el}}}\right]^{\beta_3/\beta_2 - 1} \left[\frac{1}{1-A_0}\left(1-\frac{T}{T_{\text{N\acute{e}el}}}\right)\right]^{2\beta_3},\tag{67}$$

where

$$\beta_3 = \frac{1}{2} \left( 1 - \frac{8}{\pi^2 N} \right) \tag{68}$$

is the true 3D critical exponent for the magnetization. It should be noted that we have not to perform the replacement  $N \rightarrow N-2$  in Eq. (68) and other contributions which come from essentially three-dimensional integrals. We get for N=3 the value  $\beta_3 \approx 0.36$ . The result (68) coincides with that of the 1/N expansion in the  $\phi^4$  model<sup>23</sup> at d=3, in agreement with the universality hypothesis. The dependence (67) is to be compared with that in the Tyablikov approximation (16) where  $\beta = 1/2$  and the dimensional crossover is absent.

Consider now the self-energy  $\Sigma(k,k_z,0)$  at  $T=T_{\text{N\acute{e}el}}$ . At  $\alpha^{1/2} \ll k \ll T_{\text{N\acute{e}el}}$  the self-energy has the same form as in the 2D case<sup>12</sup> with  $\xi$  being replaced by  $\xi_{J'}$ :

$$\Sigma(k,k_z,0) = k^2 \left[ \eta \ln \frac{N\Lambda}{16\rho_s} + \frac{1}{N} \ln \frac{\ln(2T_{\text{N\'eel}}^2/\alpha)}{\ln(2k^2/\alpha)} + \frac{1}{N} \right].$$
(69)

Thus the expression for Green's function reads  $(G = G_t = G_l)$ 

$$G(k,k_z,0) = \frac{1}{k^2} \left[ \frac{(N-2)T_{\text{N\'eel}}}{4\pi\rho_s} \ln \frac{2k^2}{\alpha} \right]^{1/(N-2)} \times \frac{N-1}{N} \left[ 1 - \eta \ln \frac{N\Lambda}{16\rho_s} \right],$$
(70)

$$\alpha^{1/2} \ll k \ll T_{\text{Néel}}.$$

At  $k \ll \alpha^{1/2}$ ,  $k_z \ll 1$  the *k* dependence of the Green's function changes. After integration and frequency summation in (36) (which are analogous to the calculation of the functions *R* and *F* in Appendix B) we have

$$\Sigma(k,k_z,0) = A_1 k^2 + \frac{\alpha}{2} A_2 k_z^2 + \frac{\eta}{2} \left( k^2 + \frac{\alpha}{2} k_z^2 \right) \ln \frac{\alpha}{k^2 + \alpha k_z^2/2}.$$
(71)

Here

$$A_{1} = \eta \ln \frac{N\Lambda}{16\rho_{s}} + \frac{1}{N} \ln \ln \frac{2T^{2}}{\alpha} + \frac{0.4564}{N}, \qquad (72)$$
$$A_{2} = -0.6122/N,$$

and

$$\eta = 8/(3\,\pi^2 N) \tag{73}$$

is the 3D critical exponent for the asymptotics of the correlation function at the phase transition point in the first order in 1/N. For N=3 we have  $\eta \approx 0.09$ . Using Eq. (71) we find

$$G^{-1}(k,k_z,0) = (1+A_1) \alpha_c^{\eta/2} \left( k^2 + \frac{\alpha_c}{2} k_z^2 \right)^{1-\eta/2}$$
(74)  
$$k \ll \alpha^{1/2}, \quad k_z \ll 1.$$

The quantity

$$\alpha_c = \alpha (1 + A_2) / (1 + A_1) \tag{75}$$

can be interpreted as the renormalized interlayer coupling at  $T = T_{\text{N\acute{e}el}}$ .

Using Eq. (51) we find the following relation between the renormalized coupling parameters at low T and at  $T = T_{\text{Néel}}$ :

$$\alpha_{c} = \alpha_{r} \left( 1 + \frac{1.0686}{N} \right) \left[ \frac{(N-2)T_{\text{N\acute{e}el}}}{4\pi\rho_{s}} \right]^{1/(N-2)}.$$
 (76)

When deriving Eq. (76) we have transformed the term with  $\ln \ln(2T^2/\alpha)$  into a power and then replaced  $N \rightarrow N-2$  in the exponent. As in SSWT (see Sec. II), the renormalized interlayer coupling at  $T_{\text{N\'eel}}$  is lower than the low-temperature one, but the concrete expression at N=3 is slightly different from these in SSWT.

Using Eq. (76) we get the following equation for  $T_{\text{Neel}}$  in terms of  $\alpha_c$ :

$$T_{\text{N\acute{e}el}} = 4 \pi \rho_s \bigg[ (N-2) \ln \frac{2T_{\text{N\acute{e}el}}^2}{c^2 \alpha_c} + 2 \ln \frac{4 \pi \rho_s}{(N-2)T_{\text{N\acute{e}el}}} + 1.0117 \bigg]^{-1},$$
(77)

where c is the fully renormalized spin-wave velocity; in SSWT we have  $c = \sqrt{8} \gamma(0)S$  (see Sec. II). For N=3 we have

$$T_{\rm N\acute{e}el} = 4 \,\pi \rho_s / \ln \left[ 5.5005 \frac{(4 \,\pi \rho_s)^2}{c^2 \,\alpha_c} \right], \tag{78}$$

which is similar to the result of the Tyablikov approximation (17), but the bare value of  $\alpha$  is replaced by its renormalized value at the critical temperature (76) and  $\rho_s$  is also replaced by its renormalized value. Besides that, the result (78) does not violate the scaling form (21).

Finally, we consider the spin-correlation function

$$S(R,R_z) = -\frac{1}{\pi} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} e^{i(\mathbf{k}\mathbf{R}+k_z R_z)} \times \sum_m \int d\omega \mathrm{Im}\chi^{mm}(k,k_z,\omega) \frac{1}{e^{\omega/T}-1}$$
(79)

at  $T = T_{\text{N\'eel}}$ . For N = 3 we have

$$S(R,R_z) = |\langle \mathbf{S}_i(\mathbf{r})\mathbf{S}_{i+R_z}(\mathbf{r}+\mathbf{R})\rangle|.$$

The static approximation is sufficient to determine the asymptotics of the correlation function. Using Eqs. (30) and (49) we derive (cf. Ref. 12)

$$S(R,R_z) = \frac{T\overline{S}_0^2}{\rho_s} \left[ 1 + \eta \ln \frac{N\Lambda}{16\rho_s} \right]$$
$$\times \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} G(k,k_z,0) e^{i(\mathbf{kR}+k_zR_z)}.$$
(80)

One can see that at  $R^2 \alpha + R_z^2 \ge 1$  the asymptotics of the integral in Eq. (80) is determined by the region  $k \ll \alpha^{1/2}$  and  $k_z \ll 1$  where  $G(k, k_z, 0)$  is calculated above [see Eq. (74)]. Substituting Eq. (74) into Eq. (80) we have

$$S(\mathcal{R}) = \frac{1}{4\pi} \frac{T_{\text{N\'eel}} \overline{S}_0^2}{\rho_s} (1 - A_1 - \eta C) \left[ 1 + \eta \ln \frac{N\Lambda}{16\rho_s} \right] \\ \times \left( \frac{2}{\alpha_c^{1+\eta} \mathcal{R}^{2+2\eta}} \right)^{1/2}, \tag{81}$$

where  $\mathcal{R} = (R^2 + 2R_z^2/\alpha_c)^{1/2}$  and  $C \approx 0.5772$  is the Euler constant. Using the value of  $A_1$  [Eq. (72)] and transforming the term with  $(1/N) \ln(2T^2/\alpha)$  into power we obtain the final result for the spin-correlation function at  $T = T_{\text{N\acute{e}el}}$  and  $\mathcal{R}\alpha_c^{1/2} \ge 1$ :

$$S(\mathcal{R}) = \frac{T_{\text{N\acute{e}el}} \overline{S}_{0}^{2}}{4 \pi \rho_{s}} \left[ \frac{(N-2)T_{\text{N\acute{e}el}}}{4 \pi \rho_{s}} \right]^{1/(N-2)} (1 - \overline{A}_{1} - \eta C) \\ \times \left( \frac{2}{\alpha_{c}^{1+\eta} \mathcal{R}^{2+2\eta}} \right)^{1/2},$$
(82)

where  $\overline{A}_1 = 0.4564/N$ . Thus  $S(\mathcal{R})$  enables one to determine the value of  $\alpha_c$ . As one should expect, being rewritten through renormalized parameters  $\rho_s$  and  $\alpha_c$ ,  $S(\mathcal{R})$  does not contain the cutoff parameter  $\Lambda$  and is thereby completely universal.

At  $1 \ll R \ll \alpha_c^{1/2}$  we derive from Eqs. (70) and (80) the leading term of asymptotics of the correlation function within a plane (N=3)

$$S(R,0) = \frac{\overline{S}_0^2}{3\rho_s} \left(\frac{T}{4\pi\rho_s}\right)^2 \ln^2 \frac{8}{\alpha_c R^2}.$$
 (83)

Thus we have in this case a logarithmic decrease of the correlation function, as well as in the 2D case at  $1 \le R \le \xi$ .<sup>11</sup>

In the above treatment we analyzed the sublattice magnetization  $\overline{S}$  of a quasi-2D quantum antiferromagnet  $(T_{\text{N\acute{e}el}} \ll JS)$ . At temperatures  $T \ll (JJ')^{1/2}$  the behavior  $\overline{S}(T)$  is satisfactorily decribed by the standard spin-wave theory. For  $T \gg (JJ')^{1/2}$  we have obtained Eq. (52) which determines  $\overline{S}$  to first order in the formal small parameter 1/N. We have three temperature intervals (the boundaries of the intervals are presented for N=3):

(i) The case of low temperatures

$$T\ln(2T^2/JJ')/(4\pi JS^2) \ll \overline{S}^2/\overline{S}_0^2$$
 (84)

 $[\overline{S}_0 = \overline{S}(T=0); \ \overline{S}_0 = S - 0.196$  for the square lattice] where the results of SSWT are reproduced.

(ii) The case of the intermediate temperatures Eq. (61), or equivalently

$$\overline{S}^2 / \overline{S}_0^2 \ll T \ln(2T^2 / JJ') / (4\pi JS^2),$$
  
$$1 - T / T_{\text{N\acute{e}el}} \gg (1 - A_0) (T / 4\pi JS^2)^{1/2}$$
(85)

 $(1-A_0 \approx 0.0365)$ , where a 2D-like critical behavior, which is similar to that in SSWT, takes place. However, the corrections to SSWT modify considerably the numerical factors, so that the Néel temperature is considerably lowered.

(iii) The vicinity of the Néel temperature Eq. (63), or

$$1 - T/T_{\text{N\'eel}} \ll (1 - A_0) (T/4\pi J S^2)^{1/2}, \tag{86}$$

where we obtain the critical behavior  $\overline{S} \sim (T_{\text{N\'eel}} - T)^{\beta_3}$ ,  $\beta_3 \simeq 0.36$ .

The detailed description of the temperature region between (ii) and (iii), where  $\overline{S}^2/\overline{S}_0^2 \sim T/4\pi\rho_s$ , cannot be obtained within the first order in 1/N, since Eq. (52) is transformed in different ways in these regions to derive the results (54) and (64), respectively. Note, that in region (ii) the "2Dlike" behavior of the system enables one to calculate corrections to SSWT in a regular way, e.g., by using the 1/N expansion in the  $CP^{N-1}$  model.

We have also derived the expressions for the magnetic transition temperature Eqs. (65) and (77), which contain the renormalized quantities  $\alpha_{r,c} = 2 \gamma'_{r,c} / \gamma$  where  $\gamma'_{r,c}$  are the experimentally observable (renormalized) interlayer exchange parameters at low temperatures and  $T = T_{\text{Néel}}$ , respectively, and  $\gamma \simeq 1.1571J$  is the value of renormalized intralayer coupling parameter which is weakly temperature dependent. Therefore these expressions have universal form, in agreement with the scaling analysis. Unlike the corresponding results of the spin-wave approaches (see Sec. II), they contain the terms of order of  $\ln\ln(T_{\text{N\'eel}}^2/JJ')$  and unity, which are formally small as compared to the leading term of order of  $\ln(T_{\text{N\acute{e}el}}^2/JJ')$ . However, the lnln terms result in a significant lowering of  $T_{\text{Néel}}$  in comparison with the SSWT value (10) at not too large  $\ln(J/J')$ . The regular terms yield small corrections only, so that one may expect that the higher-order terms in  $1/\ln(T_{\text{Néel}}^2/JJ')$  may be neglected.

The experimental temperature dependence<sup>24</sup> of the sublattice magnetization in  $La_2CuO_4$  is shown in Fig. 1. For comparison, the results of spin-wave approximations (SWT, SSWT, and the Tyablikov theory; see Sec. II) and the result



FIG. 1. The theoretical temperature dependences of the relative sublattice magnetization  $\overline{S}/\overline{S}_0$  from different spin-wave approximations and from the 1/N expansion in the O(N) model [Eqs. (54) and (64)], and the experimental points for La<sub>2</sub>CuO<sub>4</sub> (Ref. 24).

of 1/N expansion are also presented. The renormalized value of the in-plane exchange parameter  $\gamma \approx 1850$  K can be found from the experimental data<sup>25</sup> and the value  $\gamma'_r/\gamma = 5 \times 10^{-4}$ was chosen from the best fit to SWT at low temperatures T < 100 K). The experimental results for  $\gamma'/\gamma$  are not reliable, and it is difficult to compare our value of  $\gamma'/\gamma$  with experiment. For example, the result of Ref. 26,  $\gamma'/\gamma = 5 \times 10^{-5}$ , is by an order lower than that found from the fit in the spin-wave region. It is also important that the value of  $\gamma'/\gamma$  has an appreciable temperature dependence because of renormalizations. In particular, we have from Eq. (76) for above parameters  $\alpha_c/\alpha_r = \gamma'_c/\gamma'_r \approx 0.13$ . Thus experiments at different temperatures may give different results.

One can see that SWT and SSWT yield satisfactory results for  $T < 0.6T_{\text{N\'eel}}$  and  $T < 0.8T_{\text{N\'eel}}$ , respectively. At higher temperatures the sublattice magnetization in SWT and SSWT is still linear in temperature, so that the critical exponent is  $\beta_{SW}=1$ , instead of the experimental one,  $\beta_{exp} \approx 0.33$ . Besides that, both theories give large values of the Néel temperature  $T_{N\acute{e}el}^{SWT} = 672$  K,  $T_{N\acute{e}el}^{SSWT} = 537$  K. This fact is often not taken into account when treating experimental data. At the same time, TT gives the value  $T_{\text{N\acute{e}el}}^{\text{TT}} = 454 \text{ K}$ which is much lower than those in SWT and SSWT and the magnetization critical exponent  $\beta_{TT} = 1/2$ . Thus the Tyablikov approximation seems to describe the experimental data more satisfactorily. However, this approximation may be justified in fact only in the case of "classical" magnets with  $T_{\text{N\acute{e}el}} \gg JS$ . Besides that, TT has a number of drawbacks: mean-field values of critical exponents, absence of crossover from 2D-like to 3D behavior of magnetization, neglect of quantum effects at high temperatures (in particular,  $T_{\text{N\acute{e}el}} = T_{\text{C}}$  for the same |J|).

The result of the 1/N expansion to first order in 1/N (65) is  $T_{\text{N\acute{e}el}}=345$  K which is considerably lower than in the Tyablikov approximation and is in a good agreement with the experimental value,  $T_{\text{N\acute{e}el}}^{\text{exp}}=325$  K. The spin-wave region ex-

tends up to 300 K, and the crossover region from 320 to about 340 K; the critical 3D region is narrow (about 1 K). The results of the numerical solution of Eq. (54) in the temperature regions (i) and (ii) and the dependence (64) in the region (iii) turn out to be smoothly joined. One can see also that the result of the 1/N expansion is most close to the experimental data and demonstrates a correct critical behavior. One may assume that higher-order 1/N corrections will give a precise description of the experimental situation. Thus we may conclude that using the 1/N expansion in the O(N) model improves considerably the results of standard spin-wave approximations in the Heisenberg model.

Recent experiments demonstrate existence of a gap for the out-of-plane spin-wave excitations<sup>24</sup> in La<sub>2</sub>CuO<sub>4</sub>, which is assumed to be determined by the easy-plane anisotropy. The possible role of easy-axis anisotropy was also discussed, see, e.g., Ref. 27. Therefore an extension of the present approach to 2D systems with a weak anisotropy is of interest. The results may be expected to be similar to those in the quasi-2D case, since SSWT gives similar descriptions of both the types of magnets with small ordering temperature<sup>15</sup>.

The case of "classical" spins cannot be treated consistently in the continual limit since in this case the natural upper limit cutoff parameter (which is the temperature in the quantum case) is absent, and the integrals are determined by the whole Brillouin zone. Therefore the continual models may be used to calculate the critical exponents, but not the temperature dependence of magnetization in a broad interval and the Néel temperature.

It would be also interesting to perform similar calculations of thermodynamic properties for a ferromagnet. The results should coincide with those for a antiferromagnet only in the classical case. Unfortunately, the nonlinear- $\sigma$  model for ferromagnet has the Berry phase term  $\mathbf{A}(\boldsymbol{\sigma})\partial\boldsymbol{\sigma}/\partial\tau$  in the action (**A** is the vector potential of unit magnetic monopole), see, e.g., Ref. 4. This term cannot be eliminated in the quantum case and prevents constructing the 1/N expansion. Due to the Berry phase term, the singular contributions for a quantum ferromagnet ( $T_C \ll JS$ ) differ from those for an antiferromagnet by the replacement

$$\ln(T^2/8S^2\gamma\gamma'_{r,c}) \rightarrow \ln(T/\gamma'_{r,c}S)$$
(87)

(as well as in SSWT; see Ref. 15). Taking into account only such terms, the expression for the Curie temperature has the form  $(\gamma'_r = J')$ 

$$T_{C} = 4 \pi \rho_{s} \left[ (N-2) \ln \frac{T_{C}}{J'S} + 3 \ln \frac{2 \pi \rho_{s}^{0}}{(N-2)T_{C}} + \mathcal{O}(1) \right]^{-1}$$
(88)

or, in terms of the renormalized exchange parameter at the Curie temperature,

$$T_{C} = 4 \pi \rho_{s} \left[ (N-2) \ln \frac{T_{C}}{\gamma_{c}' S} + 2 \ln \frac{2 \pi \rho_{s}^{0}}{(N-2) T_{C}} + \mathcal{O}(1) \right]^{-1},$$
(89)

where

$$\gamma_{c}' = A_{\gamma} J' \left[ \frac{(N-2)T_{\rm C}}{4\pi\rho_{s}} \right]^{1/(N-2)}$$
 (90)

and  $A_{\gamma} \sim 1$ . One may expect that, as well as in Eqs. (65) and (77), the nonsingular terms will influence weakly the value of the ordering point. These regular contributions may be calculated for a ferromagnet within the 1/N expansion in the SU(*N*) model (cf. Ref. 4). However, as discussed in the Introduction, this expansion gives poor results at not too large *N* for *d* not too close to 2, so that only the "2D-like" region can be described satisfactory. The description of the 3D critical behavior of a quasi-2D ferromagnet requires other methods.

#### ACKNOWLEDGMENT

We are grateful to M. I. Katsnelson for stimulating discussions.

#### APPENDIX A: ANALYTICAL RESULTS FOR THE FUNCTIONS $\Pi(q,q_z,\omega_n)$ AND $I(q,q_z,\omega_n)$

Here we present a list of results for the polarization operator  $\Pi(q,q_z,\omega_n)$ , Eq. (39) and the function  $I(q,q_z,\omega_n)$ determined by Eq. (42) at  $\alpha^{1/2} \ll T$ , and the asymptotic forms of these functions. Due to inequality  $\alpha^{1/2} \ll T$ , the possible values of  $q,\omega_n$  may be divided into two regions. The first region is  $\omega_n=0$ ,  $q \ll T$ , while in the second region  $q^2 + \omega_n^2 \gg \alpha$ , i.e., either  $\omega_n=0$  and  $q \gg \alpha^{1/2}$  or  $\omega_n \neq 0$  at arbitrary q.

It may be checked that at  $q \ll T$  and  $\omega_n = 0$  the main contribution to  $\Pi$  comes from the term with  $\omega_m = 0$ . After integrating over  $\mathbf{k}, k_z$  with the use of the Feynman identity (see, e.g., Ref. 28) we get

$$\Pi(q,q_z,0) = \frac{TK_2}{2} \int_0^1 \frac{dz}{\sqrt{z(1-z)}} \frac{1}{\sqrt{z(1-z)q^4 + 2\,\widetilde{\alpha}(q,q_z)}},$$
$$q \ll T \tag{A1}$$

where  $\widetilde{\alpha}(q,q_z) = \alpha[q^2 + \alpha(1 - \cos q_z)]$ . At large  $q \ge \alpha^{1/2}$  the function  $\Pi(q,q_z,0)$  has a 2D form (cf. Ref. 12)

$$\Pi(q,q_z,0) \simeq \frac{T}{2\pi q^2} \ln \frac{2q^2}{\alpha}, \quad \alpha \ll q^2 \ll T.$$
 (A2)

In the opposite limit the form of function  $\Pi(q,q_z,0)$  changes from 2D to 3D:

$$\Pi(q,q_z,0) \simeq \frac{T}{4\sqrt{2\,\widetilde{\alpha}(q,q_z)}}, \quad q^2 \ll \alpha.$$
(A3)

Consider now the case  $q^2 + \omega_n^2 \ge \alpha$ . Picking out the terms with m=0 and m=-n (if  $n \ne 0$ ) we have

$$\Pi(q,q_z,\omega_n) = \frac{T}{2\pi(q^2+\omega_n^2)} \ln \frac{2(q^2+\omega_n^2)^2}{q^2\alpha} + \Pi_{qu}(q,\omega_n),$$
$$q^2+\omega_n^2 \ge \alpha \tag{A4}$$

where the quantum contribution  $\Pi_{qu}$  is given by

$$\Pi_{qu}(q,\omega_n) = \frac{T}{\pi} \sum_{m \neq 0} \frac{1}{\sqrt{(\omega_n^2 + q^2 + 2\omega_m \omega_n)^2 + 4q^2 \omega_m^2}} \\ \times \operatorname{arctanh} \frac{\omega_n^2 + q^2 + 2\omega_m \omega_n}{\sqrt{(\omega_n^2 + q^2 + 2\omega_m \omega_n)^2 + 4q^2 \omega_m^2}}.$$
(A5)

In all the further calculations we will need only the asymptotic form of  $\prod_{qu}(q, \omega_n)$  for  $q^2 + \omega_n^2 \ge T^2$ . In this limit we find

$$\Pi_{qu}(q,\omega_n) = \frac{T}{\pi(q^2 + \omega_n^2)} \ln \frac{qT}{q^2 + \omega_n^2} + \frac{1}{8\sqrt{q^2 + \omega_n^2}},$$
$$q^2 + \omega_n^2 \gg T^2.$$
(A6)

For  $\omega_n = 0$  and  $q \ll T$  we obtain by analogy with the calculation of  $\Pi(q, q_z, 0)$  the result

$$I(q,q_z,0) = \frac{T}{4\pi} \frac{1}{q^2 + \alpha(1 - \cos q_z)} \int_0^1 \frac{dz}{\sqrt{z(1-z)}} \times \frac{q^2 z(1-z) + \alpha z(1 - \cos q_z)}{[q^4 z(1-z) + 2\,\widetilde{\alpha}(q,q_z)]^{3/2}}, \quad q \ll T$$
(A7)

and its asymptotic form

$$I(q,q_z,0) \simeq \frac{T}{2\pi q^4} \bigg[ \ln \frac{2q^2}{\alpha} - \frac{3 + \cos q_z}{2} \bigg], \quad \alpha \ll q^2 \ll T^2.$$
(A8)

In the region with  $q^2 + \omega_m^2 \gg \alpha$  we have

$$I(q,q_{z},\omega_{n}) = \frac{Tq^{2}}{2\pi(q^{2}+\omega_{m}^{2})^{3}} \ln \frac{2(q^{2}+\omega_{m}^{2})^{2}}{q^{2}\alpha} + \frac{T}{4\pi} \frac{\omega_{n}^{2} - 3q^{2} - (q^{2}+\omega_{n}^{2})\cos q_{z}}{(q^{2}+\omega_{n}^{2})^{3}} + I_{qu}(q,\omega_{n}), \quad q^{2}+\omega_{n}^{2} \ge \alpha$$
(A9)

with

$$I_{qu}(q,\omega_{n}) = \frac{T}{\pi_{m\neq0}} \sum_{\substack{m\neq0 \\ [(\omega_{n}^{2}+q^{2}+2\omega_{m}\omega_{n})^{2}+4q^{2}\omega_{m}^{2}]^{3/2}}} \\ \times \operatorname{arctanh} \frac{\omega_{n}^{2}+q^{2}+2\omega_{m}\omega_{n}}{\sqrt{(\omega_{n}^{2}+q^{2}+2\omega_{m}\omega_{n})^{2}+4q^{2}\omega_{m}^{2}}} \\ + \frac{T}{4\pi_{m\neq0}} \sum_{\substack{m\neq0 \\ w_{m}^{2}[(\omega_{n}^{2}+q^{2}+2\omega_{m}\omega_{n})^{2}+4q^{2}\omega_{m}^{2}]}} \\ (A10)$$

In the ultraviolet limit  $q^2 + \omega_n^2 \ge T^2$  the following asymptotic takes place:

$$I_{qu}(q,\omega_n) = \frac{Tq^2}{\pi (q^2 + \omega_n^2)^3} \ln \frac{qT}{q^2 + \omega_n^2} + \frac{T}{\pi} \frac{\omega_n^2 - q^2}{(q^2 + \omega_n^2)^3},$$
$$q^2 + \omega_n^2 \gg T^2.$$
(A11)

## APPENDIX B: CALCULATION OF 1/N CORRECTIONS TO THE CONSTRAINT AT $T \leq T_{Neel}$

Consider briefly the calculation of the functions *R* [Eq. (44)] and *F* [Eq. (45)] which determine, according to Eq. (43), the corrections to the constraint to first order in 1/*N*. First we introduce intermediate cutoff parameters *C* and *C'* determined by  $\alpha^{1/2} \ll C \ll T \ll 2\pi C' \ll \Lambda$  and divide the region of summation and integration  $q^2 + \omega_n^2 < \Lambda^2$  into four regions: (1)  $\omega_n = 0$ , q < C, (2)  $\omega_n = 0$ ,  $C < q < 2\pi C'$ , (3)  $\omega_n \neq 0$ ,  $q^2 + \omega_n^2 < 2\pi C'$ , (4)  $2\pi C' < q^2 + \omega_n^2 < \Lambda$ . Further we denote the contributions from *i*th region to *R* and *F* as  $R_i(T, x_{\overline{\sigma}})$  and  $F_i(T, x_{\overline{\sigma}})$ .

In the first region we can use the expressions for the functions  $\Pi(q,q_z,0)$  and  $I(q,q_z,0)$  at  $q^2 \ll T$ , Eqs. (A1) and (A7), and their asymptotics (A2), (A3), (A8). Then

$$R_{1}(T, x_{\overline{\sigma}}) = \frac{T}{2\pi N} \ln \frac{2C^{2}}{\alpha} - \frac{(3+2x_{\overline{\sigma}})T}{4\pi N} \ln \frac{\ln(2C^{2}/\alpha) + x_{\overline{\sigma}}}{x_{\overline{\sigma}}} + \frac{T}{4\pi N} I_{1}(x_{\overline{\sigma}}), \qquad (B1)$$

where

$$\begin{split} I_{1}(x_{\overline{\sigma}}) &= \frac{4}{N} \int_{0}^{\infty} q dq \int_{-\pi}^{\pi} \frac{dq_{z}}{2\pi} \Bigg[ \frac{1}{q^{2} + 1 - \cos q_{z}} \\ &\times \frac{I(q, q_{z}, 0) - \widetilde{\Pi}(q, q_{z}, 0)}{\widetilde{\Pi}(q, q_{z}, 0)} + \frac{3 + 2x_{\overline{\sigma}}}{2q^{2}} \frac{\theta(q^{2} - 1/2)}{\ln(2q^{2}) + x_{\overline{\sigma}}} \Bigg]. \end{split}$$
(B2)

 $\theta(x)$  is the step function. In the second and third regions we use the expressions for the functions  $\Pi(q,q_z,0)$  and  $I(q,q_z,0)$  at  $q^2 \ge \alpha$ , Eqs. (A4) and (A9):

$$R_{2}(T, x_{\overline{\sigma}}) = \frac{T}{\pi N} \bigg[ \ln \frac{T}{C} - \frac{3 + 2x_{\overline{\sigma}}}{4} \ln \frac{4\pi \rho_{s}/NT}{\ln(2C^{2}/\alpha) + x_{\overline{\sigma}}} + \ln \frac{2\pi C'}{T} \frac{\ln(2T^{2}/\alpha)}{\ln(2T^{2}/\alpha) + x_{\overline{\sigma}}} \bigg],$$
(B3)

$$R_{3}(T, x_{\overline{\sigma}}) = \frac{T}{\pi N} \frac{\ln(2T^{2}/\alpha)}{\ln(2T^{2}/\alpha) + x_{\overline{\sigma}}} \left[\frac{4C'}{3T} + \frac{1}{2} - \ln\frac{2\pi C'}{T}\right],$$
(B4)

where we have used the identity

$$\ln(2T^2/\alpha) + x_{\overline{\sigma}} = 4\pi\rho_s/NT \tag{B5}$$

which is satisfied in the zeroth order in 1/N. In the fourth region we obtain

$$R_{4}(T, x_{\bar{\sigma}}) = \frac{8T}{3\pi^{3}N} \ln \frac{2T^{2}}{\alpha} \ln \frac{N\Lambda}{16\rho_{s}} - \frac{2T}{3\pi^{3}N} \ln \frac{N\Lambda}{16\rho_{s}} - \frac{4C'}{3\pi N} \frac{\ln(2T^{2}/\alpha)}{\ln(2T^{2}/\alpha) + x_{\bar{\sigma}}},$$
(B6)

where we have used the asymptotic forms (A6), (A11), and the identity (B5). After collecting all  $R_i$  (i=1...4) the intermediate cutoff parameters C, C' are canceled and we find the result (47) of the main text.

Analogously, we obtain the contribution from the first region to F in the form

$$F_1(T, x_{\overline{\sigma}}) = \frac{1}{N} \ln \frac{\ln(2C^2/\alpha) + x_{\overline{\sigma}}}{x_{\overline{\sigma}}} + I_2(x_{\overline{\sigma}}), \qquad (B7)$$

where

$$I_{2}(x_{\overline{\sigma}}) = \frac{4}{N} \int_{0}^{\infty} q dq \int_{-\pi}^{\pi} \frac{dq_{z}}{2\pi} \left[ \frac{1}{(q^{2}+1-\cos q_{z})^{2}} \frac{1}{\widetilde{\Pi}(q,q_{z},0)} - \frac{1}{2q^{2}} \frac{\theta(q^{2}-1/2)}{\ln(2q^{2})+x_{\overline{\sigma}}} \right].$$
 (B8)

Contributions from other three regions are also easily calculated:

$$F_2(T, x_{\overline{\sigma}}) = \frac{1}{N} \ln \frac{4 \pi \rho_s / NT}{\ln(2C^2/\alpha) + x_{\overline{\sigma}}},$$
 (B9)

$$F_3(T, x_{\overline{\sigma}}) = \mathcal{O}[1/\ln(2T_{\text{N\'eel}}^2/\alpha)], \qquad (B10)$$

$$F_4(T, x_{\overline{\sigma}}) = \frac{8}{\pi^2 N} \ln \frac{N\Lambda}{16\rho_s}.$$
 (B11)

Summing up all  $F_i$  (i=1, ..., 4) we find the result (48) of the main text.

### APPENDIX C: THE ORDER PARAMETER AND TRANSITION TEMPERATURE AT $d=2+\varepsilon$

In this appendix we consider the calculation of the sublattice magnetization to first order in 1/N in the space with the dimensionality  $d=2+\varepsilon$ . We will be interested in the terms of the leading order in  $\varepsilon$  at not too small temperatures  $T \ge Je^{-1/\varepsilon}$  (which is an analog of the renormalized classical regime in the 2D case), so that only the contributions with zero Matsubara frequences will be taken into account. Consider first the results for the functions  $\Pi$  and *I*. Evaluating the integrals in Eqs. (39) and (42) at an arbitrary space dimensionality 2 < d < 4 (see, e.g., Ref. 28 for the procedure of calculation of such integrals) we have

$$\Pi(q,0) = \frac{TK_d A_d}{q^{4-d}},\tag{C1}$$

$$I(q,0) = \frac{TK_d A_d(3-d)}{q^{6-d}},$$
 (C2)

where q is the d-dimensional vector,

$$A_{d} = \frac{\Gamma(d/2)\Gamma(2-d/2)\Gamma^{2}(d/2-1)}{2\Gamma(d-2)},$$
  
$$K_{d}^{-1} = 2^{d-1}\pi^{d/2}\Gamma(d/2).$$
 (C3)

 $\Gamma(x)$  is the Euler gamma function. At  $d=2+\varepsilon$  we find to leading order in  $\varepsilon$ 

$$\Pi(q,0) = q^2 I(q,0) = \frac{2TK_2}{\varepsilon q^{2-\varepsilon}}, \quad K_2 = \frac{1}{2\pi}.$$
 (C4)

The constraint equation to first order in 1/N Eq. (43) takes the form

$$1 - \frac{g T^{1+\varepsilon} K_2}{\varepsilon} \left( 1 - \frac{2}{N} \right) = \overline{\sigma}^2 \left[ 1 - \frac{K_2}{N} \ln \frac{T^{1+\varepsilon/\varepsilon} + \overline{\sigma}^2/g}{\overline{\sigma}^2/g} \right].$$
(C5)

Using the identity

$$gT^{1+\varepsilon}/\varepsilon + \overline{\sigma}^2 = 1, \qquad (C6)$$

which is satisfied in the zeroth order in 1/N and transforming the logarithmic term in Eq. (C5) into a power, we obtain

$$\overline{\sigma} = (1 - T^{1+\varepsilon} / T^{1+\varepsilon}_{\text{N\'eel}})^{\beta_{2+\varepsilon}}, \qquad (C7)$$

$$\beta_{2+\varepsilon} = (1+1/N)/2 + \mathcal{O}(1/N^2,\varepsilon).$$
(C8)

The Néel temperature is determined by

$$T_{\text{N\'eel}}^{1+\varepsilon} = \frac{\varepsilon}{gK_2(1-2/N)} = \frac{2\pi\rho_s\varepsilon}{N-2}.$$
 (C9)

This result coincides with the result of the RG analysis.<sup>10</sup> The RG result for the critical exponent  $\beta$  reads

$$\beta_{2+\varepsilon} = \frac{1}{2} \left( 1 + \frac{1}{N-2} \right) + \mathcal{O}(\varepsilon).$$
 (C10)

Thus one has to replace  $N \rightarrow N-2$  in Eq. (C8). Such a replacement is analogous to this in the renormalized classical regime of Ref. 12 and may be justified by the calculations of terms of order of  $1/N^2$ , which we did not carry out. As demonstrated in Ref. 12 by calculations of analogous contributions up to  $1/N^2$ , this replacement should be indeed performed. Since the denominator in Eq. (C9) is of order of N, the replacement  $N \rightarrow N-2$  occurs already in the first-order expression for the transition temperature, Eq. (C9).

According to Eq. (C7), two regimes are possible in the temperature dependence of the order parameter. At  $Je^{-1/\varepsilon} \ll T \ll T_{\text{N\acute{e}el}}$  we have the spin-wave behavior

$$\overline{\sigma} = 1 - \frac{(N-1)T^{1+\varepsilon}}{4\pi\rho_s\varepsilon}.$$
(C11)

For N=3 this result is analogous to the quasi-2D case result (10) in the quantum spin case. At  $1 - T/T_{\text{N\acute{e}el}} \ll 1$  the temperature dependence of the sublattice magnetization changes from the linear one to the power behavior with the critical exponent  $\beta_{2+\varepsilon}$ .

The two temperature regimes above correspond to different pictures of the excitation spectrum. In the lowtemperature regime  $T \ll T_{\text{N\acute{e}el}}$  we have from Eq. (40) at quasimomenta q < T (only such q give a contribution to thermodynamic quantities) the zeroth-order longitudinal Green's function

$$G_l^{N=\infty}(q,0) = \frac{g}{2} \Pi(q,0) = \frac{gTK_2}{\varepsilon q^{2-\varepsilon}},$$
 (C12)

which corresponds to spin-wave excitations. Near the phase

- \*Electronic address: aoa@newton.usu.ru
- <sup>1</sup>Magnetic Properties of Layered Transition Metal Compounds, edited by L. J. de Jongh (Kluwer, Dordrecht, 1989).
- <sup>2</sup>D. Yoshioka, J. Phys. Soc. Jpn. 58, 3733 (1989).
- <sup>3</sup>M. Takahashi, Phys. Rev. B **40**, 2494 (1989); Progr. Theor. Phys. Suppl. **101**, 487 (1990).
- <sup>4</sup>A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer-Verlag, New York, 1994).
- <sup>5</sup>S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).
- <sup>6</sup>N. Read and S. Sachdev, Phys. Rev. B 42, 4568 (1990).
- <sup>7</sup>O. A. Starykh, Phys. Rev B **50**, 16 428 (1994).
- <sup>8</sup>A. V. Chubukov and O. A. Starykh, Phys. Rev. B **52**, 440 (1995).
- <sup>9</sup>V. Yu. Irkhin, A. A. Katanin, and M. I. Katsnelson, Phys. Rev. B 54, 11 953 (1996).
- <sup>10</sup>E. Brezin and J. Zinn-Justin, Phys. Rev. B **14**, 3110 (1976).
- <sup>11</sup>S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B 39, 2344 (1989).
- <sup>12</sup>A. V. Chubukov, S. Sachdev, and J. Ye, Phys. Rev. B 49, 11 919 (1994).
- <sup>13</sup>S. Hikami, Progr. Theor. Phys. 64, 1425 (1980).
- <sup>14</sup>V. Yu. Irkhin, A. A. Katanin, and M. I. Katsnelson, Phys. Lett. A 157, 295 (1991).

transition point we have at an arbitrary q [except for the exponentially narrow hydrodynamic region  $q < (2\overline{\sigma}^2/g)^{1/\varepsilon}$ ]

$$G_l^{N=\infty}(q,0) = \frac{1}{q^2},$$
 (C13)

which corresponds to critical (non-spin-wave) excitations. As follows from Eqs. (C12) and (C13), the difference of the excitation spectra is of the order of  $\varepsilon \ln q$ .

- <sup>15</sup>V. Yu. Irkhin, A. A. Katanin, and M. I. Katsnelson, Fiz. Met. Metalloved. **79**, N1, 65 (1995).
- <sup>16</sup>B.-G. Liu, J. Phys. Condens. Matter 5, 149 (1993).
- <sup>17</sup> M. I. Kaganov and A. V. Chubukov, Usp. Fiz. Nauk **153**, 537 (1987) [Sov. Phys. Usp. **30**, 1015 (1987)].
- <sup>18</sup>R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, New York, 1982).
- <sup>19</sup>E. L. Nagaev, *Magnetics with Complex Exchange Interactions* (in Russian) (Nauka, Moscow, 1988).
- <sup>20</sup>F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
- <sup>21</sup>J. Igarashi, Phys. Rev. B 46, 10 763 (1992).
- <sup>22</sup>R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989).
- <sup>23</sup>S.-K. Ma, *Modern Theory of Critical Phenomena* (Benjamin-Cummings, Reading, 1976).
- <sup>24</sup>B. Keimer *et al.*, Phys. Rev. B **45**, 7430 (1992); **46**, 14 034 (1992).
- <sup>25</sup>G. Aeppli *et al.*, Phys. Rev. Lett. **62**, 2052 (1989); K. B. Lyons *et al.*, Phys. Rev. B **37**, 2353 (1988).
- <sup>26</sup>T. Thio et al., Phys. Rev. B 38, 905 (1988); 41, 231 (1990).
- <sup>27</sup>T. Aoki, J. Phys. Soc. Jpn. **61**, 2909 (1992).
- <sup>28</sup>L. H. Ryder, *Quantum Field Theory* (Cambridge University Press, Cambridge, England, 1985).