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

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Abstract

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, Neel 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 Neel temperature. The thermodynamic quantities calculated are universal functions of the renormalized interlayer coupling parameter. The renormalization of interlayer coupling parameter turns out to be considerably temperature dependent. A good agreement with experimental data on La$_2$CuO$_4$ is obtained. The application of the approach used to the case of a ferromagnet is discussed.

75.10.-b, 75.10.Jm, 75.40.Cx

1. Introduction

Last time, great interest is paid to properties of quasi-two-dimensional (quasi-2D) antiferromagnets in connection with the investigations of layered perovskites and copper-oxide systems, including high-$T_c$ superconductors. In particular, La$_2$CuO$_4$ gives one of the best known example 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 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 $J$ (Ref. 8). 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 magnetic transition temperature. Recently, the self-consistent spin-wave theory (SSWT) has been proposed which takes into account partially the interaction between spin waves. However, the value of the Neel 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 which is based on the random-phase decoupling of equations of motion for the transverse spin Green’s function. This approach yields often 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 perturbation theory which describes correctly 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 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 $M \to \infty$ limit corresponds to SSWT (see, e.g., Ref. 7), at finite $M$ thermodynamics is described in terms of the spin-wave picture of excitation spectrum. The second way 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 $N \to \infty$ 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. 8) and $d = 2 + \varepsilon$ (Ref. 10) the results in the $SU(M)$ model coincide in the zeroth order in $1/M$ with those of the one-loop 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.[4]) 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[3] and in the classical case at an arbitrary dimensionality $2 < d < 4$ (see, e.g., Ref.[5]), lead to results which are close to those obtained by other methods. The applicability of the $1/N$-expansion at arbitrary dimensionality $2 \leq d \leq 4$ is important for the investigation of quasi-2D systems since they demonstrate the dimensional crossover from 2D to 3D behavior (see, e.g., Ref.[6]). On the other hand, the renormalization group $\varepsilon$-expansion is not applicable 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 $d = 2$ 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 Sect.2 we review various approximations in the theory of quasi-2D systems since they are based on the spin-wave picture of excitation spectrum, and analyze the corresponding expressions for the Neel temperature. In Sect.3 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[5] for the 2D case. In Sect.4 we calculate the magnetization, Neel temperature and spin correlation function to first order in $1/N$. In Sect.5 we discuss our results and compare them with experimental data on La$_2$CuO$_4$.

2. Spin-wave approximations in the theory of quasi-2D antiferromagnets

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

$$ H = \frac{1}{2} \sum_{ij} J_{ij} S_i S_j $$ (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 Neel temperature. First we consider the standard spin-wave theory. The spectrum of spin waves has the form

$$ E_q^{\text{SWT}} = S(J_0^2 - J_q^2)^{1/2} $$ (2)

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

$$ J_q = 2J(\cos q_x + \cos q_y) + 2J' \cos q_z $$ (3)

The sublattice magnetization is determined by

$$ S = S_0 - \frac{1}{2} \sum_q \frac{J_q S}{2E_q} \coth \frac{E_q}{2T} $$ (4)

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

$$ T_{\text{Neel}}^{\text{SWT}} = 4\pi JS^2 \times \left\{ \begin{array}{ll} 1/\ln(T_{\text{Neel}}/8JS^2) & \ln(J/J') \gg 2\pi S \\ 1/\ln(Jq_0^2/J') & 1 \ll \ln(J/J') \ll 2\pi S \end{array} \right. $$ (5)

Here $q_0 \simeq \pi$ 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 wavevector comes from the region with $q \leq T$, while in the classical case the value of $T_{\text{Neel}}$ is determined by the whole Brillouin zone.

The spin-wave spectrum in SSWT and the Tyablikov approach is renormalized in different ways. SSWT 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[4]. We will follow to approach of Ref.[3] which gives more satisfactory results at small $J'/J$. The spin-wave spectrum in SSWT has the form

$$ E_q^{\text{SSWT}} = S(\gamma_0^2 - \gamma_q^2)^{1/2} $$ (6)

$$ \gamma_q = 2\gamma(\cos q_x + \cos q_y) + 2\gamma' \cos q_z $$

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

$$ \gamma/J = \sum_q \frac{\gamma_q S}{E_q} \cos q_x \coth \frac{E_q}{2T} + 2S(T) $$ (7)

$$ \gamma'/J' = \sum_q \frac{\gamma_q S}{E_q} \cos q_y \coth \frac{E_q}{2T} + 2S(T) $$ (8)

The sublattice magnetization is given by
\[ \mathcal{S} = S + \frac{1}{2} - \sum_q \frac{\gamma_0 S}{2E_q} \coth \frac{E_q}{2T} \tag{9}\]

At small values of \( J'/J \) we have
\[ \mathcal{S} = \mathcal{S}_0 - \frac{T}{4\pi\gamma S} \times \left\{ \ln(T^2/8\gamma' S^2) - \ln(\gamma_0^2/\gamma') \right\} S(JJ')^{1/2} \ll T \ll JS \approx J S^2 \tag{10}\]

where \( \mathcal{S}_0 \) is the sublattice magnetization in the ground state. The quantity \( \gamma \) varies slowly with temperature in the whole region \( T < T_{\text{Neel}} \) and may be replaced by its zero-temperature value \( \gamma(0) \). According to Refs.\[\text{[I]}\], we have
\[ \gamma(0) = 1.1571J, \quad \mathcal{S}_0 = 0.3034 \tag{11}\]

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

As follows from \( \text{[I]} \), the Neel temperature is determined by the equation of Ref.\[\text{[I]}\] (note that some coefficients in this paper are incorrect)
\[ T_{\text{Neel}}^{SSWT} = 4\pi\gamma_S S \mathcal{S}_0 \times \left\{ \frac{1}{\ln(T^2(8\gamma \gamma' S^2))} - \frac{1}{\ln(\gamma_0^2/\gamma')} \right\} \ln(J/J') \gg 2\pi S \leq 2\pi S \tag{12}\]

Here \( \gamma_c \simeq \gamma(0) \) and \( \gamma'_c \) are the renormalized exchange parameters at \( T = T_{\text{Neel}} \). The value of \( \gamma_c' \) determined from \( \text{[I]} \) is
\[ \gamma'_c = (T_{\text{Neel}}/4\pi \gamma_S S^2)J' \tag{13}\]

in both the quantum and classical regimes. Note that the renormalization of the interlayer coupling in \( \text{[I]} \) plays a crucial role in lowering the Neel temperature in comparison with its SWT value \( \text{[I]} \) since \( \gamma_c'J/J' = T_{\text{Neel}}/4\pi JS^2 \ll 1 \).

In the Tyablikov theory\[\text{[II]}\] (TT) the excitation spectrum has the form
\[ E_q^{TT} = \mathcal{S}(J_0^2 - J_q^2)^{1/2} \tag{14}\]

As well as in a ferromagnet, the proportionality of the spectrum to \( \mathcal{S} \) 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.\[\text{[II]}\]). The equation for \( \mathcal{S} \) at \( S = 1/2 \) reads
\[ 1/\mathcal{S} = \sum_q J_0 \mathcal{S} q \coth \frac{E_q}{2T} \tag{15}\]

and has a more complicated form for higher spins\[\text{[II]}\]. Near the Neel temperature \( TT \) yields at arbitrary \( S \) and any space dimensionality \( d > 2 \)
\[ \mathcal{S} = \left[ 2\Gamma_S T_{\text{Neel}}^{TT} \left( 1 - \frac{T}{T_{\text{Neel}}^{TT}} \right) \right]^{1/2} \tag{16}\]

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
\[ T_{\text{Neel}}^{TT} \approx \frac{4\pi JS^2}{\ln(\gamma_0^2/\gamma')} \tag{17}\]

The result \( \text{[II]} \) is lower than SSWT value \( \text{[I]} \) and closed to experimental data (see Sect.5). On the other hand, the result \( \text{[II]} \) coincides with that of the spherical model\[\text{[II]}\] (which is adequate only in the classical limit \( S \to \infty \)) and with the result of the spin-wave approximation \( \text{[II]} \) in the classical regime \( T_{\text{Neel}} \gg JS \).

The Tyablikov approximation gives the same result \( \text{[II]} \) (with the replacement \( J \to -J, J' \to -J' \) 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 the theoretical point of view.

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

To improve the description of the critical region and obtain a better approximation for the Neel temperature in the quantum case, it is necessary to take into account fluctuation corrections to the spin-wave theory result for \( T_{\text{Neel}} \) 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.

3. 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
In the 2D case this model was applied in Refs. 13, 14. The large value of the correlation length \( \xi \gg a \) (a is the lattice parameter in the plane) plays the crucial role in the Haldane’s mapping of an antiferromagnetic Heisenberg model \( ( i ) \) to quantum nonlinear sigma-model (see e.g. Ref. 13). 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 \( \xi(T \leq T_{\text{Neel}}) = \infty. \) However, at small \( q \) we have

\[
J_0 - J_q \simeq J(a q)^2 + 2 J' (1 - \cos q_z) \tag{18}
\]

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 \( \alpha = 2 J'/J a^2 \) is the interlayer coupling parameter; in this paper we consider only the case where \( \alpha < 1 \).

On the scale of order of \( \xi_{J'} \) the regime of fluctuations changes from 2D to 3D one. 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

\[
L_T = c/T \tag{20}
\]

(\( c \sim JSa \) is the fully renormalized spin-wave velocity), three regimes are possible

(i) \( L_T \sim \xi_{J'} \), or, equivalently, \( T \sim \alpha^{1/2} c \sim (J J')^{1/2} \). This is an analog of the quantum critical regime \( L_T \sim \xi \) in the 2D case[8,9,11].

(ii) \( a \ll L_T \ll \xi_{J'} \), i.e. \( \alpha^{1/2} c \ll T \ll c \) which is an analog of the renormalized classical regime \( a \ll L_T \ll \xi \) in the 2D case and

(iii) the classical regime \( L_T \ll a \) (i.e. \( JS \ll T \).

Since the regime (i) is well described by the standard spin-wave theory (or by SSWT), we do not treat the thermodynamics at temperatures of order of \( (J J')^{1/2} \). From (i) and (ii) one can see that \( T_{\text{Neel}} \gg (J J')^{1/2} \). In the regimes (ii) and (iii) implementation of principles of finite-size scaling gives

\[
T_{\text{Neel}} = \rho_s \Phi(\xi_{J'}/L_T, \xi_{J'})/a \tag{21}
\]

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

\[
T_{\text{Neel}} = \rho_s \Phi(\xi_{J'}/L_T, \infty) = \rho_s \Phi_a(T_{\text{Neel}}/\alpha^{1/2} c) \tag{22}
\]

while in the regime (iii) \( \xi_{J'}/L_T \gg \xi_{J'}/a \) and

\[
T_{\text{Neel}} = \rho_s \Phi(\infty, \xi_{J'}/a) = \rho_s \Phi_a(1/\alpha^{1/2} a) \tag{23}
\]

Note that the results of SWT \( ( i ) \) and SSWT \( ( i i ) \) for the Neel temperature agree with \( ( i i i ) \) for the quantum regime and with \( ( i i ) \) for the classical regime. At the same time, the result of the Tyablikov approximation \( ( i i i ) \) satisfies the classical regime scaling form \( ( i i ) \) for all spin values, which confirms the absence of quantum fluctuations at the critical temperature in this approximation. As follows from \( ( i i ) \), the value of Neel temperature in the classical regime depends on fluctuations on a scale of order of lattice constant, i.e. is non-universal. 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 \( ( i i i ) \) (see full discussion in Ref. 13) to integrate out “fast” modes. Thus the partition function has in terms of a path integral the form

\[
Z = \int D\sigma_i(\tau) \exp \left\{ -\frac{\chi_0}{2} \int_0^{1/T} d\tau \int d\tau' \sum_i (\partial_\tau \sigma_i)^2 \right. \\
\left. - \frac{1}{2} S^2 \int_0^{1/T} d\tau \int d\tau' \sum_{ij} (\sigma_i - \sigma_j)^2 \right\} \prod_i \delta(\sigma_i^2 - 1) \tag{24}
\]

where \( \sigma_i \) is a three-component unit-vector field, \( i \) is the index of a site, \( \chi_0 \) is the uniform magnetic susceptibility. In the continual limit we reproduce the standard three-dimensional quantum nonlinear-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: \( \sigma_i(\tau) \to \sigma_{i z}(r, \tau) \) where \( r \) is a 2D vector, \( i_z \) is the index of a layer. The partition function takes the form

\[
Z = \int D\sigma_{i z}(r, \tau) \exp \left\{ -\frac{\rho_s^0}{2} \int_0^{1/T} d\tau \int d^2 r \sum_{i z} \left[ \frac{1}{c_0^2} (\partial_\tau \sigma_{i z})^2 \right. \\
\left. + (\nabla \sigma_{i z})^2 + \frac{\alpha}{2} (\sigma_{i z+1} - \sigma_{i z})^2 \right] \right\} \delta(\sigma_{i z}^2 - 1) \tag{25}
\]

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 three-component field \( \sigma_{i z}(r, \tau) \) by the \( N \)-component one \( \sigma^m_{i z}(r, \tau), m = 1...N \). The constraint condition \( \sigma^2 = 1 \) may be taken into account by introducing the slave field \( \lambda_{i z}(r, \tau) \). To calculate the dynamic susceptibility we also introduce the external non-uniform time-dependent
magnetic field $h_i^m(r, \tau)$. Then we obtain the partition function of the $O(N)$ model in the form:

$$ Z[h] = \int D\sigma D\lambda \exp \left\{ -\frac{1}{2g} \int_0^{1/T} d\tau \int d^2r \sum_i \left[ \frac{1}{2} (\partial_\tau \sigma_i)^2 + (\nabla \sigma_i)^2 + \frac{\alpha}{2} (\sigma_{i+1} - \sigma_i)^2 + i\lambda (\sigma_i^2 - 1) - 2gh_i_i \sigma_i - \sigma_i \right] \right\} $$

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

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

$$ S_{eff}[\lambda, h] = \frac{1}{2} \ln \det \tilde{G}_0 + \frac{1}{2g} (1 - \bar{\sigma}^2) \text{Sp}(i\lambda) $$

$$ + \frac{1}{2g} \text{Sp} \left[ (i\lambda \sigma - h/\rho_s^0) \tilde{G}_0 (i\lambda \sigma - h/\rho_s^0) \right] $$

where

$$ \tilde{G}_0 = [\partial^2/\epsilon_0^2 + \nabla^2 + \alpha \Delta_z]^{-1} $$

$$ \Delta_z \sigma_i(r, \tau) = \sigma_{i+1}(r, \tau) - \sigma_i(r, \tau) $$

Since $N$ enters only as a prefactor in the exponent, expanding near the saddle point generates a series in $1/N$. At $T < T_{\text{Neel}}$ we have the saddle point value $i\lambda = 0$ and $\bar{\sigma}^2 \neq 0$. The Green’s function of the field $\bar{\sigma}$ is defined by

$$ G^{m,n}(q, q_z, \omega_n) = \frac{\rho_s^0}{Z[0]} \int \frac{d^2p}{(2\pi)^2} \int \frac{dz}{2\pi} \sum_i \frac{\partial^2 Z[h]}{\partial h^m(p, p_z, \omega_l) \partial h^n(q - p, q_z - p_z, \omega_l - \omega)} \bigg|_{h=0} $$

where $h(p, p_z, \omega)$ is the Fourier transform of $h_i_i(r, \tau)$. Note that only diagonal elements $G^{m,n}$ are nonzero, and they are proportional to the non-uniform dynamic spin susceptibility:

$$ G^{m,n}(q, q_z, \omega) = \rho_s^0 S \chi^{m,n}(q + Q, q_z + \pi, \omega) \delta_{mn} $$

where $Q = (\pi, \pi)$ is the wavevector of antiferromagnetic structure in the plane; for $N = 3$

$$ \chi^{\alpha\beta}(q, q_z, \omega) = \sum_i e^{i(q \cdot R_i + q_z \cdot z_i)} \langle \sigma_i^\alpha | S_i^\beta \rangle_{\omega} $$

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 $\sigma^m = \sigma_0^m N$ where $\sigma$ plays the role of the relative sublattice magnetization $\sigma/\bar{\sigma}$. Then $G^{N,N}$ corresponds to the longitudinal Green’s function, $G_1$, while other diagonal components (which are all equal) to the transverse Green’s function, $G_{\perp}$. At $T < T_{\text{Neel}}$, the value of $\bar{\sigma}$ is determined by the constraint $\langle \sigma^2 \rangle = 1$ which takes the form

$$ 1 - \bar{\sigma}^2 = \frac{T}{\rho_s^0} \sum_m \sum_n \int \frac{d^2k}{(2\pi)^2} \int \frac{dk_z}{2\pi} G^{mn}(k, k_z, \omega_n) $$

(25)

We use the relativistic (hard) cutoff $\omega_0^2 + k^2 < \Lambda^2$ 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 put to be equal to unity except for the final results.

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

$$ G_0(k, k_z, \omega_n) = [\omega_0^2 + k^2 + \alpha(1 - \cos k_z)]^{-1} $$

After evaluation of the integrals and frequency summation in (32) we obtain the Neel temperature in the limit $N \to \infty$

$$ T_{\text{Neel}}^0 = \frac{4\pi \rho_s N^{\infty}}{N \ln(2T_{\text{Neel}}/\alpha c^2)} $$

(34)

where $\rho_s^{N^{\infty}} = N(1 - 1/\gamma_c)$ is the renormalized spin stiffness in zeroth order in $1/N$, $\gamma_c = 2\pi^2/\Lambda$. To compare the result (34) with the result of the SSWT we note that the value of spin stiffness in SSWT is $\rho_s^{SSWT} = \gamma S$ for $S = 1/2$ this equals to 0.176J which is somewhat lower than the result of two-loop RG analysis and numerical calculation $\rho_s = 0.181J$ and the value of the spin-wave velocity is $c^{SSWT} = \sqrt{\gamma S}$. 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, $\alpha^{SSWT} = 2\gamma_c/\gamma_c < \alpha$). Further we will show that, as well as in the calculation of the correlation length in the 2D-case in the first order in $1/N$,

(i) the factor of $N$ in the denominator of (34) is to be replaced by $N - 2$

(ii) $\rho_s^{N^{\infty}}$ and $\alpha$ in (34) are to be replaced by their renormalized values, $\rho_s$ and $\alpha$.

(iii) terms of order of $\ln(2T^2/\alpha)$ and unity, which do not enter the SSWT result for $T_{\text{Neel}}$, occur in the denominator of (34).

The exact Green’s function may be expressed as
\[ G^{mm}(k, k_z, \omega_n) = \left[ \omega_n^2 + k^2 + \alpha(1 - \cos k_z) \right] + \Sigma(k, k_z, \omega_n)^{-1} - C(k, k_z, \omega_n) \delta_{mN} \]

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:

\[
\Sigma(k, k_z, \omega_n) = \frac{2T}{N} \sum_{\omega_m} \int \frac{d^2q}{(2\pi)^2} \int \frac{dq_z}{2\pi} \Pi(q, q_z) \left( G_0(k + q, k_z + q_z, \omega_n + \omega_m) - G_0(q_z, \omega_m) \right) \frac{\Pi(q, \omega_m)}{\Pi(k, \omega_m)}
\]

\[
C(k, k_z, \omega_n) = \frac{2\sigma^2}{g} \frac{1}{\Pi(k, k_z, \omega_n)}
\]

where

\[
\Pi(q, q_z, \omega_n) = \Pi(q, q_z, \omega_n) + \frac{2\sigma^2}{g} G_0(q, q_z, \omega_n)
\]

\[
\Pi(q, q_z, \omega_n) = T \sum_{\omega_m} \int \frac{d^2p}{(2\pi)^2} \int \frac{dp_z}{2\pi} G_0(p, p_z, \omega_l) \times G_0(p + q, p_z + q_z, \omega_l + \omega_n).
\]

Note that the quantity \(C\) in (35) 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 \(1/N\):

\[
G_{1=0}^N(q, q_z, \omega_n) = \frac{\Pi(q, q_z, \omega_n)}{q^2 \Pi(q, q_z, \omega_n) + 2\sigma^2/g}.
\]

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

\[
1 - \sigma^2 = gT \sum_{\omega_m} \int \frac{d^2k}{(2\pi)^2} \int \frac{dk_z}{2\pi} G_0(k, k_z, \omega_m)
\]

\[ - gT \sum_{\omega_m} \int \frac{d^2k}{(2\pi)^2} \int \frac{dk_z}{2\pi} G_0^2(k, k_z, \omega_m) \Sigma(k, k_z, \omega_m)
\]

\[ - \frac{2\sigma^2T}{N} \sum_{\omega_m} \int \frac{d^2k}{(2\pi)^2} \int \frac{dk_z}{2\pi} \frac{G_0^2(k, k_z, \omega_m)}{\Pi(k, k_z, \omega_m)}.
\]

Following to (35) we introduce the function

\[
I(k, k_z, \omega_m) = T \sum_{\omega_n} \int \frac{d^2q}{(2\pi)^2} \int \frac{dq_z}{2\pi} G_0(q, q_z, \omega_n) (42)
\]

\[ \times \left[ G_0(k + q, k_z + q_z, \omega_m + \omega_n) - G_0(k, k_z, \omega_m) \right]
\]

and represent the equation (31) in the following convenient form

\[
R(T, x_T) = \frac{2T}{N} \sum_{\omega_m} \int \frac{d^2k}{(2\pi)^2} \int \frac{dk_z}{2\pi} I(k, k_z, \omega_m),
\]

\[
F(T, x_T) = \frac{2T}{N} \sum_{\omega_m} \int \frac{d^2k}{(2\pi)^2} \int \frac{dk_z}{2\pi} \frac{G_0^2(k, k_z, \omega_m)}{\Pi(k, k_z, \omega_m)},
\]

and

\[
x_T = 4\pi\sigma^2/gT
\]

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. The expressions (34)-(36) enable one to investigate the magnetization and to calculate the Neel temperature for a quantum quasi-2D antiferromagnet.

4. The sublattice magnetization, Neel temperature and correlation functions

As discussed in the beginning of previous section, we consider the quantum case with \(\alpha\) being small enough to satisfy the condition \(\ln(2T_{\text{Neel}}^2/\alpha^2) \gg 1\). The calculation of the functions \(R\) and \(F\) at \(T \gg \alpha^{1/2}\) (i.e. (41) \(\gg (JJ')^{1/2}\)) is discussed in Appendix B. Neglecting the terms of order of \(1/\ln(2T_{\text{Neel}}^2/\alpha^2)\) we have

\[
R(T, x_T) = \frac{T}{2\pi N} \ln \frac{2T^2}{\alpha} - \frac{(3 + 2x_T)T}{4\pi N} \ln \frac{4\pi \rho_s}{NT x_T}
\]

\[ + \frac{T}{2\pi N} \ln(2T^2/\alpha/\alpha) + x_T \]

\[ + \frac{8T}{3\pi^3 N} \ln \frac{2T^2}{\alpha/\alpha} + x_T \]

\[ - \frac{2T}{3\pi^3 N} \ln \frac{NA}{16\rho_s} + \frac{T}{4\pi} \ln 1(x_T)
\]

and

\[
F(T, x_T) = \frac{1}{N} \ln \frac{4\pi \rho_s}{NT 3x_T} + \frac{8}{\pi^2 N} \ln \frac{NA}{16\rho_s} + I_2(x_T)
\]
where the functions $I_1(x\sigma), I_2(x\sigma)$ are defined in Appendix B. After substituting (17), (18) into the constraint equation (14) and using the results of Ref. 4 for the renormalized ground-state sublattice magnetization $\sigma_0 = \sigma(T = 0) = S_0/S$ and the spin stiffness $\rho_s$ of a quantum 2D antiferromagnet,

$$\frac{\sigma^2}{\rho_s} = \frac{g}{N} \left(1 - \frac{8}{3\pi^2 N} \ln \frac{NA}{16\rho_s}\right), \quad (49)$$

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

one can see that the sublattice magnetization, being expressed in terms of quantum-renormalized $\rho_s$ and $\sigma_0$, still depends on $\Lambda$, i.e. is non-universal. To make the sublattice magnetization completely universal we have to introduce the renormalized parameter of the interlayer coupling

$$\sigma = \alpha \left[1 - \frac{8}{3\pi^2 N} \ln \frac{NA}{16\rho_s}\right]. \quad (51)$$

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 (14) reads

$$1 - \frac{NT}{4\pi \rho_s} \left[(1 - \frac{2}{N}) \ln \frac{2T^2}{\alpha_r} + \frac{3}{N} \ln \frac{4\pi \rho_s}{NT \sigma} \right]$$

$$+ \frac{2}{N} \ln \frac{2T^2}{\alpha_r} + x\sigma - I_1(x\sigma)$$

$$= \frac{\sigma}{\sigma_0} \left[1 + \frac{1}{N} \ln \frac{4\pi \rho_s}{NT \sigma} - I_2(x\sigma)\right]. \quad (52)$$

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

First we consider the case $x\sigma = 1$, or, equivalently,

$$NT/4\pi \rho_s \ll \sigma^2/\sigma_0 \quad (53)$$

Since $x\sigma$ is the decreasing function of temperature, this inequality is satisfied at low enough temperatures. In this case the integrals $I_1(x\sigma)$ and $I_2(x\sigma)$ are of order of $1/\beta_2$, 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 $1/\varepsilon \rightarrow \ln(2/\alpha_r)$, which corresponds to the limit $\varepsilon \rightarrow 0$ with simultaneous cutting the integrals over quasimomentum on the scale $1/\xi$. Similar to the $d = 2 + \varepsilon$ case (Appendix C) we transform the logarithmic term in the right-hand side of (52) into power and replace $N \rightarrow N - 2$. Then we have

$$(\sigma/\sigma_0)^{1/\beta_2} \left[1 - I_2(x\sigma)\right], \quad (54)$$

$$= 1 - \frac{NT}{4\pi \rho_s} \left[(1 - \frac{2}{N}) \ln \frac{2T^2}{\alpha_r} + \frac{3}{N} \ln \frac{\sigma_0}{\sigma} \right]$$

$$+ \frac{2}{N} \ln \frac{2T^2}{\alpha_r} + x\sigma - I_1(x\sigma) \quad (52)$$

where, being expressed through the renormalized parameters,

$$x\sigma = \frac{4\pi \rho_s}{(N-2) T \sigma_0^2} \quad (55)$$

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

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

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

$$T(N - 2) \ln(2T^2/\alpha_r)/4\pi \rho_s \ll \sigma^2/\sigma_0 \quad (57)$$

In this region

$$\sigma = \sigma_0 \left[1 - \frac{T(N - 1)}{8\pi \rho_s} \ln \frac{2T^2}{\alpha_r c_T}\right]. \quad (58)$$

At $N = 3$ we reproduce the result of SSWT (10) with $2\gamma'/\gamma$ being replaced by $\alpha_r$. The factor $N - 1$ in (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 $\sigma(T)$. 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 (60) we get

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

irrespective of $k_z$. Thus we have

$$G_{t}^{-1}(k, k_z, 0) = k^2 \left[1 + \frac{8}{3\pi^2 N} \ln \frac{NA}{16\rho_s} + \alpha(1 - \cos k_z)\right] \quad (60)$$

$$= Z^{-1} \left[k^2 + \alpha_r(1 - \cos q_z)\right].$$
We see that the renormalized Green’s function differs from the bare one by the renormalization factor $Z$ and by replacement $\alpha \to \alpha_r$ only. Thus the experimentally observed (fully renormalized) interlayer coupling is just $\alpha_r$. At higher temperatures the temperature renormalization of interlayer coupling, which will be calculated below, becomes important.

At intermediate temperatures where

$$(N-2)T/4\pi\rho_s \ll \sigma^2/\sigma_0^2 \ll (N-2)T\ln(2T^2/\alpha)/4\pi\rho_s$$

(61)

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

$$\left(\sigma/\sigma_0\right)^{1/\beta_2} = 1 - \frac{T}{4\pi\rho_s} \left[ (N-2)\ln\frac{2T^2}{\alpha_r} + 3\ln\frac{\sigma_0}{\sigma} - 2 \right]$$

(62)

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

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

$$\sigma^2/\sigma_0^2 \ll (N-2)T/4\pi\rho_s$$

(63)

After expanding (62) near $T = T_{\text{Neel}}$, $\sigma = 0$, picking out the logarithmically divergent parts of $I_1(\sigma)$ and $I_2(\sigma)$ at small $\sigma$ analytically, and evaluating numerically the integrals we have

$$1 - \frac{T}{T_{\text{Neel}}} = \frac{\sigma^2}{\sigma_0^2} \left[ 1 + \frac{1}{N} \ln\frac{4\pi\rho_s}{(N-2)T_{\text{Neel}}} + \frac{8}{\pi^2 N} \ln x_\sigma - A_0 \right]$$

(64)

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

$$T_{\text{Neel}} = 4\pi\rho_s \left[ (N-2)\ln\frac{2T_{\text{Neel}}^2}{\alpha_r} + 3\ln\frac{4\pi\rho_s}{(N-2)T_{\text{Neel}}} - 0.6660 \right]^{-1}.$$  

(65)

As will be clear below the second term in the denominator, which is of order of $\ln(2T_{\text{Neel}}^2/\alpha)$ leads to a significant lowering of Neel temperature in comparison with SSWT (where only the first term is taken into account). We collect separately the logarithmic terms in (64) which comes from the quasimomenta $q \gg \alpha^{1/2}$ (2D regime) and $q \ll \alpha^{1/2}$ (3D regime):

$$1 - \frac{T}{T_{\text{Neel}}} = \frac{\sigma^2}{\sigma_0^2} (1 - A_0) \left[ 1 + \frac{1}{N} \ln\frac{4\pi\rho_s}{(N-2)T_{\text{Neel}}} \right]$$

$$\times \left[ 1 + \frac{8}{\pi^2 N} \ln x_\sigma \right]$$

(66)

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

$$\frac{\sigma^2}{\sigma_0^2} = \left[ \frac{4\pi\rho_s}{(N-2)T_{\text{Neel}}} \right]^{\beta_3/\beta_2 - 1} \left[ 1 - \frac{T}{T_{\text{Neel}}} \right]^{2\beta_3}$$

(67)

where

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

(68)

is the true 3D critical exponent for the magnetization. It should be noted that we have not to perform the replacement $N \to N - 2$ in (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 at $d = 3$, in agreement with the universality hypothesis. The dependence (67) is to be compared with that in the Tyablikov approximation (69) where $\beta = 1/2$ and the dimensional crossover is absent.

Consider now the self-energy $\Sigma(k, k_z, 0) = T = T_{\text{Neel}}$. At $\alpha^{1/2} \ll k \ll T_{\text{Neel}}$ the self-energy has the same form as in the 2D case (69) with $\xi$ being replacing by $\xi'$:

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

(69)

Thus the expression for Green’s function reads ($G = G_i = G_l$)

$$G(k, k_z, 0) = \frac{1}{k^2} \left[ \frac{(N-2)T_{\text{Neel}}}{4\pi\rho_s} \ln\frac{2k^2}{\alpha} \right]^{1/(N-2)}$$

$$\times \left( \frac{N-1}{N} \right) \left[ 1 - \eta \ln\frac{N\Lambda}{16\rho_s} \right]$$

(70)

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

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 (69) (which are analogous to the calculation of the functions $R$ and $F$ in Appendix B) we have
\[ \Sigma(k, k_2, 0) = A_1 k^2 + \frac{\alpha}{2} A_2 k_2^2 + \frac{\eta}{2} (k^2 + \frac{\alpha}{2} k_2^2) \ln k^2 + \frac{\alpha}{2} k_2^2 / 2. \] (71)

Here
\[ A_1 = \frac{\eta}{2} N A \frac{1}{16 \rho_s} + \frac{1}{N} \ln \ln \frac{2T^2}{2\pi} + \frac{0.4564}{N}, \] (72)
\[ A_2 = -0.6122 / N. \]

and
\[ \eta = 8 / (3\pi^2 N) \]
(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 \(\eta \simeq 0.09\). Using (73) we find
\[ G^{-1}(k, k_2, 0) = (1 + A_1) \alpha^{\eta/2} \left( k^2 + \frac{\alpha}{2} k_2^2 \right)^{(1-\eta/2)} \]
(74)

\(k \ll \alpha^{1/2}, k_2 \ll 1\).

The quantity
\[ \alpha_c = \alpha (1 + A_2) / (1 + A_1) \]
(75)
can be interpreted as the renormalized interlayer coupling at \(T = T_{\text{Neel}}\).

Using (73) we find the following relation between the renormalized coupling parameters at low \(T\) and at \(T = T_{\text{Neel}}\):
\[ \alpha_c = \alpha_c \left( 1 + \frac{1.0686}{N} \right) \left[ \frac{(N - 2) T_{\text{Neel}}}{4\pi \rho_s} \right]^{1/(N-2)}. \] (76)

When deriving (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 well as in SSWT (see Sect.2), the renormalized interlayer coupling at \(T_{\text{Neel}}\) is lower than the low-temperature one, but the concrete expression at \(N = 3\) is slightly different from these in SSWT.

Using (74) we get the following equation for \(T_{\text{Neel}}\) in terms of \(\alpha_c\):
\[ T_{\text{Neel}} = 4\pi \rho_s \left[ (N - 2) \ln \frac{2 T_{\text{Neel}}}{e^2 \alpha_c} + 2 \ln \frac{4\pi \rho_s}{(N - 2) T_{\text{Neel}}} + 1.0117 \right]^{-1}. \] (77)

where \(c\) is the fully-renormalized spin-wave velocity: in SSWT we have \(c = \sqrt{8\gamma}(0) S\) (see Sect.2). For \(N = 3\) we have
\[ T_{\text{Neel}} = 4\pi \rho_s / \ln \left[ 5.5005 (4\pi \rho_s)^2 / e^2 \alpha_c \right], \]
(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
\[ S(R, R_z) = -\frac{1}{\pi} \int \frac{d^2 k}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} e^{i(k_R + k_z) R_z} \]
(79)
\[ \times \sum_m \int d\omega \text{Im} \chi^{mm}(k, k_z, \omega) \frac{1}{e^{\omega/T} - 1} \]

at \(T = T_{\text{Neel}}\). For \(N = 3\) we have
\[ S(R, R_z) = \left| \langle S_i(r) S_{i+R_z}(r + R) \rangle \right| \]

The static approximation is sufficient to determine the asymptotics of the correlation function. Using (80), (81) we derive (cf. Ref.3)
\[ S(R, R_z) = \frac{T_{\text{Neel}}}{\rho_s} \left[ 1 + \eta \ln \frac{N A}{16 \rho_s} \right] \]
(80)
\[ \times \int \frac{d^2 k}{(2\pi)^2} \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} \chi(k, k_z, 0) e^{i(k_R + k_z) R_z}. \]

One can see that at \(R^2 \alpha + R_z^2 \gg 1\) the asymptotics of the integral in (81) is determined by the region \(k \ll \alpha^{1/2}\) and \(k_z \ll 1\) where \(\chi(k, k_z, 0)\) is calculated above (see (74)). Substituting (74) into (80) we have
\[ S(R) = \frac{1}{4\pi} \frac{T_{\text{Neel}} \tilde{\rho}_S}{\rho_s} (1 - A_1 - \eta C) \left[ 1 + \eta \ln \frac{N A}{16 \rho_s} \right] \]
(81)
\[ \times \left( \frac{2}{\alpha_c + \eta R^2 + 2\eta} \right)^{1/2} \]
where \(R^2 = (R^2 + 2R_z^2 / \alpha_c)^{1/2}\) and \(C \simeq 0.5772\) is the Euler constant. Using the value of \(A_1\) (72) and transforming the term with \(1/N \ln \ln (2T^2/\alpha)\) into power we obtain the final result for the spin correlation function at \(T = T_{\text{Neel}}\) and \(R \alpha_c^{1/2} \gg 1\):
\[ S(R) = \frac{1}{4\pi} \frac{T_{\text{Neel}} \tilde{\rho}_S}{\rho_s} \left[ (N - 2) T_{\text{Neel}} \right]^{1/(N-2)} \]
(82)
\[ \times (1 - A_1 - \eta C) \left( \frac{2}{\alpha_c + \eta R^2 + 2\eta} \right)^{1/2} \]
where $T_1 = 0.4564/N$. Thus $S(R)$ enables one to determine the value of $\alpha_c$. As one should expect, being rewritten through renormalized parameters $\rho_s$ and $\alpha_c$, $S(R)$ does not contain the cutoff parameter $\Lambda$ and is thereby completely universal.

At $1 \ll R \ll \alpha_c^{-1/2}$ we derive from (74), (75) the leading term of asymptotics of the correlation function within a plane ($N = 3$)

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

Thus we have in this case a logarithmic decrease of the correlation function, as well as in the 2D case at $1 \ll R \ll \alpha_c^{-1/2}$.

5. Discussion and conclusions

In the above treatment we analyzed the sublattice magnetization $\overline{S}$ of a quasi-2D quantum antiferromagnet ($T_{Neel} \ll JS$). At temperatures $T \leq (JJ')^{1/2}$ the behavior $\overline{S}(T)$ is satisfactorily described by the standard spin-wave theory. For $T \gg (JJ')^{1/2}$ we have obtained the equation (22) 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

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

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

(ii) the case of the intermediate temperatures (23), or equivalently

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

$$1 - T/T_{Neel} \gg (1 - A_0)/(4\pi JS^2)^{1/2} \tag{85}$$

$(1 - A_0 \simeq 0.0365)$, 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 Neel temperature is considerably lowered.

(iii) the vicinity of the Neel temperature (24), or

$$1 - T/T_{Neel} \ll (1 - A_0)(T/4\pi JS^2)^{1/2} \tag{86}$$

where we obtain the critical behaviour $\overline{S} \sim (T_{Neel} - T)^{\beta_3}$, $\beta_3 \simeq 0.36$.

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 the equation (22) is transformed in different ways in these regions to derive the results (24) and (25) respectively. Note, that in the region (ii) the “2D-like” 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 $CDN^{-1}$ model.

We have also derived the expressions for the magnetic transition temperature (26), (27) which contain the renormalized quantities $\alpha_{c,T} = 2\gamma_r/J_S$ where $\gamma_r$ are the experimentally observable (renormalized) interlayer exchange parameters at low temperatures and $T = T_{Neel}$ respectively, and $\gamma \simeq 1.1571J$ is the value of renormalized intralayer coupling parameter which is weakly temperature dependent. Therefore these expressions have an universal form, in agreement with the scaling analysis. Unlike the corresponding results of the spin-wave approaches (see Sect.2), they contain the terms of order of $\ln \ln(T_{Neel}/JJ')$ and unity, which are formally small as compared to the leading term of order of $\ln(T_{Neel}/JJ')$. However, the $\ln$-terms result in a significant lowering of $T_{Neel}$ in comparison with the SSWT value (11) 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 $1/\ln(T_{Neel}/JJ')$ may be neglected.

The experimental temperature dependence of the sublattice magnetization in La$_2$CuO$_4$ is shown in Fig.1. For comparison, the results of spin-wave approximations (SWT, SSWT and the Tyablikov theory, see Sect.2) and the result of $1/N$ expansion are also presented. The renormalized value of the in-plane exchange parameter $\gamma \simeq 1850K$ can be found from the experimental data[3] and the value $\gamma_r/J_S = 5 \cdot 10^{-4}$ 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.4, $\gamma'/\gamma = 5 \cdot 10^{-5}$, 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 (74) for above parameters $\alpha_{c}/\alpha_r = \gamma_r'/\gamma_c' \simeq 0.13$. Thus experiments at different temperatures may give different results.

One can see that SWT and SSWT yield satisfactory results for $T < 0.6T_{Neel}$ and $T < 0.8T_{Neel}$ 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, $\beta_{exp} \simeq 0.33$. Besides that, both theories give large values of the Neel temperature $T_{SW}^{Neel} = 672K, T_{SSWT}^{Neel} = 537K$. This fact is often not taken into account when treating experimental data. At the same time, TT gives the value $T_{TT}^{Neel} = 454 K$ 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 $T_{\text{Neel}} \gg JS$. 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, $T_{\text{Neel}} = T_{\text{Curie}}$ for the same $| J |$).

The result of the $1/N$-expansion to first order in $1/N$ is $T_{\text{Neel}} = 345$ K which is considerably lower than in the Tyablikov approximation and is in a good agreement with the experimental value, $T_{\text{exp}} = 325$ K. The spin-wave region extends up to $300$ K, while the 2D-like region from $320$ K to about $340$ K; the critical 3D region is narrow (about $1$ K). The results of the numerical solution of equation (64) 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 in La$_2$CuO$_4$, 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. 13. Therefore an extension of the present approach up 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.

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 Neel temperature.

It would be also interesting to perform similar calculations of thermodynamic properties for a ferromagnet. The results should coincide with those for an antiferromagnet only in the classical case. Unfortunately, the nonlinear-sigma model for ferromagnet has the Berry phase term $A(\sigma) \partial \sigma / \partial \tau$ in the action ($A$ is the vector potential of unit magnetic monopole), see, e.g., Ref. 14. This term cannot be eliminated in the quantum case and prevents constructing the $1/N$-expansion. For singular contributions, the results for a quantum ferromagnet ($T_{\text{Curie}} \ll JS$) differ from those for an antiferromagnet by the replacement

$$\ln(T^2/8S^2\gamma_{r,c}') \to \ln(T/\gamma_{r,c}'S)$$

(as well as in SSWT, see Ref. 12). Taking into account only such terms, the expression for the Curie temperature has the form

$$T_{\text{Curie}} = 4\pi\rho_s \left[ (N - 2) \ln \frac{T_{\text{Curie}}}{\gamma_{c}' S} + \frac{2\pi\rho_s}{(N - 2)T_{\text{Curie}}} + O(1) \right]^{-1}$$

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

$$T_{\text{Curie}} = 4\pi\rho_s \left[ (N - 2) \ln \frac{T_{\text{Curie}}}{\gamma_{c}' S} + 2 \ln \frac{2\pi\rho_s}{(N - 2)T_{\text{Curie}}} + O(1) \right]^{-1}$$

where

$$\gamma_{c}' = A_{\gamma c}' \left( \frac{(N - 2)T_{\text{Curie}}}{4\pi\rho_s} \right)^{1/(N - 2)}.$$

and $A_{\gamma} \sim 1$. One may expect that, as well as in Ref. 13, 17, the non-singular 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. 11). 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 satisfactorily. The description of the 3D critical behavior of a quasi-2D ferromagnet requires other methods.

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 $\Pi(q, q_z, \omega_n)$ (93) and the function $I(q, q_z, \omega_n)$ determined by (12) 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 $\omega_m = 0$. 

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After integrating over $k_z$ with the use of the Feynman identity (see, e.g., Ref. [3] we get

$$\Pi(q, q_z, 0) = \frac{T K_F}{2} \int_0^{2\pi q^2} \frac{d\alpha}{\sqrt{1-\alpha^2}} \frac{1}{\sqrt{\alpha(z)}} \ln \frac{q^2}{\alpha}$$

where $\alpha(q, q_z) = \alpha[2 + \alpha(1 - \cos q_z)]$. At large $q \gg \alpha^{1/2}$ the function $\Pi(q, q_z, 0)$ has a 2D form (cf. [3])

$$\Pi(q, q_z, 0) \approx \frac{T}{2\pi q^2} \ln \frac{q^2}{\alpha}, \quad \alpha \ll q^2 \ll T. \quad (92)$$

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

$$\Pi(q, q_z, 0) \approx \frac{T}{4\sqrt{2\alpha(q, q_z)}}, \quad q^2 \ll \alpha. \quad (93)$$

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

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

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

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

$$\times \ln \frac{\omega_n^2 + q^2 + 2\omega_m \omega_n}{\sqrt{(\omega_n^2 + q^2 + 2\omega_m \omega_n)^2 + 4q^2 \omega_n^2}} \times \text{Arc tanh}$$

$$(95)$$

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

$$\Pi_{qu}(q, \omega_n) \approx \frac{Tq^2}{\pi (q^2 + \omega_n^2)^{3/2}} \ln \frac{qT}{q^2 + \omega_n^2} + \frac{T}{4\pi} \sum_{m \neq 0} \frac{\omega_n^2 - q^2}{(q^2 + \omega_n^2)^{3/2}}, \quad q^2 + \omega_n^2 \gg T^2 \quad (101)$$

Appendix B. Calculation of 1/N-corrections to the constraint at $T \leq T_{Neel}$.

Consider briefly the calculation of the functions $R$ and $F$ which determine, according to (43), the corrections to the constraint to first order in $1/N$. First we introduce intermediate cutoff parameters $C$ and $C'$ determined by $\alpha^{1/2} < C \ll T < 2\pi C' \ll \Lambda$ 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. $\omega_n = 0$, $C < q \ll 2\pi C'$
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 $R_i(T, x, x')$ and $F_i(T, x, x')$.

In the first region we can use the expressions for the $1/N$ corrections to the $\Pi(q, q_z, 0)$ and $I(q, q_z, 0)$ functions of Ref. [14] and [17] and their asymptotics (92), (93), (95). Then
\[ R_1(T, x_\sigma) = \frac{T}{2\pi N} \ln \frac{2C^2}{\alpha} - \frac{(3 + 2x_\sigma)T}{4\pi N} \times \ln \frac{2C^2/\alpha + x_\sigma}{x_\sigma} + \frac{T}{4\pi N} I_1(x_\sigma) \]  

where

\[ I_1(x_\sigma) = \frac{4}{N} \int_0^\infty dq \int_0^{\pi} dq_z \frac{d q_z}{2\pi} \left[ 1 \ln q^2 + 1 - \cos q_z \right] \times \frac{I(q, q_z, 0) - \Pi(q, q_z, 0)}{\Pi(q, q_z, 0)} + \frac{3 + 2x_\sigma}{2q^2} \frac{\theta(q^2 - 1/\rho_s)}{\ln(2q^2 + x_\sigma)} \]

\( \theta(x) \) 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 \( q^2 \gg \alpha \), \( K_4 \) and \( I_4 \):

\[ R_2(T, x_\sigma) = \frac{T}{\pi N} \left[ \ln \frac{2T^2/\alpha}{(2T^2/\alpha) + x_\sigma} + \frac{4\pi C^2/\alpha}{\ln(2T^2/\alpha)} \right] + \frac{T}{\pi N} \left[ \ln \frac{2T^2/\alpha}{(2T^2/\alpha) + x_\sigma} \right] \]

\[ R_3(T, x_\sigma) = \frac{T}{\pi N} \left[ \ln \frac{2T^2/\alpha}{(2T^2/\alpha) + x_\sigma} \right] \frac{4C'/T}{3T} + \frac{1}{2} \ln \frac{2T^2/\alpha}{x_\sigma} \]

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

\[ R_4(T, x_\sigma) = \frac{8T}{3\pi^2 N} \ln \frac{2T^2}{\alpha} \ln \frac{NA}{16\rho_s} - \frac{2T}{3\pi^2 N} \ln \frac{NA}{16\rho_s} - \frac{4C'}{3\pi N} \ln \frac{2T^2/\alpha}{x_\sigma} \]

Contributions from other three regions are also easily calculated:

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

\[ F_3(T, x_\sigma) = O(1/\ln(2T^2/\alpha)) \]

\[ F_4(T, x_\sigma) = \frac{8}{\pi N} \ln \frac{NA}{16\rho_s} \]

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 \( T \gg J e^{-1/\varepsilon} \) (which is an analog of the renormalized classical regime in the 2D case), so that only the contributions with zero Matsubara frequencies will be taken into account. Consider first the results for the functions \( \Pi \) and \( I \). Evaluating the integrals in \( K_4 \) and \( I_4 \) at an arbitrary space dimensionality \( 2 < d < 4 \) (see, e.g., Ref. \( K_4 \) for the procedure of calculation of such integrals) we have

\[ \Pi(q, 0) = \frac{TKdA_d}{q^{1-d}} \]

\[ I(q, 0) = \frac{TKdA_d(3 - d)}{q^{3-d}} \]

where \( q \) is the \( d \)-dimensional vector,

\[ A_d = \frac{\Gamma(d/2)\Gamma(2 - d/2)}{2\Gamma(d - 2)} \]

\[ K_d^{-1} = 2^{d-1}\pi^d/2\Gamma(d/2) \]

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

\[ \Pi(q, 0) = q^2 I(q, 0) = \frac{2TK_2}{q^{2-\varepsilon}} \]

The constraint equation to first order in \( 1/N \) \( K_4 \) takes the form

\[ 1 - \frac{q^2}{\varepsilon} \frac{T^{1+\varepsilon} K_2}{N} (1 - 2) = \frac{\varepsilon^2}{4} \left[ 1 - \frac{K_2}{N} \ln \frac{T^{1+\varepsilon}/q^2 + \varepsilon^2}{\sigma^2} \right] \]
Using the identity
\[ g T^{1+\varepsilon}/\varepsilon + \sigma^2 = 1 \] (118)
which is satisfied in the zeroth order in \( 1/N \) and transforming the logarithmic term in (117) into a power, we obtain
\[ \sigma = \left(1 - T^{1+\varepsilon}/T_{\text{Neel}}^{1+\varepsilon}\right)^{\beta_{2+\varepsilon}} \] (119)
\[ \beta_{2+\varepsilon} = (1 + 1/N)/2 + O(1/N^2, \varepsilon) \] (120)
The Neel temperature is determined by
\[ T_{\text{Neel}}^{1+\varepsilon} = \frac{\varepsilon}{gK_2(1 - 2/\varepsilon)} \] (121)
This result coincides with the result of the RG analysis in (10). The RG result for the critical exponent \( \beta \) reads
\[ \beta_{2+\varepsilon} = \frac{1}{2} \left(1 + \frac{1}{N - 2}\right) + O(\varepsilon) \] (122)
Thus one have to replace \( N \to N - 2 \) in (121). Such a replacement is analogous to this in the renormalized classical regime of Ref. [4] 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. [4] by calculations of analogous contributions up to \( 1/N^2 \), this replacement should be indeed performed. Since the denominator in (121) is of order \( 1/N \), the replacement \( N \to N - 2 \) occurs already in the first-order expression for the transition temperature.

According to (119), two regimes are possible in the temperature dependence of the order parameter. At \( J \varepsilon^{-1/\varepsilon} \ll T \ll T_{\text{Neel}} \) we have the spin-wave behavior
\[ \sigma = 1 - \frac{(N - 1)T^{1+\varepsilon}}{4\pi\rho_\varepsilon \varepsilon} \] (123)
For \( N = 3 \) this result is analogous to the quasi-2D case result in (110) in the quantum spin case. At \( 1 - T/T_{\text{Neel}} \ll 1 \) the temperature dependence of the sublattice magnetization changes from the linear one to the power behavior with the critical exponent \( \beta_{2+\varepsilon} \).

Two above temperature regimes correspond to different pictures of the excitation spectrum. In the low-temperature regime \( T \ll T_{\text{Neel}} \) we have from (111) at quasimomenta \( q < T \) (only such \( q \) give a contribution to thermodynamic quantities) the zeroth order longitudinal Green’s function
\[ G_1^{N=\infty}(q, 0) = \frac{g}{2} \Pi(q, 0) = \frac{gTK_2}{\varepsilon q^{2+\varepsilon}} \] (124)
which corresponds to spin-wave excitations. Near the phase transition point we have at an arbitrary \( q \) (except for the exponentially-narrow hydrodynamic region \( q \ll (2\varepsilon q^2/g)\varepsilon^{1/\varepsilon} \))
\[ G_1^{N=\infty}(q, 0) = \frac{1}{q^2} \] (125)
which corresponds to critical (non-spin-wave) excitations.

**Figure Caption**

Fig.1. The theoretical temperature dependences of the relative sublattice magnetization \( S_x/S_0 \) from different spin-wave approximations and from the \( 1/N \)-expansion in the \( O(N) \) model (equations (54) and (14)), and the experimental points for La\(_2\)CuO\(_4\) (Ref. [4]).
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