

## THERMODYNAMIC PROPERTIES OF TWO-LAYER QUASI-TWO-DIMENSIONAL ANTIFERROMAGNETS

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For two-layer quasi-two-dimensional antiferromagnets of type  $\text{YBaCuO}$  in the Tyablikov approximation, we investigate the dependences of the energy spectrum and the temperature of transition into an ordered state on both the quasi-two-dimensionality parameter and the intensity of the exchange coupling of spin moments located in two close planes. We assume that the exchange parameters inside the  $\text{CuO}_2$  planes are much greater than the exchange parameters resulting in coupling between a spin located on a plane of an elementary cell and a spin on another plane of a different elementary cell. The obtained expressions for the Néel temperature and for the sublattice magnetic moment at zero temperature describe the dependences of these quantities on the parameters of interplane exchange interactions.

**Keywords:** antiferromagnetism, high-temperature superconductor, Tyablikov approximation, Green's function

### 1. Introduction

The compound  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  drew much attention after the high-temperature superconducting phase was discovered [1]. Studies of the crystallographic structure of  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  revealed the two-layer structure [2] of this compound: two  $\text{CuO}_2$  planes are separated by  $3.2 \text{ \AA}$  in one elementary cell. These planes are responsible for the transport and magnetic properties of the system and are separated only by the yttrium ion, while the planes separated by the charge reservoir and belonging to different elementary cells are separated by  $8.2 \text{ \AA}$ . Studying the magnetic properties revealed the presence of antiferromagnetic ordering in the system under a small doping [3]. Copper ions  $\text{Cu}^{2+}$  in the  $\text{CuO}_2$  planes have spin moments  $S = 1/2$  and are antiferromagnetically ordered; the spin moments are then in the  $\text{CuO}_2$  plane with no selected direction.

The thermodynamic properties of two-dimensional antiferromagnets were studied in [4], where, in particular, the expression for the Néel temperature  $T_N$  depending on the anisotropy field was obtained and the magnetization at absolute zero temperature was calculated. It was later shown in [5] that in the two-dimensional antiferromagnet with the easy-axis anisotropy, we have  $T_N \sim J/\log(J/\lambda)$ , where  $J$  is the exchange interaction parameter and  $\lambda$  is the anisotropy parameter, and this agreed with the calculations in [4]. In [6], the influence of the interplane interaction on the properties of an easy-axis quasi-two-dimensional antiferromagnet was investigated. The magnon spectrum and the calculated expression for the Néel temperature were obtained, and the Néel temperature and the magnetization at absolute zero temperature were calculated numerically. But an explicit analytic expression for the Néel temperature as a function of the interplane exchange parameter was not obtained. The authors calculated for the case  $S = 1$  corresponding to the compound  $\text{K}_2\text{NiF}_4$ .

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Studies of antiferromagnetic systems with the spin  $S = 1/2$  continue currently. For example, the ground state of a two-dimensional antiferromagnet was investigated in [7], [8] at various values of the spin moment. One of the most recent papers on antiferromagnets with the spin  $S = 1/2$  is [9], where the importance of taking the exchange interaction with next-to-nearest neighbors in antiferromagnets with FCC lattices into account was demonstrated.

Two-layer systems with an exchange interaction of the antiferromagnetic type were studied in [10], [11]. In the first of those papers, the behavior of a two-layer spin system in the vicinity of the antiferromagnet-paramagnet phase transition was considered. In the second paper, the authors concentrated on peculiarities of the system energy spectrum in the paramagnetic phase and, correspondingly, on the antiferromagnet susceptibility. Moreover, the renormalization of the energy spectrum by doping the  $\text{CuO}_2$  planes was shown in [11]. But the interaction between the two-layer systems was neglected in both cases.

In this respect, studying thermodynamic properties of quasi-two-dimensional two-layer antiferromagnets where the quasi-two-dimensionality parameter is determined by two exchange integrals characterizing the couplings between spin moments belonging to two planes from the same elementary cell and the exchange couplings between spin moments belonging to planes from nearest-neighbor elementary cells is relevant. Solving this problem is our objective here.

## 2. The Heisenberg model for the two-layer antiferromagnetic system

We consider the subsystem of spin moments corresponding in an ordered phase to the antiferromagnetic state of  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ . Taking the presence of two  $\text{CuO}_2$  planes in an elementary cell into account, we split the sites with spin moments into two magnetic sublattices  $F$  and  $G$ . For definiteness, we assume that the spin moments in the sublattice  $F$  are oriented along the quantization axis and those in the sublattice  $G$  are oriented oppositely. When describing the quasi-two-dimensionality and the two-layer structure of the system, we use three indices to label the spin moment coordinates. We use the first index  $(f, f', g, g')$  corresponding to two coordinates to describe the spin positions in the  $\text{CuO}_2$  planes. The second index  $(n)$  corresponds to the  $z$  component of an elementary cell. We label each of the two  $\text{CuO}_2$  planes in one elementary cell using the third index  $(\alpha = \pm 1)$  and set  $\bar{\alpha} = -\alpha$ . In Fig. 1, we show how the value of  $\alpha$  corresponds to the plane position in an elementary cell.

We define the Heisenberg Hamiltonian for a magnetic subsystem of the quasi-two-dimensional two-layer antiferromagnet in the form  $H = H_{\text{in}} + H_{\text{ext}}$ , where the operator  $H_{\text{in}}$  describes the collection of mutually disjoint two-dimensional spin subsystems with the exchange interaction between the spin moments in the same plane (for fixed indices  $n$  and  $\alpha$ ),

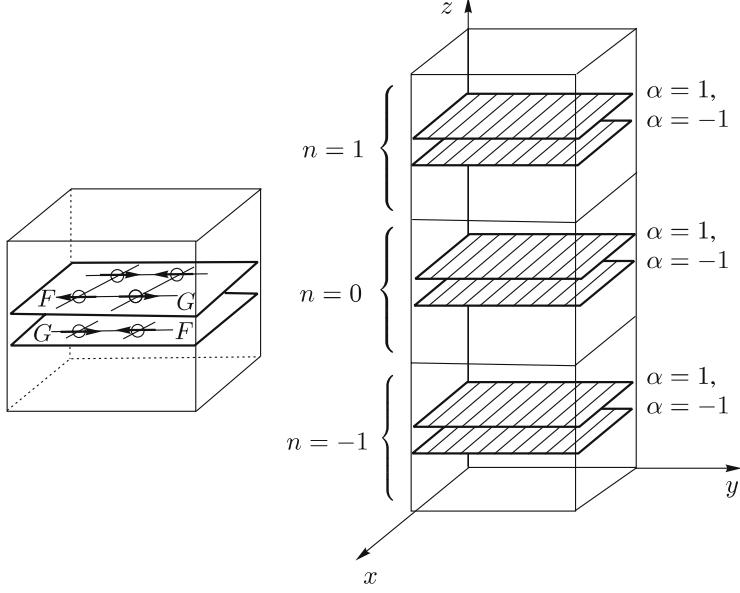
$$H_{\text{in}} = \sum_{n,\alpha} \left[ \sum_{f,g} J_{fg} (\vec{S}_{fn\alpha} \vec{S}_{gn\alpha}) - \frac{1}{2} \sum_{f,f'} I_{ff'} (\vec{S}_{fn\alpha} \vec{S}_{f'n\alpha}) - \frac{1}{2} \sum_{g,g'} I_{gg'} (\vec{S}_{gn\alpha} \vec{S}_{g'n\alpha}) \right],$$

and  $H_{\text{ext}} = H_{\text{ext}}^{(1)} + H_{\text{ext}}^{(2)}$  takes the exchange couplings between spin moments in different planes into account,

$$H_{\text{ext}}^{(1)} = \sum_{n,\alpha} \left\{ \sum_{f,g} K_{fg} (\vec{S}_{fn\alpha} \vec{S}_{gn\bar{\alpha}}) - \frac{1}{2} \sum_{f,f'} L_{ff'} (\vec{S}_{fn\alpha} \vec{S}_{f'n\bar{\alpha}}) - \frac{1}{2} \sum_{g,g'} L_{gg'} (\vec{S}_{gn\alpha} \vec{S}_{g'n\bar{\alpha}}) \right\},$$

$$H_{\text{ext}}^{(2)} = \sum_{n,\alpha} \left\{ \sum_{f,g} K'_{fg} (\vec{S}_{fn\alpha} \vec{S}_{g(n+\alpha)\bar{\alpha}}) - \frac{1}{2} \sum_{f,f'} L'_{ff'} (\vec{S}_{fn\alpha} \vec{S}_{f'(n+\alpha)\bar{\alpha}}) - \frac{1}{2} \sum_{g,g'} L'_{gg'} (\vec{S}_{gn\alpha} \vec{S}_{g'(n+\alpha)\bar{\alpha}}) \right\}.$$

The operator  $H_{\text{ext}}^{(1)}$  here takes the exchange interaction between spin moments located at two most closely situated planes (see Fig. 1) into account, and the operator  $H_{\text{ext}}^{(2)}$  describes the exchange interactions of



**Fig. 1.** The parameterization of the CuO<sub>2</sub> planes and enumeration of sites for the quasi-two-dimensional two-layer ferromagnet.

spins on two nearest planes belonging to different elementary cells. The constants  $J_{fg}$  and  $I_{gg'}$  and  $I_{ff'}$  correspond to the intraplane exchange interaction between spins belonging to different sublattices and the same sublattice, the constants  $K_{fg}$ ,  $L_{ff'}$ , and  $L_{gg'}$  correspond to interactions of ions in the nearest planes, and the constants  $K'_{fg}$ ,  $L'_{ff'}$ , and  $L'_{gg'}$  correspond to interactions in planes located in different elementary cells. In what follows, we assume that the exchange interaction constants correspond to the antiferromagnetic ordering both in the planes and in the direction orthogonal to the planes.

We note that the sublattices  $F$  and  $G$  in neighboring planes are shifted by the vector of the nonmagnetic elementary cell, which is perpendicular to the  $z$  axis. An ion of the sublattice  $G$  is therefore situated just below an ion of the sublattice  $F$ . This property is manifested when passing to the quasimomentum representation.

To find the elementary excitation spectrum, we write the equations of motion for the spin operators  $S_{fn\alpha}^+$  and  $S_{gn\alpha}^+$  in the Tyablikov approximation [12]:

$$\begin{aligned} i\dot{S}_{fn\alpha}^+ &= (J_0 + I_0 + K_0 + L_0)RS_{fn\alpha}^+ + R \sum_g J_{fg} S_{gn\alpha}^+ - R \sum_{f'} I_{ff'} S_{f'n\alpha}^+ + \\ &+ R \sum_g (K_{fg} S_{gn\bar{\alpha}}^+ + K'_{fg} S_{g(n+\alpha)\bar{\alpha}}^+) - R \sum_{f'} (L_{ff'} S_{f'n\bar{\alpha}}^+ + L'_{ff'} S_{f'(n+\alpha)\bar{\alpha}}^+), \\ i\dot{S}_{gn\alpha}^+ &= -(J_0 + I_0 + K_0 + L_0)RS_{gn\alpha}^+ - R \sum_f J_{fg} S_{fn\alpha}^+ + R \sum_{g'} I_{gg'} S_{g'n\alpha}^+ - \\ &- R \sum_f (K_{fg} S_{fn\bar{\alpha}}^+ + K'_{fg} S_{f(n+\alpha)\bar{\alpha}}^+) + R \sum_{g'} (L_{gg'} S_{g'n\bar{\alpha}}^+ + L'_{gg'} S_{g'(n+\alpha)\bar{\alpha}}^+). \end{aligned}$$

Correlation effects are neglected in this approximation. We can go beyond the framework of this approximation using the method of irreducible Green's functions [13]. In presenting the equations of motion, we

use the notation

$$\begin{aligned} J_0 &= \sum_g J_{fg}, & I_0 &= \sum_{f'} I_{ff'} = \sum_{g'} I_{gg'}, \\ K_0 &= \sum_g (K_{fg} + K'_{fg}), & L_0 &= \sum_{f'} (L_{ff'} + L'_{ff'}), \end{aligned}$$

and  $R = \langle S_f^z \rangle = -\langle S_g^z \rangle$ , where  $R$  is the mean of the projection of the spin momentum of an ion belonging to the sublattice  $F$  on the quantization axis in the antiferromagnetic phase.

We calculate the thermodynamic characteristics using the method of two-time retarded Green's functions constructed based on the spin operators [12]. Standardly defining the Green's function,

$$\langle\langle S_{ln\alpha}^+(t) | S_{jm\beta}^-(t') \rangle\rangle = -i\theta(t-t') \langle [S_{ln\alpha}^+, S_{jm\beta}^-] \rangle,$$

we perform the Fourier transformation

$$G(E, q)_{A\alpha B\beta} = \frac{4}{N} \sum_q \int \langle\langle S_{ln\alpha}^+(t) | S_{jm\beta}^-(t') \rangle\rangle e^{iE(t-t')-iq(R_{ln\alpha}-R_{jm\beta})} dE.$$

The indices  $A$  and  $B$  here take the values  $F$  or  $G$  depending on which sublattice the ions with the indices  $ln\alpha$  and  $jm\beta$  belong to.

Introducing the notation for the exchange interaction parameters in the quasimomentum representation,

$$\begin{aligned} \tilde{J}_0(q) &= J_0 + I_0 + K_0 + L_0 - \tilde{I}(q), \\ \tilde{I}(q) &= \sum_{f'} I_{ff'} e^{-iq(R_{fn\alpha}-R_{f'n\alpha})}, & \tilde{J}(q) &= \sum_g J_{fg} e^{-iq(R_{fn\alpha}-R_{gn\alpha})}, \\ \tilde{K}(q) &= \sum_g K_f e^{-iq(R_{fn(-1)}-R_{gn1})} + \sum_g K'_{fg} e^{-iq(R_{fn(-1)}-R_{g(n-1)1})}, \\ \tilde{L}(q) &= \sum_{f'} L_{ff'} e^{-iq(R_{fn(-1)}-R_{f'n1})} + \sum_{f'} L'_{fg} e^{-iq(R_{fn(-1)}-R_{f'(n-1)1})}, \end{aligned}$$

we obtain the expression for the energy spectrum  $E(q)$  of the quasi-two-dimensional two-layer antiferromagnet system:

$$E_{1,2}^2(q) = R^2 (\tilde{J}_0^2 + |\tilde{L}|^2 - \tilde{J}^2 - |\tilde{K}|^2 \pm D(q)),$$

where

$$D(q) = [4\tilde{J}^2|\tilde{K}|^2 - 2|\tilde{L}|^2|\tilde{K}|^2 + 4\tilde{J}_0^2|\tilde{L}|^2 - 4\tilde{J}_0\tilde{J}(\tilde{K}\tilde{L}^* + \tilde{L}\tilde{K}^*) + \tilde{K}^2(\tilde{L}^*)^2 + \tilde{L}^2(\tilde{K}^*)^2]^{1/2}.$$

### 3. The nonfrustrated antiferromagnet

We restrict ourself to the nearest-neighbor approximation. The parameters of the exchange interaction in the quasimomentum representation then become

$$\begin{aligned} \tilde{J}(q) &= 4J_1 \cos \frac{q_x}{2} \cos \frac{q_y}{2}, & \tilde{I}(q) &= 0, & \tilde{L}(q) &= 0, \\ \tilde{K}(q) &= Ke^{-iq_z\delta_\perp} + K'e^{iq_z\delta'_\perp}, & |\tilde{K}(q)|^2 &= K^2 + (K')^2 + 2KK' \cos q_z, \end{aligned}$$

and  $\tilde{J}_0(q)$  no longer depends on the quasimomentum:  $\tilde{J}_0 = 4J_1 + K + K'$ , where  $J_1$  is the constant of the exchange interaction between the nearest spin moments on the same plane,  $K$  and  $K'$  are constants of the exchange interaction between spin moments on nearest-neighbor planes, and  $\delta_\perp$  and  $\delta'_\perp$  are the distances between the corresponding planes (in units of the elementary cell height).

The expression for the energy spectrum in the considered case becomes

$$E_{1,2}(q) = R\omega_{1,2}, \quad \omega_{1,2} = \sqrt{\tilde{J}_0^2 - (\tilde{J} \pm |\tilde{K}|)^2}.$$

This expression in the limit  $K' = 0$  coincides with the energy spectrum obtained in [14]. The energy spectrum is characterized by two branches, one of which is a Goldstone branch with a zero gap. We find that  $E_q \sim q$  at small quasimomentum values for this branch.

At the spin moment  $S = 1/2$ , the self-consistency equation can be written as

$$\langle S_{fn\alpha}^+ S_{fn\alpha}^- \rangle = \frac{1}{2} + \langle S_{fn\alpha}^z \rangle.$$

By virtue of the spectral theorem, the spin correlation function in this equation can be written as

$$\langle S_{fn\alpha}^+ S_{fn\alpha}^- \rangle = \frac{4}{N} \sum_q \int \frac{e^{E/T}}{e^{E/T} - 1} \left\{ -\frac{1}{\pi} \operatorname{Im} G_{F\alpha F\alpha} \right\} dE,$$

where the Green's function  $G_{F\alpha F\alpha}$  is

$$G_{F\alpha F\alpha} = \frac{2R(E + \tilde{J}_0 R)(E^2 - R^2(\tilde{J}_0^2 - \tilde{J}^2 - |\tilde{K}|^2))}{(E^2 - E_1^2)(E^2 - E_2^2)}.$$

After simple algebra, we obtain the self-consistency equation

$$R = \frac{1}{I_1 + I_2}, \quad I_j = \frac{4}{N} \sum_q \frac{\tilde{J}_0}{\omega_j} \coth \frac{\omega_j R}{2T}, \quad j = 1, 2. \quad (1)$$

Using the obtained equation, we can find the Néel temperature  $T_N$  and the sublattice magnetization  $R(0)$  at absolute zero. We obtain the Néel temperature from the vanishing condition for  $R$ . As  $R \rightarrow 0$ , we can keep only the leading term of the hyperbolic cotangent expansion, setting  $\coth(\omega_j R / 2T) \simeq 2T/\omega_j R$ . The Néel temperature for the two-layer antiferromagnet in the nearest-neighbor approximation then becomes

$$T_N = \left( 2\tilde{J}_0 \frac{4}{N} \sum_q \left[ \frac{1}{\omega_1^2} + \frac{1}{\omega_2^2} \right] \right)^{-1}.$$

It hence follows that if the integral diverges, then the antiferromagnetic phase is absent, and the system becomes a spin liquid [7], [8]. We can easily see that the integral determined by the gapless branch of the energy spectrum develops a logarithmic singularity in the vicinity of  $q = 0$  in the two-dimensional case (when at least one of the parameters  $K$  and  $K'$  vanishes). This corresponds to absence of the magnetic transition temperature. If both the parameters  $K$  and  $K'$  are nonzero, then the integral becomes finite, and the Néel temperature is also finite.

The expression for  $\tilde{K}$  simplifies for  $K = K'$ , becoming  $\tilde{K} = 2K \cos(q_z/2)$ , and we can evaluate integrals over  $q_z$  explicitly:

$$I_1 = \frac{1}{\pi^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left[ \frac{\arctan \sqrt{(A_- + 2K)/(A_- - 2K)}}{\sqrt{A_-^2 - (2K)^2}} + \frac{\arctan \sqrt{(A_+ - 2K)/(A_+ + 2K)}}{\sqrt{A_+^2 - (2K)^2}} \right] dq_x dq_y,$$

$$I_2 = \frac{1}{\pi^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left[ \frac{\arctan \sqrt{(A_- - 2K)/(A_- + 2K)}}{\sqrt{A_-^2 - (2K)^2}} + \frac{\arctan \sqrt{(A_+ + 2K)/(A_+ - 2K)}}{\sqrt{A_+^2 - (2K)^2}} \right] dq_x dq_y,$$

where we introduce the notation  $A_{\pm} = 4J_1(1 \pm \cos(q_x/2) \cos(q_y/2)) + 2K$  for brevity.

In the quasi-two-dimensional case where  $K \ll J_1$ , the values of the integrals  $I_1$  and  $I_2$  are dominated by terms containing  $A_-$  because those are the terms that contain the logarithmic divergence of integrals in the vicinity of the point  $q_x = q_y = 0$  at  $K = 0$ . In our approximation, these integrals can be transformed into the form

$$I_{1,2}^{(1)} = \frac{1}{\pi J_1} \int_0^{\sqrt{J_1 Q / 8K}} \frac{dx}{\sqrt{1+x^2}},$$

where  $Q$  is the radius of the domain of applicability of the expansion  $\cos(q_x/2) \cos(q_y/2) = 1 - q^2/8$ ,  $q^2 = q_x^2 + q_y^2$ , and we have  $K/J_1 \ll Q^2$  for the parameter ratio. The sum of the integrals then becomes

$$I_1^{(1)} + I_2^{(1)} = \frac{1}{\pi J_1} \log \frac{J_1}{K}.$$

The Néel temperature in the case where  $K' = K \ll J_1$  is then determined by the expression

$$T_N = \frac{\pi J_1}{\log(J_1/K) + C_1},$$

where  $C_1$  is the constant determined by contributions of neglected terms in the integrals  $I_1$  and  $I_2$  and by integrations outside the chosen domain of radius  $Q$ . Estimating these contributions at  $Q = 0.1$  gives  $C_1 \approx 3.5$ .

We now pass to the case where the two-layer structure of a system is manifested more clearly, i.e., to the case where one of the interplane exchange interactions is much weaker than the other,  $K' \ll K$ . Then  $\tilde{K} = K + K' \cos q_z$ , and the integrals  $I_1$  and  $I_2$  become

$$\begin{aligned} I_1 &= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left[ \frac{1}{\sqrt{A_-^2 - (K')^2}} + \frac{1}{\sqrt{A_+^2 - (K')^2}} \right] dq_x dq_y, \\ I_2 &= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \left[ \frac{1}{\sqrt{B_-^2 - (K')^2}} + \frac{1}{\sqrt{B_+^2 - (K')^2}} \right] dq_x dq_y, \end{aligned}$$

where, as in the above case, for brevity, we introduce the concise notation

$$\begin{aligned} A_{\pm} &= 4J_1 \left( 1 \pm \cos \frac{q_x}{2} \cos \frac{q_y}{2} \right) + K' + K \pm K, \\ B_{\pm} &= 4J_1 \left( 1 \pm \cos \frac{q_x}{2} \cos \frac{q_y}{2} \right) + K' + K \mp K. \end{aligned}$$

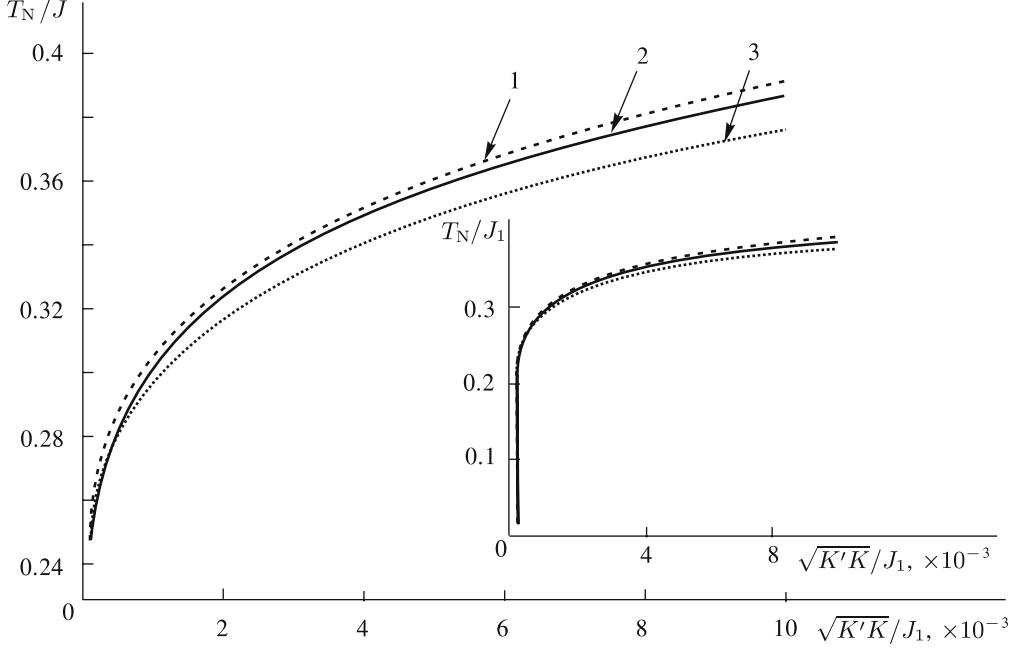
Analogously to the case  $K' = K \ll J_1$ , we can easily obtain the expressions for the integrals in question in the case where  $K' \ll K \ll J_1$ :

$$I_1^{(1)} + I_2^{(1)} = \frac{1}{\pi J_1} \log \frac{J_1}{\sqrt{K'K}}.$$

The Néel temperature then becomes

$$T_N = \frac{\pi J_1}{\log(J_1/\sqrt{K'K}) + C_2}. \quad (2)$$

We can easily see that  $C_2 \approx C_1$  for  $K \ll J_1$ .



**Fig. 2.** The Néel temperature dependence on the ratio  $\sqrt{K'K}/J_1$ : line 1 corresponds to the numerical solution at  $K' = K$ , line 2 is given by formula (2), and line 3 is the solution at  $K' = K/10$ .

As can be seen, we obtain the same result in both limit cases, which implies that the Néel temperature presumably manifests the same dependence of form (2) (see Fig. 2) for any value of the ratio of the parameters  $K$  and  $K'$  if  $K, K' \ll J_1$ . The graph in Fig. 2 coincides qualitatively with the graph obtained in [6] for the spin  $s = 1$ .

From self-consistency equation (1), we can find the expression determining the spin moment projection value as the temperature tends to zero:

$$R(0) = \left( \sum_j W_j \right)^{-1}, \quad W_j = \frac{4}{N} \tilde{J}_0 \sum_q \frac{1}{\omega_j}, \quad j = 1, 2. \quad (3)$$

As above, we work in the quasi-two-dimensionality domain  $K, K' \ll J_1$ . The integrals in (3) can then be written as a sum:

$$W_j = W_{2D} + \Delta W_j, \quad W_{2D} = \frac{1}{(2\pi)^2} \iint \frac{dq_x dq_y}{\sqrt{1 - (\cos(q_x/2) \cos(q_y/2))^2}}.$$

Here,  $W_{2D}$  is the integral in the two-dimensional case, and  $\Delta W_j$  is the correction to this integral. The leading part of the correction obviously comes from integration in the vicinity of the point  $q_x = q_y = 0$ . Taking this into account, we consider the integral  $W_1$  in the cylindric domain of radius  $Q$  and height  $2\pi$ :

$$\begin{aligned} W_{1Q} &= \frac{2}{(2\pi)^2} \int_0^Q \int_{-\pi}^{\pi} \frac{q dq dq_z}{\sqrt{q^2 + 2(K + K')(1 - \gamma_z)/J_1}} \approx \\ &\approx \frac{1}{\pi^2} \int_0^\pi \left( Q - \sqrt{\frac{2(K + K')}{J_1}(1 - \gamma_z)} \right) dq_z, \end{aligned}$$

where

$$\gamma_z = \sqrt{1 - \frac{2K'K(1 + \cos q_z)}{(K + K')^2}}.$$

Writing the analogous expression  $W_{2Q}$  for the integral  $W_2$ , we obtain the sought correction to the integrals,

$$\Delta W_1 + \Delta W_2 \approx -\frac{1}{\pi^2} \sqrt{\frac{2(K + K')}{J_1}} \int_0^\pi (\sqrt{1 - \gamma_z} + \sqrt{1 + \gamma_z}) dq_z.$$

The value of the spin moment projection  $R(0)$  at absolute zero and at small parameters of the interplane exchange interaction is

$$R(0) \approx R_{2D}(0) + R_{2D}^2(0)|\Delta W_1 + \Delta W_2|,$$

where

$$\Delta W_1 + \Delta W_2 \approx \begin{cases} -\frac{8}{\pi^2} \sqrt{\frac{2K}{J_1}}, & K' = K, \\ -\frac{2}{\pi} \sqrt{\frac{K}{J_1}} \left(1 + \frac{2}{\pi} \sqrt{\frac{K'}{K}}\right), & K' \ll K, \end{cases}$$

and  $R_{2D}(0)$  is the magnetization at absolute zero in the two-dimensional case.

We consider the behavior of the spin moment projection  $R$  as a function of temperature at a small temperature and at a temperature close to  $T_N$ . The expression for  $R$  in the low-temperature limit is

$$R(T)|_{T \rightarrow 0} = \left( \frac{4}{N} \tilde{J}_0 \sum_q \left[ \frac{1}{\omega_1} + \frac{1}{\omega_2} \right] + \Delta I \right)^{-1},$$

where

$$\Delta I = 2\tilde{J}_0 \int \frac{g(\omega)}{\omega} e^{-R(0)\omega/T} (1 + e^{-R(0)\omega/T}) d\omega,$$

in which we take into account that only magnon excitations corresponding to the gapless energy spectrum are relevant at a small temperature because the gap width is of the order  $\sqrt{KJ_1}$ . In the last equality,  $g(\omega)$  is the density of states,

$$g(\omega) = \frac{1}{(2\pi)^3} \iiint \delta(\omega - \omega_1(q)) dq_x dq_y dq_z.$$

The density of states in the low-energy domain can be written in the form

$$g(\omega) = \frac{\omega^2}{(4\pi J_1)^2 \sqrt{J_1 K' K / (K + K')}}.$$

The sought integral  $\Delta I$  is then

$$\Delta I = \frac{5}{4} \frac{T^2}{2\pi^2 R^2(0) J_1 \sqrt{J_1 K' K / (K + K')}}.$$

The final expression for the low-temperature magnetization of a sublattice then becomes

$$R(T) = R(0) - \alpha T^2, \quad \alpha = \frac{5}{8\pi^2} \frac{1}{J_1} \frac{1}{\sqrt{KJ_1}} \sqrt{\frac{K + K'}{K'}}.$$

In the vicinity of the Néel temperature, the expression for the magnetization has the form corresponding to the Landau theory

$$R(T) = \sqrt{3 \frac{T_N - T}{\tilde{J}_0}}.$$

## 4. Conclusions

We have investigated the thermodynamic properties of a quasi-two-dimensional two-layer antiferromagnet. We first obtained the analytic expression for the Néel temperature  $T_N$  as a function of the two interplane exchange interaction constants  $K$  and  $K'$  in the limit  $K, K' \ll J_1$ . We showed that the Néel temperature is expressed in terms of the geometric mean of the interplane exchange parameters determining the two-layer structure of the system. In the low-temperature domain, we established that the coefficient of the term quadratic in the temperature, which describes the magnetization decrease, is expressed nonanalytically in terms of combinations of the exchange parameters.

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