Effect of frustrations on magnetism in the Ru double perovskite Sr_2YRuO_6

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Localized Ru^{5+} spins in Sr_2YRuO_6 form a fcc lattice with an antiferromagnetic (AFM) nearest-neighbor (NN) coupling $J \approx 25$ meV and rather low Néel temperature $T_N = 26$ K. Analysis of the electronic structure of Sr_2RuO_4 results in the effective Heisenberg model. We have studied the effect of frustrations on the AFM type-I structure of Sr_2YRuO_6 in the spin-wave approximation. In the model with only NN coupling the AFM state is unstable due to frustrations, and $T_N = 0$. Stabilization of the AFM state occurs due to the next-nearest-neighbor coupling I or due to the magnetic anisotropy D. Very small values $D/J \sim I/J \leqslant 10^{-3}$ are enough to obtain the experimental values of T_N and sublattice magnetization $m = 1.85\mu_B$/Ru (62% from the nominal $S = 3/2$ value).

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I. INTRODUCTION

Mixed ruthenates with perovskite-based crystal structures have been intensively studied during the past ten years. The primary interest results from the recent discovery of the superconductivity in Sr_2RuO_4 (Ref. 1) that is the only oxide superconductor without Cu isostructural to La_2CuO_4. Then it was found that other ruthenates have quite interesting magnetic and electronic properties. A very complex phase diagram is observed in the $Sr_{2-x}Ca_xRuO_4$ layered perovskite alloy system with several structural phase transitions, strong competition of the ferromagnetic (FM) and antiferromagnetic (AFM) spin correlations, and the metal-insulator transition.[2,3] The corresponding three-dimensional (3D) perovskite $SrRuO_3$ is a robustly ferromagnetic metal with $T_C = 165$ K,[4,5] which makes it rather unique among the $4d$ oxides. Sr_2YRuO_6 provides an interesting counterpoint to these materials. Like them, it features a perovskite derived structure with strong Ru-O hybridization and magnetism. However, its double perovskite structure, in which every second Ru is substituted by Y, disrupts the Ru-O perovskite structural motif of intersecting 1D chains. As a result, the compound shows more localized electronic and magnetic behavior than most of the perovskite derived ruthenates (an exception is Ca_2RuO_4, which is a Mott insulator). In particular, Sr_2YRuO_6 displays an antiferromagnetic, insulating ground state,[6,7] and according to local spin density approximation (LSDA) calculations should be described as a local-moment system. Its magnetic properties are strongly suppressed in comparison with typical three-dimensional antiferromagnetism where one would expect $T_N \sim J$ and sublattice magnetization $m \approx 2S$.

The nearest-neighbor (NN) coupling J has been obtained by the first-principles spin-polarized electronic structure calculations,[8] $J \approx 25-30$ meV. The observed Néel temperature $T_N = 26$ K is less than 10% of J. One explanation is that the value of J reported is from LSDA calculations, which often give an overestimate. However, in this well hybridized $4d$ oxide, on-site Hubbard correlations should be weak compared with $3d$ oxides and the nature of the gap between different manifolds of $4d$ derived states is different from the underestimated gaps of semiconductors such as Si or GaAs. Thus it is unclear whether this is the correct explanation. Similarly, for Ru^{5+} $S = 3/2$ while $m = 1.85\mu_B$/Ru measured by neutron diffraction is near 60% of its nominal value $3\mu_B$/Ru. Our primary interest in Sr_2YRuO_6 is to gain an understanding of the suppression of magnetism in this compound. The secondary motivation is provided by recent reports[9,10] of superconductivity up to 60 K when the compound is doped with Cu. The fcc lattice of Ru spin in Sr_2YRuO_6 with the AFM NN coupling is known to be frustrated. For the AFM type-I state with FM ordered xy planes that are staggered along z axes, all four in-plane couplings are frustrated while eight out-plane couplings are not frustrated. On the mean-field level, the effective molecular field acting on each spin is reduced to $4J$ instead of zJ ($z = 12$ is the NN number) for the unfrustrated lattice. Similarly, in the Ising model, frustration also reduces T_N (Ref. 11) but not so strongly as in the experiment. We have shown in this paper that the transverse spin fluctuations are the most important in the frustrated fcc lattice resulting in the total suppression of the AFM state in the Heisenberg model with only NN coupling. Weak next-nearest-neighbor (NNN) coupling or small anisotropy gives stabilization of the AFM state with reduced T_N and m.

II. ELECTRONIC STRUCTURE AND MAGNETIC COUPLING IN Sr_2YRuO_6

The substitution of every second Ru by nonmagnetic Y justifies the cluster approach to the electronic and magnetic properties of Sr_2YRuO_6. Indeed, each RuO_6 cluster has no common oxygen with the NN cluster. The coupling occurs

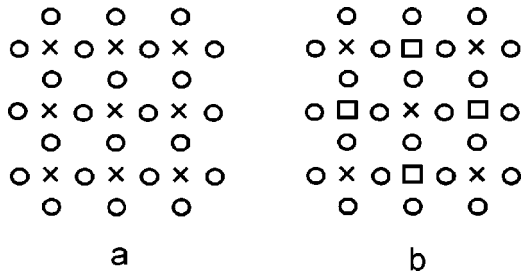

FIG. 1. The ordered diamagnetic substitution of every second Ru by Y in $SrRuO_3$ (a) results in the Sr_2YRuO_6 lattice (b). Here notations are × (Ru), ○ (O), □ (Y).

via Ru-O-O-Ru bonds. That is why the results of the tight-binding calculations of the electronic structure of Sr_2YRuO_6 with RuO_6 cluster as the fcc lattice site are very similar to the *ab initio* linearized augmented plane wave (LAPW) calculations.[8] Substituted nonmagnetic Y ions can be considered as a diamagnetic substitution in perovskite $SrRuO_3$ with concentration of vacancies 0.5 and their space ordering (Fig. 1). These vacancies have strong influence on the magnetic coupling of the NN Ru spins. While in the $SrRuO_3$ the coupling is FM, in the Sr_2RuO_4 there is strong competition of FM and AFM interactions,[12] in the system $Sr_{2-x}Ca_xRuO_4$ the AFM becomes stronger with increasing Ca concentration (see a review paper[13] on ruthenates), and in the Sr_2YRuO_6 there is quite strong AFM NN coupling. Thus in ruthenates, the magnetic properties have more variety than in cuprates with the AFM NN coupling.

The origin of this variety is the specific feature of the electronic structure of ruthenates formed by $(t_{2g}-p)$-π bonding. An orbital degeneracy of t_{2g} Ru states results in the multiband self-doping metallic state in $SrRuO_3$ and Sr_2RuO_4. An estimation of the electron correlation effects gives $U \leqslant W$, where U is the Hubbard intra-atomic Coulomb interaction, and W is the electron band half-width, $W=z|t|$ for the nearest-neighbor hopping case. Due to diamagnetic substitution by the ordered vacancies in Sr_2YRuO_6, the hopping Ru-Ru parameter t is sharply decreasing, the $W \ll U$ ratio results in strong electron correlation regime in Sr_2YRuO_6 with the insulator (semiconductor) ground state, although the possibility that Sr_2YRuO_6 is a band insulator has not yet to be excluded. In zero approximation on t, we have a system of uncoupled RuO_6 clusters. The electronic structure of RuO_6 cluster has been studied in the paper.[8] Here we will present some results of Ref. 8 that are important for the exchange interaction analysis.

The crystal field in RuO_6 cluster splits the Ru d orbital in t_{2g} and e_g states. The Op orbitals are involved both in $pd\pi$ and $pd\sigma$ bonding with Ru. The intracluster p-d hopping results in the following molecular orbital (MO):[8] 13 nonbonding MO's, $4\times E_0(p_\sigma)+9\times E_0(p_\pi)$; five bonding MO's, $2\times E_-(E_g)+3\times E_-(T_{2g})$; five antibonding MO's, $2\times E_+(E_g)+3\times E_+(T_{2g})$. Here E_0 is the electron energy of the atomic orbital in the crystal field, and the bonding (antibonding) energies are equal to

$$E_\pm(E_g)=0.5\{E_0(p_\sigma)+E_0(e_g)\pm[(E_0(p_\sigma)-E_0(e_g))^2+16t_\sigma^2]^{1/2}\}, \quad (1a)$$

$$E_\pm(T_{2g})=0.5\{E_0(p_\pi)+E_0(t_{2g})\pm[(E_0(p_\pi)-E_0(t_{2g}))^2+16t_\pi^2]^{1/2}\}. \quad (1b)$$

A sequence of terms is the following:

$$E_-(T_{2g}) \approx E_-(E_g) < E_0(p_\sigma) < E_0(p_\pi) < E_+(T_{2g}) < E_+(E_g).$$

These terms are occupied by 39 valence electrons. The states $E_-(T_{2g})$, $E_-(E_g)$, $E_0(p_\sigma)$, $E_0(p_\pi)$ take 36 electrons and the rest three electrons form high spin $S=3/2$ configuration with half-filled $E_+(T_{2g})$ term. The symmetry of T_{2g} MO is the same as the t_{2g} atomic Ru orbital.

The NN AFM coupling results from the intercluster hopping. In the standard superexchange approach, it is the Ru-O-O-Ru interaction. The same interaction can be considered as a result of the intercluster hopping between the NN RuO_6 clusters, the xy-xy hopping with the amplitude $\tau_\sigma = 0.75t_{dd\sigma}$. The corresponding exchange energy (per cluster) is equal to $2J_0 \sim \tau_\sigma^2/\Delta$, where Δ is the Hund-type exchange splitting of the T_{2g} MO. The estimation of the parameters from the LAPW calculation[8] gives $2J=0.05$ eV. This value is consistent also with the difference in energy of the AFM and FM states obtained by *ab initio* spin-polarized band-structure calculation.[8] For simplified tetragonal structure of the Sr_2YRuO_6 (Fig. 1), the value $\Delta E = E_{FM} - E_{AFM} = 0.12$ eV, due to the tilting of RuO_6 octahedral and the monoclinic lattice distortion $\Delta E = 0.095$ eV. The NNN coupling I results from the Ru-O-O-Ru-O-O-Ru or Ru-O-Y-O-Ru bonding and can be estimated to be

$$I \sim \tau_\sigma^4/\Delta^3 \leqslant 10^{-2} \text{ J}.$$

The magnetic properties of the localized spins in Sr_2YRuO_6 will be discussed in the framework of the isotropic Heisenberg model,

$$H=-\frac{1}{2}\sum_{f,R} J(R)\vec{S}_f\cdot\vec{S}_{f+R}, \quad (2a)$$

$$J(\vec{R})=J(-\vec{R}), \quad J(0)=0. \quad (2b)$$

The NN distance will be denoted as $R_1=1/\sqrt{2}$ (lattice parameter $a=1$), the NNN distance $R_2=1$. In the fcc lattice, there are $z_1=12$ NN's with interaction $J(\vec{R}_1)=-J$, $J>0$ and $z_2=6$ NNN interactions $J(\vec{R}_2)=I$, $I>0$. We introduce two sublattices A and B with sites $\vec{\alpha}$ belonging to A and $\vec{\beta}$ to B, $\langle S_A^z\rangle = -\langle S_B^z\rangle \equiv \overline{S}$. For the AFM type-I phase, we have FM xy planes with alternating AFM order along z direction. It is convinient to substitute NN spin in two groups, inside the xy plane with $\vec{R}_1 \equiv \vec{d}$ and outside the xy plane with $\vec{R}_2 \equiv \vec{\delta}$. Here,

$$\vec{d}=\left(\pm\frac{1}{2},\ \pm\frac{1}{2},\ 0\right)(xy), \quad \vec{\delta}_1=\left(0,\ \pm\frac{1}{2},\ \pm\frac{1}{2}\right)(yz),$$

$$\vec{\delta}_2=\left(\pm\frac{1}{2},\ 0,\ \pm\frac{1}{2}\right)(xz).$$

In these notations, we have

$$\langle S^z_{\vec{\alpha}}\rangle=\overline{S},\quad \langle S^z_{\vec{\alpha}+\vec{d}}\rangle=\overline{S},\quad \langle S^z_{\vec{\alpha}+\vec{\delta}}\rangle=-\overline{S},\quad \langle S^z_{\vec{\alpha}+\vec{a}}\rangle=\overline{S}, \tag{3a}$$

$$\langle S^z_{\vec{\beta}}\rangle=-\overline{S},\quad \langle S^z_{\vec{\beta}+\vec{d}}\rangle=-\vec{S},\quad \langle S^z_{\vec{\beta}+\vec{\delta}}\rangle=\overline{S},\quad \langle S^z_{\vec{\beta}+\vec{a}}\rangle=-\overline{S}. \tag{3b}$$

Due to FM order in the xy planes, all four NN AFM couplings in this plane are frustrated. Nevertheless, the eight out-plane AFM couplings are energetically favored. Thus, in the mean-field approximation (MFA), frustrations decrease the value of the effective field $\overline{h}$ acting on each spin. Without frustrations one would expect $\overline{h}=z_1J\overline{S}=12J\overline{S}$, due to frustrations $\overline{h}=4J\overline{S}$. In the MFA, the Néel temperature is given by $T_N=Jz_1S(S+1)/3$ that is much higher than the experimental value $T_N=26$ K. Decrease of $\overline{h}$ due to frustrations decreases T_N by a factor of 3 but it is still rather large. Similarly, in the Ising model the suppression of T_N due to frustrations is also known[8] and results in $T_N\approx 700$–900 K that is also too large. Thus we have to consider at least the transverse spin fluctuations.

III. SPIN-WAVE THEORY OF FRUSTRATED ANTIFERROMAGNET ON THE fcc LATTICE

The exact equation of motion for S^+_f operator after the Tyablikov (random phase) approximation becomes linear,

$$i\dot{S}^+_{\vec{f}}\approx\sum_R J(\vec{R})(\langle S^z_{\vec{f}+\vec{R}}\rangle S^+_{\vec{f}}-\langle S^z_{\vec{f}}\rangle S^+_{\vec{f}+\vec{R}}). \tag{4}$$

Below, we will divide the Hamiltonian by the parameter z_1J to work with dimensionless values. Then Eq. (4) for two sublattices may be written as ($\lambda=I/J$)

$$i\dot{S}^+_{\vec{\alpha}}=\frac{\overline{S}}{z}\left[\sum_{\vec{d}}(S^+_{\vec{\alpha}+\vec{d}}-S^+_{\vec{\alpha}})+\sum_{\vec{\delta}}(S^+_{\vec{\alpha}+\vec{\delta}}+S^+_{\vec{\alpha}})\right]+\frac{\lambda\overline{S}}{2z_2}\sum_{\vec{a}}(S^+_{\vec{\alpha}}-S^+_{\vec{\alpha}+\vec{a}}), \tag{5a}$$

$$i\dot{S}^+_{\vec{\beta}}=-\frac{\overline{S}}{z}\left[\sum_{\vec{d}}(S^+_{\vec{\beta}+\vec{d}}+S^+_{\vec{\beta}})+\sum_{\vec{\delta}}(S^+_{\vec{\beta}+\vec{\delta}}+S^+_{\vec{\beta}})\right]-\frac{\lambda\overline{S}}{2z_2}\sum_{\vec{a}}(S^+_{\vec{\beta}}-S^+_{\vec{\beta}+\vec{a}}). \tag{5b}$$

We introduce a Fourier transform in the two-sublattice state and by the standard way find the transverse spin-fluctuation Green functions,

$$\langle\langle S^+_F(\vec{q})|S^-_G(-\vec{q})\rangle\rangle_\omega=G_{FG}(\vec{q},\omega), \tag{6}$$

$$G_{AA}=\frac{2\overline{S}(\omega+\overline{S}\alpha_q)}{D(\vec{q},\omega)}, \tag{7a}$$

$$G_{BB}=\frac{2\overline{S}(\omega-\overline{S}\alpha_q)}{D(\vec{q},\omega)}, \tag{7b}$$

$$G_{AB}=G_{BA}=-\frac{2\overline{S^2}\beta_q}{D(\vec{q},\omega)}, \tag{7c}$$

$$D(\vec{q},\omega)=\omega^2-\Omega_q^2,\quad \Omega_q=\overline{S}\varepsilon_q,\quad \varepsilon_{\vec{q}}=[\alpha_q^2(\lambda)-\beta_q^2]^{1/2}, \tag{8}$$

where $\alpha_q=0.33(1+c_xc_y)+0.5\lambda(1-\gamma_q)$, $\beta_q=0.33(c_x+c_y)c_z$, $c_i=\cos(q_i/2)$, $i=x,y,z$, $\gamma_q=0.33(\cos q_x+\cos q_y+\cos q_z)$.

We will restrict ourselves below to the simplest case of $S=1/2$ instead of $S=3/2$ for Sr_2YRuO_6. One may expect only the quantitative difference for T_N and other thermodynamic characteristics while the qualitative behavior should be the same. The most important new physics of $S=3/2$ in comparison to $S=1/2$ case results from the single-ion anisotropy. However, in Sr_2YRuO_6 the t_{2g}^3 high spin configuration is a half-filled t_{2g} shell with zero orbital moment. So there is no spin-orbital contribution to the single-ion anisotropy in the ground state and only very small contribution from the excited d^3 configuration takes place. That is why we neglect the single-ion anisotropy and will consider the exchange anisotropy in the following section.

As concerns the isotropic Heisenberg AFM, there are several random-phase-approximation (RPA) approaches for the arbitrary spin value. One of them uses a parametrized Green function,[14] another uses the representation of spin operator for arbitrary S in terms of the Hubbard operators $X^{mm'}=|m\rangle\langle m'|$, where m is a projection of S^z (Ref. 15). The main effect for the T_c and T_N is given by a trivial renormalization $J\to JS(S+1)$. We obtain J from the energy difference of the FM and AFM states, ΔE, and the main contribution to ΔE in the RPA approach is $|\Delta E|=JS^2$. Thus, the influence of the spin value S on the ratio is given by the following:

$$kT_{N/|\Delta E|}\sim S(S+1)/S^2=1+1/S\to 1,\quad S\to\infty. \tag{9}$$

For $S=1/2$ and $S=3/2$, the difference is given by a factor 5/9. We are interested in the changes of the T_N in two to three orders of magnitude due to the NNN coupling and the exchange anisotropy.

For $S=1/2$, the self-consistent equation for the AFM order parameter $\overline{S}$ has the form ($\tau=T/z_1J$)

$$\overline{S}(\tau)=\frac{1/2}{I(\tau)},\quad I(\tau)=\frac{2}{N}\sum_q\frac{\alpha_q}{\varepsilon_q}\coth\frac{\overline{S}(\tau)\varepsilon_q}{2\tau}. \tag{10}$$

At zero temperature, $\coth x\to 1$ and the zero-temperature sublattice magnetization is given by

$$\overline{S}(0)=0.5/I_1(\lambda),\quad I_1(\lambda)=2N^{-1}\sum_q\alpha_q(\lambda)/\varepsilon_q(\lambda). \tag{11}$$

In the other limit, $T \to T_N$, $\bar{S} \to 0$ $(\coth x \to 1/x)$ and one obtains for the Néel temperature

$$\tau_N = 1/4I_2(\lambda), \quad I_2(\lambda) = 2N^{-1}\sum_q \alpha_q(\lambda)/\varepsilon_q^2(\lambda). \quad (12)$$

Let us consider the integrals I_1 and I_2 near $\Gamma=(0,0,0)$ point of the Brillouin zone (BZ). After a series expansion over the small wave vector q,

$$\alpha_q \approx [2-(q_x^2+q_y^2)/8+\lambda q^2/4]/3, \quad q^2=q_x^2+q_y^2+q_z^2,$$

$$\beta_q \approx [2-(q_x^2+q_y^2)/8-q_z^2/4]/3, \quad \varepsilon_q^2=(q_z^2+\lambda q^2)/9,$$

for the integral I_1 we obtain

$$\frac{\alpha_q(\lambda)}{\varepsilon_q(\lambda)} = \frac{2-(q_x^2+q_y^2)/8+\lambda q^2/4}{(q_z^2+\lambda q^2)^{1/2}}. \quad (13)$$

If there is only NN AFM coupling J and $\lambda=0$, then the magnon spectrum in the vicinity of Γ point becomes one dimensional with the dispersion along z axis. The cancellation of the dispersion in the xy plane is the frustration effect. It results in the divergence of $I_1 \sim \int dq_z/q_z \sim \ln q_z \to \infty$ meaning $\bar{S}(0) \to 0$. Similarly for the integral I_2 near Γ point, we obtain

$$I_2 \sim \int dq_z/q_z^2 \sim 1/q_z \to \infty, \quad T_N \to \infty.$$

These instabilities of the AFM phase on the fcc lattice were known long ago.[16–18] Due to frustrations, amplitude of the transverse spin fluctuation becomes very large and the AFM state is suppressed. In our opinion, it is very likely that the main reason for the very small T_N in comparison to the LSDA value of J in Sr_2YRuO_6 is the suppression of antiferromagnetism by spin fluctuations. The stabilization of the AFM state may be caused by the NNN exchange interaction[19,20] or by the magnetic anisotropy.

IV. STABILIZATION OF THE ANTIFERROMAGNETIC STATE BY THE EXCHANGE ANISOTROPY

It is clear from Eq. (13) that the NNN coupling $\lambda \neq 0$ restores the three-dimensional magnon dispersion at small q and rules out the one-dimensional singularity. The effect of the NNN coupling has been studied in detail.[19,20] The FM NNN coupling stabilizes the AFM type I structure, while the AFM NNN coupling results in the stabilization of the AFM type III phase. The $T_N(\lambda)$ dependence has been obtained in Ref. (19) numerically; it looks very similar to the T_N versus anisotropy dependence (see Fig. 3 below). The other conclusion of Refs. 19 and 20 was that the exchange anisotropy itself without the NNN coupling λ cannot stabilize the AFM state. This conclusion is rather strange because anisotropy results in a gap in the magnon spectrum that prevents any singularities.

To study the effect of the exchange anisotropy, we start from the Hamiltonian

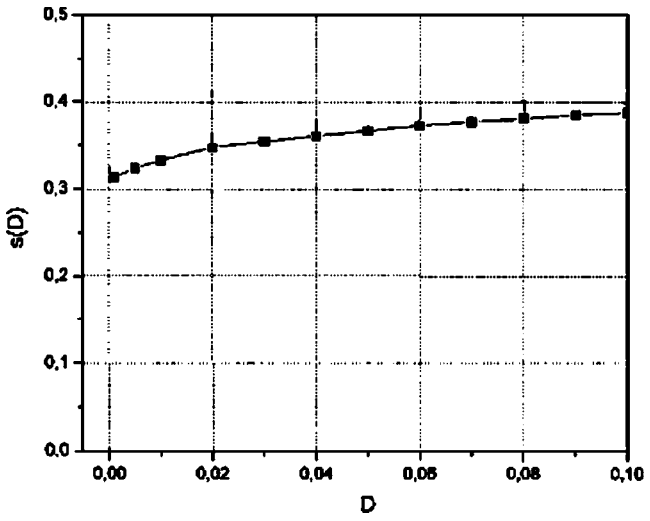

FIG. 2. The sublattice magnetization $\bar{S}$ at $T=0$ as a function of the anisotropy D.

$$H = -\frac{1}{2}\sum_{fR} J(R)(S_f^+ S_{f+R}^- + \xi_R S_f^z S_{f+R}^z), \quad \xi_R \neq 1.$$

In the simplest variant, we take into account the anisotropy only for the NN coupling and give up the anisotropy for NNN coupling. Thus we believe

$$\xi_\Delta = 1+D, \quad \xi_a = 1,$$

where D is the dimensionless anisotropy parameter, $D=(J_{||}-J_\perp)/J_\perp$. The origin of the anisotropy is the RuO_6 octahedron rotation. The angle of rotation $\varphi=12°$ is small, thus we believe $D \ll 1$.

A simple generalization of the spin-wave theory to the $D \ll 1$ case gives the renormalized Green functions (7) and (8) with substitution $\alpha_q(\lambda) \to \alpha_q(\lambda, D)$, etc., where

$$\alpha_q(\lambda, D) = 0.33(1+D+c_x c_y)+0.5\lambda(1-\gamma_q), \quad (14a)$$

$$\varepsilon_q(D) = [\alpha_q^2(\lambda, D)-\beta_q^2]^{1/2}. \quad (14b)$$

A self-consistent equation for the magnetization is derived similar to Eq. (10). The sublattice magnetization at $T=0$ is given by

$$\bar{S}(\lambda, D) = 0.5/I_1(\lambda, D), \quad (15a)$$

$$I_1(\lambda, D) = \frac{2}{N}\sum_q \alpha_q(\lambda, D)/\varepsilon_q(\lambda, D) \quad (15b)$$

and the Néel temperature reads like

$$\tau_N(\lambda, D) = 0.25/I_2(\lambda, D), \quad (16a)$$

$$I_2(\lambda, D) = \frac{2}{N}\sum_q \alpha_q(\lambda, D)/\varepsilon_q^2(\lambda, D). \quad (16b)$$

At $\lambda=0$ and $D \to 0$, both integrals I_1 and I_2 are divergent resulting in $T_N \to 0$, $\bar{S} \to 0$. To find analytically asymptotic

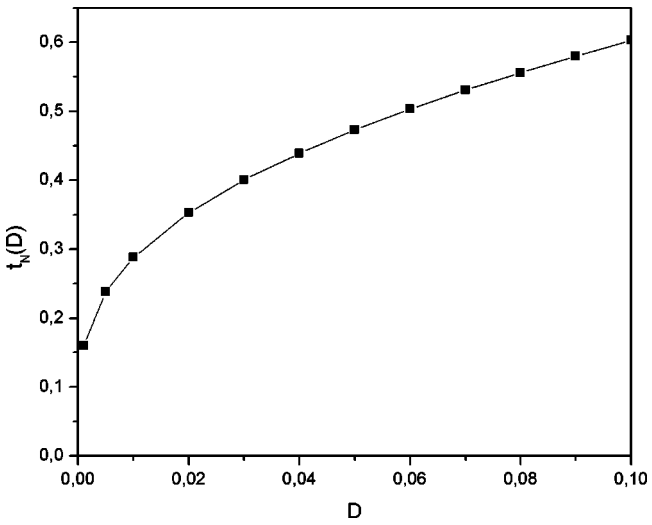

FIG. 3. The Néel temperature dependence on *D*.

behavior at $D\to 0$, we consider separately contributions from important symmetry lines in the BZ where magnon spectrum at $D=0$ is soft. The straightforward calculation gives the following asymptotic (at $\lambda = I/J = 0$):

$$\overline{S}(D) \approx \frac{1/2}{0.043(-\ln D)+1.256}, \tag{17}$$

$$T_N(D) = J\begin{cases} 4\sqrt{D}/(1+4\sqrt{D}), & 0<D<0.05 \\ 0.342+2.6D, & 0.05<D<0.1. \end{cases} \tag{18}$$

The dependence of $\overline{S}$ and T_N on the anisotropy parameter *D* is shown in Figs. 2 and 3.

V. CONCLUSIONS

The sign of the exchange anisotropy $D>0$ corresponds to the Ising-type anisotropy with $J_{||}>J_{\perp}$. In the limit $D\to\infty$, the transverse spin components become unimportant and the Heisenberg model transforms into the Ising model. As we have mentioned above, frustrations in the Ising model decrease both $\overline{S}$ and T_N (Ref. 11) but not so strongly as to get $T_N \ll J$. For each value of $D>0$, there is a gap in the magnon spectrum that results in the stabilization of the AFM type-I phase. Recently, similar problems of frustrated antiferromagnetic Heisenberg systems have been studied in Refs. 21–24 where effect of the quantum fluctuations is also important.

Comparing our calculations and the experimental data for Sr_2YRuO_6, we should remind that experimental value $S=3/2$ and monoclinic distortion of the lattice may result in the Dzyaloshinsky-Moria interaction as well as in the exchange anisotropy. It is clear that all anisotropic interactions are small versus *J*, that is why for a qualitative understanding of the experimental data we restrict ourselves to the exchange anisotropy with $D \ll J$.

To get $T_N = 30$ K with $J = 300$ K from Eq. (18), it is necessary to have $D = 8\times 10^{-4}$. That means the anisotropy of the exchange interaction $J_{||} - J_{\perp} = DJ = 0.24$ K (very small). This anisotropy in Eq. (17) results in

$$\overline{S}(8\times 10^{-4}) = 0.32$$

that is 64% from the nominal value of $S=1/2$. This value of the sublattice magnetization is in good agreement with the neutron-diffraction data.[6]

In conclusion, we have studied the effect of frustrations in the Heisenberg AFM on the fcc lattice with the NN AFM coupling. In the type-I AFM structure, frustrations result in the soft magnon modes along several dangerous lines in the BZ. For example, near the Γ point the magnon dispersion is quasi-one-dimensional that provides typical low-dimensional singularities in the spin-wave theory. Very small NNN FM coupling or Ising-type exchange anisotropy can stabilize the AFM state. We believe that this is the reason of small T_N with large *J* in the double perovskite Sr_2YRuO_6.

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