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Magnetic order and spin excitations in layered Heisenberg antiferromagnets with compass-model anisotropies

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The spin-wave excitation spectrum, the magnetization, and the Néel temperature for the quasi-two-dimensional spin-1/2 antiferromagnetic Heisenberg model with compass-model interaction in the plane proposed for iridates are calculated in the random phase approximation. The spin-wave spectrum agrees well with data of Lanczos diagonalization. We find that the Néel temperature is enhanced by the compass-model interaction and is close to the experimental value for Ba_2IrO_4.

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Spin-orbital physics in transition-metal oxides has been extensively studied in recent years. A number of theoretical models was proposed to describe a complicated nature of phase transitions induced by competing spin and orbital interactions as originally was considered in Ref. [1]. Whereas the isotropic spin interaction can be treated within the conventional Heisenberg model, to study the orientation-dependent orbital interaction the compass model is commonly used. The latter reveals a large degeneracy of ground states resulting in a complicated phase diagram. In particular, quantum and thermodynamic phase transitions in the two-dimensional (2D) compass model were studied in Refs. [2–4], where a first-order transition was found for the symmetric compass model. A generalized 2D Compass–Heisenberg (CH) model was introduced in Ref. [5], where an important role of the spin Heisenberg interaction in lifting the high degeneracy of the ground state of the compass model was stressed. In Ref. [6] a phase diagram of the CH model and excitations within Lanczos exact diagonalization for finite clusters on a square lattice were considered in detail. In particular, spin-wave excitations and column-flip excitations in nanoclusters characteristic to the compass model were analyzed.

A strong relativistic spin-orbital coupling reveals a compass-model type interaction in $5d$ transition metals. In particular, it was shown in Ref. [7], that a strong spin-orbit coupling in such compounds as Sr_2IrO_4 and Ba_2IrO_4 results in an effective antiferromagnetic (AF) Heisenberg model for the pseudospins 1/2 with the compass-model anisotropy. The model can be used to explain the AF long-range order (LRO) below the Néel temperature $T_N = 230$ K in Sr_2IrO_4 and $T_N = 240$ K in Ba_2IrO_4 (see, e.g., [8]). The spin-wave spectrum measured by magnetic resonance inelastic x-ray scattering (RIXS) in Sr_2IrO_4 shows a dispersion similar to that one in the undoped cuprate La_2CuO_4 [9].

In the present paper we calculate the spin-wave excitation spectrum and magnetization for a layered AF Heisenberg model with anisotropic compass-model interaction in the plane. To take into account the finite-temperature renormalization of the spectrum and to calculate the Néel temperature T_N, we employ the equation of motion method for the Green functions (GFs) for spin $S = 1/2$ using the random phase approximation (RPA) [10]. The results are compared with experimental data for iridates and theoretical studies of the 2D CH model in Ref. [5].

We consider the layered Heisenberg AF with the compass-model interaction in the plane. The Hamiltonian of the model can be written as

$$H = \frac{1}{2}\sum_{i,j}\Big\{J_{ij}\mathbf{S}_i\mathbf{S}_j + \Gamma^x_{ij}S^x_iS^x_j + \Gamma^y_{ij}S^y_iS^y_j\Big\}. \qquad (1)$$

Here $J_{ij} = J\,(\delta_{\mathbf{r}_j,\mathbf{r}_i\pm\mathbf{a}_x} + \delta_{\mathbf{r}_j,\mathbf{r}_i\pm\mathbf{a}_y}) + J_z\,\delta_{\mathbf{r}_j,\mathbf{r}_i\pm\mathbf{c}}$, where J is the exchange interaction between the nearest neighbors in the plane with the lattice constants $a_x = a_y = a$, and J_z is the coupling between the planes with the distance c. The compass model interaction is given by $\Gamma^x_{ij} = \Gamma_x\,\delta_{\mathbf{r}_j,\mathbf{r}_i\pm\mathbf{a}_x}$, $\Gamma^y_{ij} = \Gamma_y\delta_{\mathbf{r}_j,\mathbf{r}_i\pm\mathbf{a}_y}$. The *ab initio* many-body quantum chemistry calculations give the following parameters for Ba_2IrO_4: $J = 65$ meV, $\Gamma_x = \Gamma_y = \Gamma = 3.4$ meV, and $J_z \gtrsim (3{-}5)\,\mu$eV [11]. To compare our results with the theoretical studies of the 2D

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CH model in Ref. [5], we consider also large anisotropic compass-model interactions, $\Gamma_x > \Gamma_y > J$.

We adopt a two-sublattice (A, B) representation for the AF LRO below the Néel temperature. Then the Hamiltonian (1) with $\Gamma_x = \Gamma_y > 0$ is an easy-plane AF, where the direction of the AF order parameter (OP) – the magnetization of one sublattice in the (x, y) plane – is degenerate. To lift the degeneracy, we assume anisotropic compass-model interactions $\Gamma_x > \Gamma_y > 0$. In this case the model (1) describes an easy-axis AF with the OP $\langle S^x_{i\subset A}\rangle = -\langle S^x_{i\subset B}\rangle$ fixed along the x axis. We can consider also the limiting case, $\Gamma_x = \Gamma_y$. The AF LRO can be described by the AF wave vector $\mathbf{Q} = (\pi/a, \pi/a, \pi/c)$.

It is convenient to write the Hamiltonian (1) in terms of the circular components $S^{\pm}_i = S^y_i \pm i S^z_i$ in the form

$$H = \frac{1}{2}\sum_{\langle i,j\rangle}\Big\{J^x_{ij}\, S^x_i S^x_j + J^y_{ij}\frac{1}{2}\,\left[S^+_i S^-_j + S^-_i S^+_j\right] + \\ + \frac{1}{4}\Gamma^y_{ij}\,\left[S^+_i S^+_j + S^-_i S^-_j\right]\Big\}, \qquad (2)$$

where $J^x_{ij} = J_{ij} + \Gamma^x_{ij}$, $J^y_{ij} = J_{ij} + (1/2)\Gamma^y_{ij}$.

To calculate the spin-wave spectrum of transverse spin excitations, we introduce the retarded two-time commutator GFs [12]:

$$G^{\alpha,\beta}_{nm}(t-t') = -i\theta(t-t')\langle[S^\alpha_n(t), S^\beta_m(t')]\rangle = \\ = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\langle\langle S^\alpha_n|S^\beta_m\rangle\rangle_\omega, \qquad (3)$$

where $\alpha, \beta = (\pm)$, and $\langle\ldots\rangle$ is the statistical average. The indexes n, m run over $N/2$ lattice sites $i\,(j)$ in the sublattice $A\,(B)$.

There are four types of the GFs due to the two-sublattice representation for normal and anomalous GFs which can be written as 4×4 matrix GF

$$\hat{G}(\omega) = \left\langle\!\!\left\langle \begin{pmatrix} S^+_i \\ S^-_i \\ S^-_j \\ S^+_j \end{pmatrix} \;\Big|\; \begin{pmatrix} S^-_{i'} & S^+_{i'} & S^+_{j'} & S^-_{j'} \end{pmatrix} \right\rangle\!\!\right\rangle_\omega. \qquad (4)$$

Here the lattice sites i, i' refer to the sublattice A while the lattice sites j, j' refer to the sublattice B.

Using equations of motion for spin operators, $i(d/dt)S^{\pm}_i(t) = [S^{\pm}_i, H] = \mp\sum_n J^x_{in} S^{\pm}_i S^x_n \pm \pm\sum_n [J^y_{in}\, S^x_i S^{\pm}_n + (1/2)\Gamma^y_{in}\, S^x_i S^{\mp}_n]$, we obtain a system of equations for the matrix components of the GF (4). In particular,

$$\omega\langle\langle S^+_i|S^-_{i'}\rangle\rangle_\omega = 2\langle S^x_i\rangle\,\delta_{i,i'} - \sum_n J^x_{in}\langle\langle\, S^+_i S^x_n|S^-_{i'}\rangle\rangle_\omega + \\ + \sum_n [\, J^y_{in}\,\langle\langle\, S^x_i S^+_n|S^-_{i'}\rangle\rangle_\omega + (1/2)\Gamma^y_{in}\langle\langle\, S^x_i S^-_n\,|S^-_{i'}\rangle\rangle_\omega],$$

$$\omega\langle\langle S^-_j|S^+_{j'}\rangle\rangle_\omega = -2\langle S^x_j\rangle\,\delta_{j,j'} + \sum_m J^x_{jm}\langle\langle\, S^-_j S^x_m|S^+_{j'}\rangle\rangle_\omega - \\ - \sum_m [\, J^y_{jm}\,\langle\langle\, S^x_j S^-_m|S^+_{j'}\rangle\rangle_\omega + (1/2)\Gamma^y_{jm}\langle\langle\, S^x_j S^+_m|S^+_{j'}\rangle\rangle_\omega].$$

In the RPA [10] for all GFs the following approximation is used for the lattice sites $n \neq i$, $m \neq j$, as e.g.,

$$\langle\langle S^x_i S^\alpha_n|S^\beta_{i'}\rangle\rangle_\omega = \langle S^x_i\rangle\,\langle\langle S^\alpha_n|S^\beta_{i'}\rangle\rangle_\omega = \sigma\,\langle\langle S^\alpha_n|S^\beta_{i'}\rangle\rangle_\omega, \\ \langle\langle S^x_n S^\alpha_i|S^\beta_{i'}\rangle\rangle_\omega = \langle S^x_n\rangle\,\langle\langle S^\alpha_i|S^\beta_{i'}\rangle\rangle_\omega = -\sigma\,\langle\langle S^\alpha_i|S^\beta_{i'}\rangle\rangle_\omega, \qquad (5)$$

where $\langle S^x_i\rangle = \sigma$ for $i \in A$ while $\langle S^x_n\rangle = -\sigma$ for $n \in B$. A similar approximation is used for the B sublattice, where $\langle S^x_j\rangle = -\sigma$ for $j \in B$ while $\langle S^x_m\rangle = \sigma$ for $m \in A$. The RPA results in a closed system of equations for the components of the matrix GF (4).

To solve the obtained system of equations we introduce the Fourier representation of spin operators for $N/2$ lattice sites in two sublattices, $S^{\pm}_i = \sqrt{2/N}\sum_{\mathbf{q}} S^{\pm}_{\mathbf{q}}\,\exp(\pm i\mathbf{q}\mathbf{r}_i)$ and $S^{\pm}_j = \sqrt{2/N}\sum_{\mathbf{q}'} S^{\pm}_{\mathbf{q}'}\,\exp(\pm i\mathbf{q}'\mathbf{r}_j)$, where $\mathbf{q}$ and $\mathbf{q}'$ run over $N/2$ wave vectors in the reduced BZ of each sublattice. Using this transformation the equation for the Fourier representation of the matrix GF (4) can be written in the from

$$\hat{G}(\mathbf{q},\omega) = \{\omega\hat{I} - \hat{V}(\mathbf{q})\}^{-1}\times 2\sigma\,\hat{I}_1, \qquad (6)$$

where $\hat{I}$ is the unity matrix, $\hat{I}_1$ is a diagonal matrix with the elements $d_{11} = d_{33} = 1$ and $d_{22} = d_{44} = -1$, and the interaction matrix is given by

$$\hat{V}(\mathbf{q}) = \begin{pmatrix} A & 0 & B(\mathbf{q}) & C(\mathbf{q}) \\ 0 & -A & -C(\mathbf{q}) & -B(\mathbf{q}) \\ B(\mathbf{q}) & C(\mathbf{q}) & A & 0 \\ -C(\mathbf{q}) & -B(\mathbf{q}) & 0 & -A \end{pmatrix}. \qquad (7)$$

Here the interaction parameters are:

$$A = \sigma\, J^x(0) = \sigma\,[J(0) + 2\,\Gamma_x], \\ J(\mathbf{q}) = 2J\,(\cos q_x + \cos q_y) + 2J_z\,\cos q_z, \\ B(\mathbf{q}) = \sigma\,\Gamma_y\cos q_y,\; C(\mathbf{q}) = \sigma\,[J(\mathbf{q}) + \Gamma_y\cos q_y]. \qquad (8)$$

The spectrum of spin waves is determined from the equation

$$\mathrm{Det}\,|\omega\hat{I} - \hat{V}(\mathbf{q})| = 0. \qquad (9)$$

After some algebra we obtain the biquadratic equation for the frequency ω of spin-wave excitations:

$$\omega^4 - 2\omega^2[A^2 + B^2(\mathbf{q}) - C^2(\mathbf{q})] + [B^2(\mathbf{q}) - C^2(\mathbf{q})]^2 - \\ - 2A^2[C^2(\mathbf{q}) + B^2(\mathbf{q})] + A^4 = 0.$$

The solution of this equation reads

$$\omega_\nu(\mathbf{q}) = \pm\{A^2 + B^2(\mathbf{q}) - C^2(\mathbf{q}) + 2\nu A\, B(\mathbf{q})\}^{1/2} \equiv \equiv \pm\sigma\,\varepsilon_\nu(\mathbf{q}), \qquad (10)$$

where $\nu = \pm 1$. The energy of excitations for "acoustic" $\varepsilon_-(\mathbf{q})$ and "optic" $\varepsilon_+(\mathbf{q})$ modes are

$$\varepsilon_-(\mathbf{q}) = \Big\{J^2(0) - J^2(\mathbf{q}) + 4\,\Gamma_x[J(0)+\Gamma_x] - - 2\,\Gamma_y\,[J(0)+J(\mathbf{q})+2\,\Gamma_x]\,\cos q_y\Big\}^{1/2}, \qquad (11)$$

$$\varepsilon_+(\mathbf{q}) = \Big\{J^2(0) - J^2(\mathbf{q}) + 4\,\Gamma_x[J(0)+\Gamma_x] + + 2\,\Gamma_y[J(0)-J(\mathbf{q})+2\,\Gamma_x]\,\cos q_y\Big\}^{1/2}. \qquad (12)$$

These two branches are coupled by the relation $\varepsilon_-(\mathbf{q}+\mathbf{Q}) = \varepsilon_+(\mathbf{q})$ for the AF wave vector $\mathbf{Q}$.

For the symmetric compass-model interaction, $\Gamma_x = = \Gamma_y = \Gamma$, for $\mathbf{q}=0$ we have the gapless acoustic mode while the optic mode has a gap:

$$\varepsilon_-(0) = 0, \quad \varepsilon_+(0) = 2\sqrt{\Gamma\,J(0)+2\Gamma^2} > 0. \qquad (13)$$

For the wave vector $\mathbf{q} = \mathbf{Q}$ we have the opposite results: $\varepsilon_-(\mathbf{Q}) = \varepsilon_+(0) > 0$, $\varepsilon_+(\mathbf{Q}) = \varepsilon_-(0) = 0$. In the anisotropic case $\Gamma_x > \Gamma_y$ the spectrum of excitations has gaps both at $\mathbf{q}=0$ and $\mathbf{Q}$:

$$\varepsilon_-(0) = \varepsilon_+(\mathbf{Q}) = 2\sqrt{(\Gamma_x - \Gamma_y)\,[J(0)\,+\Gamma_x]}. \qquad (14)$$

For a conventional AF Heisenberg model with $\Gamma_x = = \Gamma_y = 0$ we have only one branch with the dispersion $\varepsilon_-(\mathbf{q}) = \varepsilon_+(\mathbf{q}) = \sqrt{J^2(0) - J^2(\mathbf{q})}$ which is gapless both at $\mathbf{q}=0$ and $\mathbf{Q}$.

A similar equation of motion method for the matrix GF (4) can be employed in the linear spin-wave theory (LSWT) using the transformation $S_i^+ = \sqrt{2S}\,a_i$, $S_i^- = \sqrt{2S}\,a_i^\dagger$, $S_i^x = S - a_i^\dagger a_i$ for the sublattice A and the similar transformation for the sublattice B $(a_i \to b_i^\dagger)$. Then keeping only linear terms in the bose-like operators $(a_i,\, a_i^\dagger)$ and $(b_i,\, b_i^\dagger)$ we obtain Eqs. (10)–(12) for the spin-wave spectrum in LSWT with the sublattice magnetization σ substituted by spin S. The same spectrum in LSWT was obtained in Refs. [5, 6]. Note that in the RPA the energy of spin excitations $\omega_\pm(\mathbf{q})$, Eq. (10), is reduced in comparison with the LSWT since $\sigma < S$ even at zero temperature due to zero-point fluctuations in the AF state. The spectrum (10) for the symmetric compass model, $\Gamma_x = \Gamma_y$, is similar to the spectrum of the anisotropic AF Heisenberg model considered in Ref. [13].

In Fig. 1 the spectrum of spin waves $\omega_\pm(\mathbf{q})$ in the plane in RPA for the parameters $J = 65$ meV, $\Gamma = 3.4$ meV found for Ba_2IrO_4 [11] is shown at

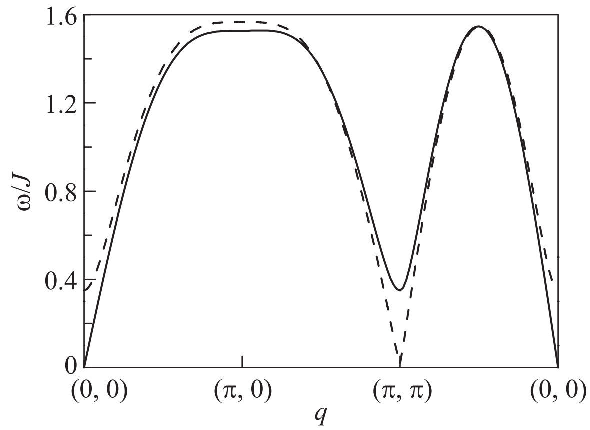

Fig. 1. Spectrum of spin-wave excitations $\omega_-(\mathbf{q})$ (bold line) and $\omega_+(\mathbf{q})$ (dashed line) along the symmetry directions in the BZ for the symmetric compass model with $\Gamma_x = \Gamma_y = \Gamma = 0.052\,J$ and $J_z = 0$

$T = 0$. The spectrum $\omega_-(\mathbf{q})$ shows a gap at the wave vector $\mathbf{Q}$ given by $\omega_-(\mathbf{Q}) = 2\,\sigma\sqrt{\Gamma\,J(0)+2\Gamma^2} \approx \approx 1.48\,J\sqrt{\Gamma/J} \approx 22$ meV for $\sigma = 0.37$. This value is comparable with the maximum energy of excitations $\omega_-^{\max}(\mathbf{Q}/2) = 4\,\sigma\,J\sqrt{1+\Gamma/J} \approx 1.5\,J$ that gives $\omega_-(\mathbf{Q})/\omega_-^{\max}(\mathbf{Q}/2) \approx 0.22$. We can suggest that the spin-wave spectrum in Ba_2IrO_4 should be similar to that one measured by RIXS in Sr_2IrO_4 [9]. The latter was fitted by a one-branch phenomenological $J{-}J'{-}J''$ model with $J = 60$ meV, $J' = -20$ meV, and $J'' = 15$ meV. The spectrum does not reveal a gap in the acoustic branch $\omega_-(\mathbf{q})$ at $\mathbf{Q}$ as for Ba_2IrO_4. However, since the intensity of scattering on magnons is proportional to $1/\omega(\mathbf{q})$, strong scattering on the gapless branch $\omega_+(\mathbf{q}) \to 0$ for $\mathbf{q} \to \mathbf{Q}$ completely suppresses scattering on the gapped $\omega_-(\mathbf{q})$ branch. To distinguish scattering on the two branches, high-resolution studies are necessary. We have found the energy of excitations at $\mathbf{q}_1 = (\pi/2, \pi/2)$, $\omega_-(\mathbf{q}_1) = \omega_+(\mathbf{q}_1)$, to be nearly equal to $\omega_\pm(\mathbf{q} = \pi, 0)$ (up to $\pm\Gamma/J$), while in the RIXS experiment $\omega(\mathbf{q}_1) \approx (1/2)\omega(\mathbf{q} = \pi, 0)$ was found. Possibly, this difference can be explained by magnon interaction with spin-orbital excitations observed in [9] which are not taken into account in the model (1).

Fig. 2 shows the spin-wave dispersion for large anisotropic interaction, $\Gamma_x = 8.9\,J$, $\Gamma_y = 4.5\,J$ used in Ref. [5] in numerical calculations with Lanczos exact diagonalization. Our RPA calculations give a similar formula for the spectrum as in LSWT except for the prefactor $\sigma = 0.44$ instead of $S = 1/2$ in LSWT. The dispersion curves are in good agreement with numerical ones shown by circles which were multiplied by the factor $10/4$, since in Ref. [5], instead of spin $1/2$ oper-

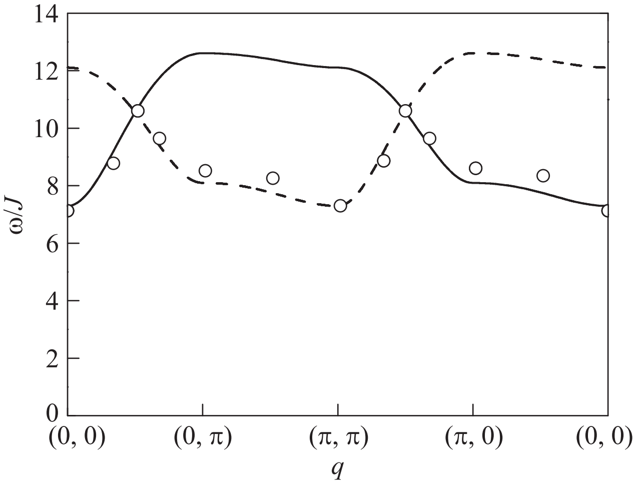

Fig. 2. Spectrum of spin-wave excitations $\omega_-(\mathbf{q})$ (bold line) and $\omega_+(\mathbf{q})$ (dashed line) along the symmetry directions in the BZ for the anisotropic compass model with $\Gamma_x = 8.9\,J$, $\Gamma_y = 4.5\,J$, $J_z = 0$. Circles are numerical results from Ref. [5]

ators, the Pauli matrices are used so that the exchange integral I corresponds to our $(1/4)\,J$ in Eq. (1), and in Fig. 4 of Ref. [5] the energy unit is $J_c = 10I$. The spectrum reveals a large gap at all wave vectors caused by the large value of Γ_x and a noticeable dispersion only along the $\Gamma(0,0) \to Y(0,\pi)$ direction due to a large, in comparison with J, interaction $\Gamma_y = 4.5\,J$.

To calculate the sublattice magnetization $\sigma = \langle S_i^x \rangle$ in RPA, we use the kinematic relation $S_i^x = 1/2 - S_i^- S_i^+$ for spin $S = 1/2$ which results in the self-consistent equation

$$\sigma = \frac{1}{2} - \frac{1}{N/2} \sum_{\mathbf{q}} \langle S_{\mathbf{q}}^- S_{\mathbf{q}}^+ \rangle. \tag{15}$$

The spin correlation function $\langle S_{\mathbf{q}}^- S_{\mathbf{q}}^+ \rangle$ can be calculated from the GF $\langle\langle S_{\mathbf{q}}^+ | S_{\mathbf{q}}^- \rangle\rangle_\omega$ which follows from the GF (6):

$$\langle\langle S_{\mathbf{q}}^+ | S_{\mathbf{q}}^- \rangle\rangle_\omega = 2\sigma \, \frac{a_{\mathbf{q}}(\omega)}{[\omega^2 - \omega_-^2(\mathbf{q})][\omega^2 - \omega_+^2(\mathbf{q})]}, \tag{16}$$

$$a_{\mathbf{q}}(\omega) = \omega^3 + A\,\omega^2 - [A^2 + B^2(\mathbf{q}) - C^2(\mathbf{q})]\,\omega - - A^3 + A\,[B^2(\mathbf{q}) + C^2(\mathbf{q})].$$

Using the spectral representation for GFs, for the correlation function we obtain

$$\langle S_{\mathbf{q}}^- S_{\mathbf{q}}^+ \rangle = 2\sigma \sum_{\mu,\nu=\pm 1} I_{\mu\nu}(\mathbf{q})\, N[\mu\omega_\nu(\mathbf{q})], \tag{17}$$

where $N(\omega) = [\exp(\omega/T) - 1]^{-1}$, and the contribution from the four poles of the GF (16) is given by

$$I_{\mu\nu}(\mathbf{q}) = \frac{a_{\mathbf{q}}[\mu\omega_\nu(\mathbf{q})]}{8\mu\nu\omega_\nu(\mathbf{q})\,AB(\mathbf{q})}. \tag{18}$$

Note that $I_{\mu\nu}(\mathbf{q})$ does not depend on σ.

Using relation (17) we perform the self-consistent solution of Eq. (15) for the magnetization σ. Fig. 3 shows

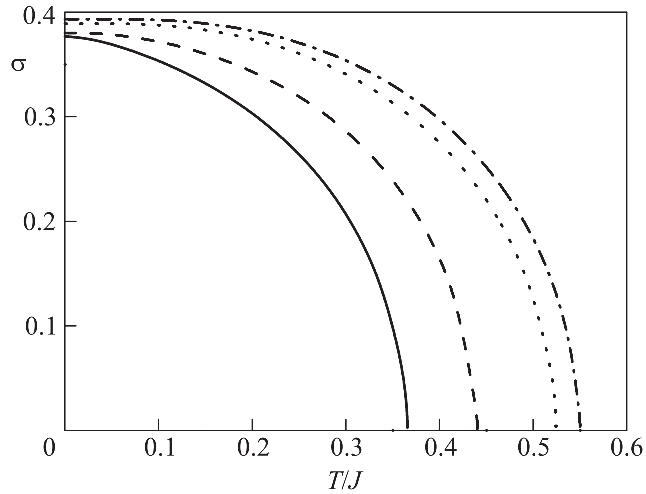

Fig. 3. Sublattice magnetization $\sigma = \langle S_i^x \rangle$ for the parameters $J_z = 5 \cdot 10^{-5}\,J$, $\Gamma_x = 0.052\,J$ for $\Gamma_y/\Gamma_x = 1$ (solid line), 0.95 (dashed line), 0.5 (dotted), and for $\Gamma_y/\Gamma_x \leqslant 0.1$ (dash-dotted)

the sublattice magnetization for $J_z = 5 \times 10^{-5}\,J$, $\Gamma_x = 0.052\,J$ for various Γ_y/Γ_x. For the symmetric compass model, $\Gamma_x = \Gamma_y = 0.052\,J$, the Néel temperature $T_{\rm N} = 0.365\,J = 275\,{\rm K}$ is close to $T_{\rm N} = 240\,{\rm K}$ observed in experiment for Ba_2IrO_4. We stress that the anisotropy of the compass-model interaction, $\Gamma_y/\Gamma_x < 1$, enhances $T_{\rm N}$.

To study the $T_{\rm N}$ dependence on the parameters of the model, we consider Eq. (15) in the limit $\sigma \to 0$. In this limit $N(\omega_\nu) \approx T/\sigma\varepsilon_\nu$, and for the Néel temperature we have the equation:

$$\frac{1}{2} = \frac{1}{N/2} \sum_{\mathbf{q}} \sum_{\mu,\nu=\pm 1} I_{\mu\nu}(\mathbf{q}) \, \frac{2\,T_{\rm N}}{\mu\varepsilon_\nu(\mathbf{q})}. \tag{19}$$

Therefore,

$$T_{\rm N} = \frac{1}{4C}, \quad C = \frac{1}{N/2} \sum_{\mathbf{q}} \sum_{\mu,\nu} \frac{I_{\mu\nu}(\mathbf{q})}{\mu\varepsilon_\nu(\mathbf{q})}. \tag{20}$$

Let us study in which cases the integral over $\mathbf{q}$ in (20) has a finite value that results in a finite $T_{\rm N}$.

At first we consider the symmetric compass model, $\Gamma_x = \Gamma_y = \Gamma$. In this case $\varepsilon_-(\mathbf{q}) = 0$ at $\mathbf{q} = 0$ and $\varepsilon_+(\mathbf{q}) = 0$ at $\mathbf{q} = \mathbf{Q}$. Since these two branches are symmetric, we can consider only the divergency of the integral in (20) at $\mathbf{q} = 0$ for $\varepsilon_-(\mathbf{q})$ given around $\mathbf{q} = 0$ by

$$\varepsilon_-^2(\mathbf{q}) = 2[J(0)+\Gamma](J\,q_x^2 + \\ + \{J + \Gamma^2/[J(0)+\Gamma]\}q_y^2 + J_z\,q_z^2). \qquad (21)$$

The integral in (20) diverges as $\int d^3\mathbf{q}/\varepsilon_-^2(\mathbf{q})$ if any coefficient before q_x, q_y or q_z in (21) is zero. In particular, for nonzero $J(0)$ there is no LRO at finite T for $J_z = 0$.

In the limiting case $\Gamma \to 0$ we have $\lim I_{\mu\nu}(\mathbf{q}) = (A + \mu\omega_{\mathbf{q}})/(4\mu\omega_{\mathbf{q}})$ with $\omega_{\mathbf{q}} = \sqrt{A^2 - C^2(\mathbf{q})}$. From Eq. (20) we get the conventional formula for $T_{\rm N}$ of the AF Heisenberg model (c.f. Ref. [14]):

$$T_{\rm N}(\Gamma = 0) = \left[\frac{8J(0)}{N}\sum_{\mathbf{q}} \frac{1}{J(0)^2 - J^2(\mathbf{q})}\right]^{-1}. \qquad (22)$$

Thus, for a symmetric 2D compass model we have no LRO at finite T. To obtain LRO, we must have finite values of both J and J_z. The Néel temperature $T_{\rm N}$ as a function of the interplane coupling J_z is shown in Fig. 4 for the interaction $\Gamma_x = \Gamma_y = 0.052\,J$ and for

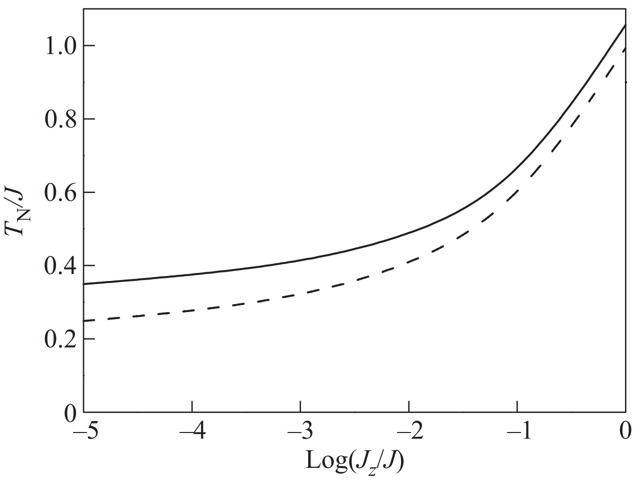

Fig. 4. Néel temperature $T_{\rm N}$ as a function of J_z with $\Gamma_x = \Gamma_y = 0.052\,J$ (solid line) and $\Gamma_x = \Gamma_y = 0$ (dashed line)

$\Gamma_x = \Gamma_y = 0$. We can conclude that the compass-model interaction enhances the Néel temperature and, in particular, the anisotropy of the compass-model interaction results in a further increase of $T_{\rm N}$ as shown in Fig. 3. In the anisotropic case $\Gamma_x > \Gamma_y$ the spectrum of excitations has a gap at $q = 0$, Eq. (14), and therefore neither branch of this spectrum ever reaches zero, so that we have a finite $T_{\rm N}$ even for $J_z = 0$. Fig. 5 demonstrates the dependence of $T_{\rm N}$ on Γ_x for $J_z = 0$, $\Gamma_y = 0.1\,\Gamma_x$, and $\Gamma_y = 0.9\,\Gamma_x$. For $\Gamma_x \to 0$ the Néel temperature goes to zero as shown in the inset.

To summarize, we have studied the spin-wave spectrum for the Heisenberg model with anisotropic compass-model interaction within the RPA. The spectrum has gaps at $\mathbf{q} = 0$ or at the AF wave vector $\mathbf{Q}$ for

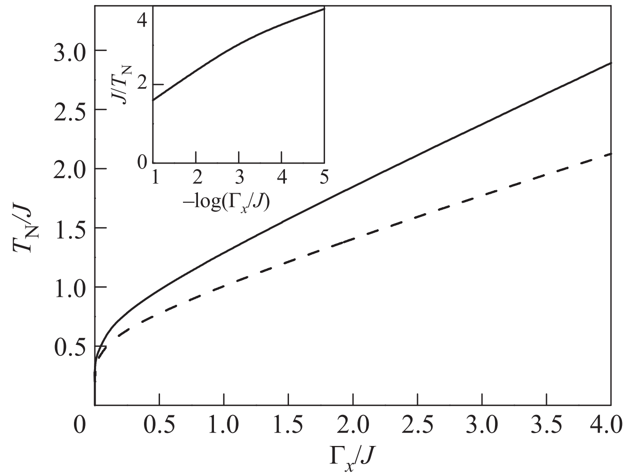

Fig. 5. Néel temperature $T_{\rm N}$ as a function of Γ_x for $J_z = 0$, $\Gamma_y = 0.1\Gamma_x$ (solid line) and $\Gamma_y = 0.9\Gamma_x$ (dashed line). In the inset the $1/T_{\rm N}$ dependence is shown in the logarithmic scale for small Γ_x

nonzero compass-model interactions. The calculation of the Néel temperature $T_{\rm N}$ shows that for the symmetric compass-model interaction, $\Gamma_x = \Gamma_y$, and a nonzero exchange interaction J, the AF LRO at finite T can exist only for a finite coupling J_z between the planes. For the anisotropic compass-model interaction, $\Gamma_x > \Gamma_y$, and a finite exchange interaction J in the plane, the AF LRO with finite Néel temperature emerges even in the 2D case as observed in finite cluster calculations [5, 6]. In any case, $T_{\rm N}$ is enhanced by the compass-model interaction.

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