Magnetic properties of antiferromagnetic bilayers analyzed in the spin and boson pictures

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Systems of antiferromagnetic bilayers [like those occurring in high-T_c cuprates ($YBa_2Cu_3O_{6+x}$ (1:2:3))], are analyzed theoretically both in spin [the random phase approximation (RPA)] and boson picture at low temperatures. Similarities and differences in excitations energies, internal energy, and magnetization are analyzed in detail, and a comparison is made to numerous existing results at $T = 0$ K and in the low-temperature range. RPA results for antiferromagnet transition temperature are analyzed in terms of spin (in-plane) and spatial anisotropies. It is shown that in-plane anisotropy plays a more important role than previously assumed.

I. INTRODUCTION

A simple magnetic system consisting of two magnetically ordered planes, coupled magnetically, the so-called magnetic bilayer, has been the subject of interest for the last decade. There are several reasons for this.

The model, although simple, is interesting by itself. Two-dimensional magnetism is already interesting since various anisotropies influence its behavior strongly.[1,2] The coupling between the planes introduces an element of three dimensionality. One can enhance this effect by building up a superlattice whose motive is this bilayer. This allows a study of dimensional crossover effects.

Experimental aspects of the problem are also interesting. Recent studies of the phenomenon of gigantic magnetoresistance (GMR) indicate that it occurs mostly in such layered systems,[3] although proper relation between the structure and GMR has not yet been established.

However, the true reason for the large interest in these systems are cuprate high-temperature superconductors. It is well known that antiferromagnetically ordered planes of Cu^{2+} ions occur, and that the magnetic system can be considered as the set of magnetic layers (La_2CuO_4) or bilayers [$YBa_2Cu_3O_{6+x}$ (1:2:3)]. The role of the magnetic subsystem in the superconductive phase is also still an issue of discussion.

The objectives of our study will be the properties of antiferromagnetically ordered bilayers which can be tested experimentally. First of all, we are interested in the energy of elementary excitations—spin waves—which are accessible by neutron scattering. A knowledge of the energies of spin-wave branches allows one to evaluate the next important quantity—sublattice magnetization—and study its low-temperature behavior as well as in the vicinity of the phase transition. We can also evaluate the magnetic contribution to the internal energy of the system, and estimate the temperature behavior of the magnetic contribution to the specific heat C_v.

There are two basic approaches occurring in the literature. One can work directly with spin operators and apply either the mean-field approximation, or use a Green's function (GF) decoupled in self-consistent manner. An alternative procedure is to use some approximate boson representation for

spin operators and than use this boson Hamiltonian as the basis for the study.

There exists numerous literature in the field, so let us comment on some of this work. One early work was performed by Matsuda and Hida[4] who considered the ground state and elementary excitations of an antiferromagnetic (AF) double layer in Bloch's approximation for spin operators. The interactions were all isotropic in spin space, with three different couplings: one within each layer and one between the layers. Their basic result is that strong interlayer coupling destroys the ground state AF long-range order. We shall later consider the result, which is of purely quantum origin, below. Hida[5] studied the low-temperature properties of this system by applying the Dyson-Maleev boson representation. Decoupling the nonlinear terms in a mean-field manner, he mainly confirmed the results of Matsuda and Hida.[4]

The particular application to cuprate superconductors was recently performed by Pratap *et al.*[6] They used simple spin-wave pictures and applied the GF formalism. Their results are important to us for the sake of comparison.

Our work will concern only the value $S = 1/2$ (which seems to correspond to Cu^{2+} ions in cuprates). Using the Green's-function formalism for both spin and boson operators, we shall study the energy and sublattice magnetization of the system. Different temperature regimes will be discussed in detail as well as the transition temperature T_N.

The structure of the paper is as follows: in Sec. II we describe the model and its relation to high-T_c superconductors. Section III is devoted to an evaluation of the expressions for all relevant physical quantities within the framework of the random-phase approximation (RPA) for spin Green's functions, while the same procedure for boson approximate representation is presented in Sec. IV. The results are discussed in detail in Sec. V, while some concluding remarks are presented in Sec. VI.

II. MODEL HAMILTONIAN

In order to be able to compare our results with the studies related to copper-oxide based HT_c superconductors, like (1:2:3) structures, we shall consider a superlattice consisting of bilayers. The elements of bilayers are antiferromagnetically ordered planes coupled antiferromagnetically. The underlying lattice is split into two magnetic sublattices a and b in such a way that each spin of one sublattice is surrounded
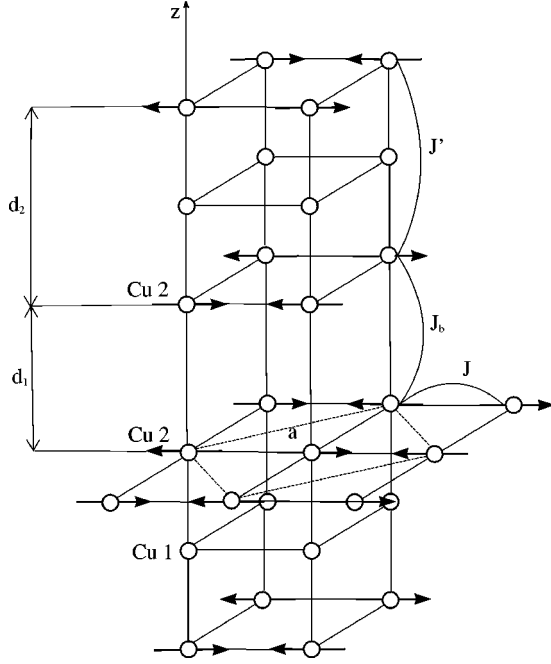
FIG. 1. Antiferromagnetic structure of $YBa_2Cu_3O_{6+x}$ following Refs. 7 and 8. Two Cu2 planes are m_1 and m_2 planes of the cell, with an in-plane interaction J and a square lattice parameter a. The intracell interaction is J_b, and the intercell interaction is J'. $c_o = d_1 + d_2$ is the period of the superlattice along the z direction.

by six neighboring spins belonging to the other sublattice. This model can be applied to the system of spins of so-called Cu2 ions in a (1:2:3) structure, as shown in Fig. 1.[7–9]

The position of each spin is defined in the following manner: $\vec{S}_{m_i,\vec{\rho}}(\alpha)$; $i=1$ and 2; $\alpha=a$, b, where m_1 and m_2 are the indices of the planes within the cell (for a superlattice) and $\vec{\rho}$ is two-dimensional vector defining the position within the plane. The basic assumption is that the atoms in the neighboring planes are positioned exactly "one above the other" looking along the $z(c)$ axis, which allows such simple notations.

Interactions are assumed to be the nearest-neighbor Heisenberg interactions, with a spin anisotropy within the plane (additional $S^z S^z$ interaction gJ) and a spatial anisotropy due to different couplings between the planes (J_b, J') and within the planes (J). The magnetic field is along the z axis.

We shall restrict ourselves to the particular case $S_a = S_b = 1/2$, since it allows a simple calculation of the system energy. It is better for this purpose to express the Hamiltonian in terms of raising and lowering operators $S^{\pm}(S_i^z = \frac{1}{2} - S_i^- S_i^+)$, so it can be written as

$$H/J = H_o + H_2 + H_4, \qquad (1)$$

$$H_o = -\frac{N_o}{8}\varepsilon - \frac{1}{2}N_o\mu\mathcal{H}, \quad \varepsilon = 4g + \lambda_b + \lambda',$$

$$\lambda_b = \frac{J_b}{J}, \quad \lambda' = \frac{J'}{J} \qquad (2)$$

(N_o is the number of paramagnetic ions),

$$H_2 = \sum_{m_i,\vec{\rho}} [\varepsilon_a \hat{S}^-_{m_i\vec{\rho}}(a)\hat{S}^+_{m_i\vec{\rho}}(a) + \varepsilon_b \hat{S}^-_{m_i\vec{\rho}}(b)\hat{S}^+_{m_i\vec{\rho}}(b)]$$

$$+\frac{1}{2}\sum_{m_i,\vec{\rho}_a,\vec{\rho}_b} (\hat{S}^+_{m_i\vec{\rho}_a}(a)\hat{S}^+_{m_i\vec{\rho}_b}(b)+\text{H.c.})$$

$$+\frac{1}{4}\sum_{m_1,\vec{\rho}} \{\hat{S}^+_{m_1\vec{\rho}}(a)[\lambda_b\hat{S}^+_{m_2\vec{\rho}}(b)+\lambda'\hat{S}^+_{m_2-1\vec{\rho}}(b)]$$

$$+\hat{S}^+_{m_1\vec{\rho}}(b)[\lambda_b\hat{S}^+_{m_2\vec{\rho}}(a)+\lambda'\hat{S}^+_{m_2-1\vec{\rho}}(a)]+\text{H.c.}\}$$

$$+\frac{1}{4}\sum_{m_2,\vec{\rho}} \{\hat{S}^+_{m_2\vec{\rho}}(a)[\lambda_b\hat{S}^+_{m_1\vec{\rho}}(b)+\lambda'\hat{S}^+_{m_1+1\vec{\rho}}(b)]$$

$$+\hat{S}^+_{m_2\vec{\rho}}(b)[\lambda_b\hat{S}^+_{m_1\vec{\rho}}(a)+\lambda'\hat{S}^+_{m_1+1\vec{\rho}}(a)]+\text{H.c.}\}, \quad (3)$$

$$H_4 = -g\sum_{m_i,\vec{\rho}_a,\vec{\rho}_b} \hat{S}^-_{m_i\vec{\rho}_a}(a)\hat{S}^+_{m_i\vec{\rho}_a}(a)\hat{S}^-_{m_i\vec{\rho}_b}(b)\hat{S}^+_{m_i\vec{\rho}_b}(b)$$

$$-\frac{1}{2}\sum_{m_1,\vec{\rho},\alpha\neq\beta=(a,b)} \hat{S}^-_{m_1\vec{\rho}}(\alpha)\hat{S}^+_{m_1\vec{\rho}}(\alpha)$$

$$\times[\lambda_b\hat{S}^-_{m_2\vec{\rho}}(\beta)\hat{S}^+_{m_2\vec{\rho}}(\beta)+\lambda'\hat{S}^-_{m_2-1\vec{\rho}}(\beta)\hat{S}^+_{m_2-1\vec{\rho}}(\beta)]$$

$$-\frac{1}{2}\sum_{m_2,\vec{\rho},\alpha\neq\beta=(a,b)} \hat{S}^-_{m_2\vec{\rho}}(\alpha)\hat{S}^+_{m_2\vec{\rho}}(\alpha)$$

$$\times[\lambda_b\hat{S}^-_{m_1\vec{\rho}}(\beta)\hat{S}^+_{m_1\vec{\rho}}(\beta)+\lambda'\hat{S}^-_{m_1+1\vec{\rho}}(\beta)\hat{S}^+_{m_1+1\vec{\rho}}(\beta)],$$

$$(4)$$

where $\varepsilon_{a/b}=\frac{1}{2}\varepsilon\pm(\mu\mathcal{H}/J)$.

III. SPIN FORMALISM

Let us start by writing the equations of motion for the operators $S^{\pm}$. They will serve two purposes: (a) to evaluate spin GF's, and (b) to derive the average energy of the system. The structure of the Hamiltonian implies a system of four coupled equations of motion for the operators $\hat{S}^+_{m_1\vec{\rho}_a}(a)$, $\hat{S}^-_{m_1\vec{\rho}_b}(b)$, $\hat{S}^+_{m_2\vec{\rho}_a}(a)$, and $\hat{S}^-_{m_2\vec{\rho}_b}(b)$, and another appears for the set of the four adjoint operators. We shall quote only one equation, while the rest of the system can be constructed by analogy. For example,

$$i\hbar\frac{d\hat{S}^+_{m_1\vec{\rho}}(a)}{dt} = \varepsilon_a\hat{S}^+_{m_1\vec{\rho}}(a) + \frac{1}{2}\sum_{\vec{\rho}_b} \hat{S}^-_{m_1\vec{\rho}_b}(b)$$

$$+\frac{1}{2}\lambda_b\hat{S}^-_{m_2\vec{\rho}}(b)+\frac{\lambda'}{2}\hat{S}^-_{m_2-1\vec{\rho}}(b)$$

$$-g\sum_{\vec{\rho}_b} \hat{S}^+_{m_1\vec{\rho}}(a)\hat{S}^-_{m_1\vec{\rho}_b}(b)\hat{S}^+_{m_1\vec{\rho}_b}(b)$$

$$-\lambda_b \hat{S}^+_{m_1\vec\rho}(a)\hat{S}^-_{m_2\vec\rho}(b)\hat{S}^+_{m_2\vec\rho}(b)$$

$$-\lambda'\hat{S}^+_{m_1\vec\rho}(a)\hat{S}^-_{m_2-1\vec\rho}(b)\hat{S}^+_{m_2-1\vec\rho}(b). \quad (5)$$

If we generalize the procedure proposed by Tyablikov[10] for a simple Heisenberg system, we arrive at the basic result

$$\frac{H}{J}=H_o+\frac{1}{2}H_2+\frac{1}{4}\sum_{m_i}\sum_{\vec\rho}\sum_{\alpha=a,b}\left[\hat{S}^-_{m_i,\vec\rho_\alpha}(\alpha)\frac{d\hat{S}^+_{m_i,\vec\rho_\alpha}(\alpha)}{dt}\right.$$

$$\left.-\frac{d\hat{S}^-_{m_i,\vec\rho_\alpha}(\alpha)}{dt}\hat{S}^+_{m_i,\vec\rho_\alpha}(\alpha)\right]. \quad (6)$$

It is important to emphasize that this is a completely exact result with no approximation involved, and it will allow us to determine the energy of the system ($\langle H\rangle$), once we know the correlation functions.

For this purpose we shall evaluate the Tyablikov's Green's functions,[10] using the equation of motion (5) and applying the RPA. The basic idea of the approximation is to neglect the correlation of the longitudinal spin components $\hat{S}^z$ with the transversal ones $\hat{S}^\pm$ at different lattice sites, so that

$$\langle\langle\hat{S}^z_i\hat{S}^\pm_j|\hat{B}\rangle\rangle\approx\langle\hat{S}^z_i\rangle\langle\langle\hat{S}^\pm_j|\hat{B}\rangle\rangle=\sigma\langle\langle\hat{S}^\pm_j|\hat{B}\rangle\rangle,$$

$$\langle S^z_i\rangle=\sigma \quad \text{(due to the translational invariance) .}$$

We arrive at two sets of four equation for the GF in the $(\vec{k},E)$ representation. The complete notation used will be $G^{\mu\nu}_{\alpha_i\beta_j}(\vec{k},E)\equiv\ll\hat{S}^\mu_{m_i\vec\rho}(\alpha)|\hat{S}^\nu_{m_j\vec\rho}(\beta)\gg_{\vec{k},E}$ ($\mu,\nu=+,-$, $\alpha,\beta=a,b$; $i,j=1,2$).

We shall quote only one set of four equations in this approximation:

$$(E-\tilde\varepsilon_a)G^{+\nu}_{a_1\beta_j}(\vec{k},E)-\sigma\gamma(\vec{k})G^{-\nu}_{b_1\beta_j}(\vec{k},E)+0$$

$$+\sigma\gamma_z G^{-\nu}_{b_2\beta_j}(\vec{k},E)=\frac{i}{2\pi}C^{+\nu}_{a_1\beta_j},$$

$$\sigma\gamma(\vec{k})G^{+\nu}_{a_1\beta_j}(\vec{k},E)+(E+\tilde\varepsilon_b)G^{-\nu}_{b_1\beta_j}(\vec{k},E)+\sigma\gamma_z G^{+\nu}_{a_2\beta_j}(\vec{k},E)$$

$$+0=\frac{i}{2\pi}C^{-\nu}_{b_1\beta_j},$$

$$0+\sigma\gamma_z^* G^{-\nu}_{b_1\beta_j}(\vec{k},E)+(E-\tilde\varepsilon_a)G^{+\nu}_{a_2\beta_j}(\vec{k},E)$$

$$-\sigma\gamma(\vec{k})G^{-\nu}_{b_2\beta_j}(\vec{k},E)=\frac{i}{2\pi}C^{+\nu}_{a_2\beta_j},$$

$$\sigma\gamma_z^* G^{+\nu}_{a_1\beta_j}(\vec{k},E)+0+\sigma\gamma(\vec{k})G^{+\nu}_{a_2\beta_j}(\vec{k},E)$$

$$+(E+\tilde\varepsilon_b)G^{-\nu}_{b_2\beta_j}(\vec{k},E)=\frac{i}{2\pi}C^{-\nu}_{b_2\beta_j}, \quad (7)$$

where

$$C^{\mu\nu}_{\alpha_i\beta_j}=\langle[\hat{S}^\mu_{m_i,\vec\rho_\alpha}(\alpha),\hat{S}^\nu_{m_j,\vec\rho_\beta}(\beta)]\rangle,$$

$$\gamma(\vec{k})=2(\cos k_x a+\cos k_y a),$$

$$\gamma_z=\lambda_b e^{ik_z d_1}+\lambda' e^{-ik_z d_2}, \quad \tilde\varepsilon_{a/b}=\tilde\varepsilon\pm\frac{\mu\mathcal{H}}{J}, \quad \tilde\varepsilon=\sigma\varepsilon.$$

There exists another set of four equations, following from the adjoint equations of motion.

Equations (7) have a determinant

$$\Delta_1(E)=\left[\left(E-\frac{\mu\mathcal{H}}{J}\right)^2-\tilde\varepsilon^2\right]^2+2\sigma^2\left[\left(E-\frac{\mu\mathcal{H}}{J}\right)^2-\tilde\varepsilon^2\right]$$

$$\times[\gamma^2(\vec{k})+|\gamma_z|^2]+\sigma^4[\gamma^2(\vec{k})-|\gamma_z|^2]^2, \quad (8)$$

while the determinant $\Delta_2(E)$ of the adjoint system satisfies

$$\Delta_2(E)=\Delta_1(-E). \quad (9)$$

We are going to study only the case when the external field is absent. In this case, there appear only two, double degenerate energy branches:

$$E_{1/2}=\sigma\sqrt{\varepsilon^2-[\gamma(\vec{k})\pm|\gamma_z|]^2}. \quad (10)$$

A long, but straightforward, calculation, which exploits the symmetry of the system, shows that for our purposes we need to know the Fourier transforms [the so-called spectral densities $I^{\mu\nu}_{\alpha_i\beta_j}(\vec{k},E)$] of only three different correlation functions:

$$I^{-+}_{\alpha_i\alpha_i}(\vec{k},E)=\frac{\sigma}{2}\left\{\left(1+\frac{\tilde\varepsilon}{E_1(\vec{k})}\right)\delta[E-E_1(\vec{k})]\right.$$

$$+\left(1-\frac{\tilde\varepsilon}{E_1(\vec{k})}\right)\delta[E+E_1(\vec{k})]$$

$$+\left(1+\frac{\tilde\varepsilon}{E_2(\vec{k})}\right)\delta[E-E_2(\vec{k})]$$

$$\left.+\left(1-\frac{\tilde\varepsilon}{E_2(\vec{k})}\right)\delta[E+E_2(\vec{k})]\right\}n(E),$$

$$\alpha=a,b, \quad i=1,2, \quad (11)$$

$$I^{++}_{\alpha_i\beta_i}(\vec{k},E)=I^{--}_{\alpha_i\beta_i}(\vec{k},E)$$

$$=-\frac{\sigma^2}{2}\left\{\frac{\gamma(\vec{k})+|\gamma_z|}{E_1(\vec{k})}\{\delta[E-E_1(\vec{k})]\right.$$

$$-\delta[E+E_1(\vec{k})]\}+\frac{\gamma(\vec{k})-|\gamma_z|}{E_2(\vec{k})}\{\delta[E-E_2(\vec{k})]$$

$$\left.-\delta[E+E_2(\vec{k})]\}\right\}n(E),$$

$$\alpha\neq\beta=a,b, \quad i=1,2, \quad (12)$$

$$I^{++}_{\alpha_i\beta_j}(\vec{k},E)=[I^{--}_{\alpha_i\beta_i}(\vec{k},E)]^*$$

$$=-\frac{\sigma^2\gamma_z}{2|\gamma_z|}\left\{\frac{\gamma(\vec{k})+|\gamma_z|}{E_1(\vec{k})}\{\delta[E-E_1(\vec{k})]\right.$$

$$-\delta[E+E_1(\vec{k})]\}-\frac{\gamma(\vec{k})-|\gamma_z|}{E_2(\vec{k})}\{\delta[E-E_2(\vec{k})]$$

$$\left.-\delta[E+E_2(\vec{k})]\}\right\}n(E),$$

$$\alpha\neq\beta=a,b,\quad i\neq j=1,2 \tag{13}$$

where $n(E)=1/(e^{E/\theta}-1)$ and $\theta=k_BT/J$. Knowing this, we are able to evaluate the energy of the system [by averaging Eq. (6)] and magnetization:

$$\frac{\langle H\rangle}{J}=H_o+\sum_{\vec{k}}\Delta E_o(\vec{k},\theta)+\sum_{\vec{k}}E(\vec{k},\theta), \tag{14}$$

$$\Delta E_o(\vec{k},\theta)=-\sigma(\theta)[\varepsilon-E_1^B(\vec{k})-E_2^B(\vec{k})$$

$$+2\tilde{\varepsilon}-E_1(\vec{k})-E_2(\vec{k})], \tag{15}$$

$$E(\vec{k},\theta)=2\sigma(\theta)\{[E_1^B(\vec{k})+E_1(\vec{k})]n[E_1(\vec{k})]$$

$$+[E_2^B(\vec{k})+E_2(\vec{k})]n[E_2(\vec{k})]\}, \tag{16}$$

$$\sigma_r(\theta)=\frac{1}{S}\sigma(\theta)=\sigma_r(0)\frac{1}{1+\sigma_r(0)F(\theta)}, \tag{17}$$

$$\sigma_r(0)=\left[\frac{\varepsilon}{2N}\sum_{\vec{k}}\left(\frac{1}{\sqrt{\varepsilon^2-[\gamma(\vec{k})+|\gamma_z|]^2}}\right.\right.$$

$$\left.\left.+\frac{1}{\sqrt{\varepsilon^2-[\gamma(\vec{k})-|\gamma_z|]^2}}\right)\right]^{-1}, \tag{18}$$

$$F(\theta)=\frac{\tilde{\varepsilon}}{N}\sum_{\vec{k}}\left[\frac{1}{E_1(\vec{k})}n[E_1(\vec{k})]+\frac{1}{E_2(\vec{k})}n[E_2(\vec{k})]\right], \tag{19}$$

where $E_{1/2}^B(\vec{k})=\frac{1}{2}\sqrt{\varepsilon^2-[\gamma(\vec{k})\pm|\gamma_z|]^2}$ are the energies in Bloch's approximation and $N=N_o/2$ is the number of magnetic elementary cells. These expressions will be the basis of our further calculations.

IV. BOSON TREATMENT

An alternative approach is to introduce Bose operators. There has been plenty of work in this field, but in our opinion, one should review the work completely. Introducing Bose operators in the Bloch approximation, we can write the following boson Hamiltonian:

$$\frac{H^B}{J}=H_o+\sum_{\vec{k}}H_{\vec{k}}, \tag{20}$$

$$H_{\vec{k}}=\sum_{i=1}^{2}\left[\varepsilon_a\hat{a}_i^+(\vec{k})\hat{a}_i(\vec{k})+\varepsilon_b\hat{b}_i^+(\vec{k})\hat{b}_i(\vec{k})\right.$$

$$+\frac{\gamma(\vec{k})}{2}[\hat{a}_i^+(\vec{k})\hat{b}_i^+(-\vec{k})+\text{H.c.}]\Bigg]$$

$$+\frac{1}{2}\{\gamma_z^*[\hat{a}_1(\vec{k})\hat{b}_2^+(-\vec{k})+\hat{b}_1^+(\vec{k})\hat{a}_2(-\vec{k})]+\text{H.c.}\}. \tag{21}$$

Here a denotes spins-up, b denotes spins-down, and indices 1 and 2 indicate the corresponding planes. This is a quadratic Hamiltonian, which can be diagonalized at least in two ways: one can use a typical Bogolyubov-Tyablikov "uv" transformation or calculate boson Green's functions. Both methods obviously lead to the same results, which are completely equivalent to the ones obtained using spin GF's. In fact, the excitation energies $E_{1/2}^B$ and the energy of the system $\langle H\rangle^B$ are obtained from Eqs. (10) and (14) by direct substitution $\sigma\to S=\frac{1}{2}$.

$$\frac{\langle H\rangle^B}{J}=H_o+\sum_{\vec{k}}\Delta E_o^B(\vec{k})+\sum_{\vec{k}}E^B(\vec{k},\theta), \tag{22}$$

$$\Delta E_o^B(\vec{k})=-[\varepsilon-E_1^B(\vec{k})-E_2^B(\vec{k})], \tag{23}$$

$$E^B(\vec{k},\theta)=2E_1^B(\vec{k})n[E_1^B(\vec{k})]+2E_2^B(\vec{k})n[E_2^B(\vec{k})]. \tag{24}$$

However, the expression for magnetization is not that simple, since here one does not apply any self-consistent approximation (this is the result in lower-order approximation). The sublattice magnetization in this case is evaluated as

$$\sigma^B=S-\langle\hat{a}_i^+\hat{a}_i\rangle=\sigma_o^B-\Delta\sigma^B(T), \tag{25}$$

$$\sigma_o^B=1-\frac{\varepsilon}{4N}\sum_{\vec{k}}\left(\frac{1}{E_1^B(\vec{k})}+\frac{1}{E_2^B(\vec{k})}\right), \tag{26}$$

$$\Delta\sigma^B(\theta)=\frac{\varepsilon}{2N}\sum_{\vec{k}}\left(\frac{n[E_1^B(\vec{k})]}{E_1^B(\vec{k})}+\frac{n[E_2^B(\vec{k})]}{E_2^B(\vec{k})}\right). \tag{27}$$

V. DISCUSSION OF THE RESULTS

Let us start our discussion with the comparison of the results of the spin (the RPA) and boson approximations for the ground state ($T=0$ K). We compare $\sigma_r(0)$, which is given by Eq. (18) for a spin formalism and Eq. (26) for a boson formalism. The results are summarized in Fig. 2 in terms of λ_b (intracell coupling). Probably unrealistically high values of λ_b are included just for the sake of comparison with the results of Refs. 4 and 5.

First of all, we must stress that the numerical values of the magnetization for a corresponding bilayer [two-dimensional (2D)] and superlattice (3D) differ only at third significant figure, so they cannot be distinguished at the plot. For this reason, the plot shows only two curves—one for the spin RPA treatment and the other for bosons.
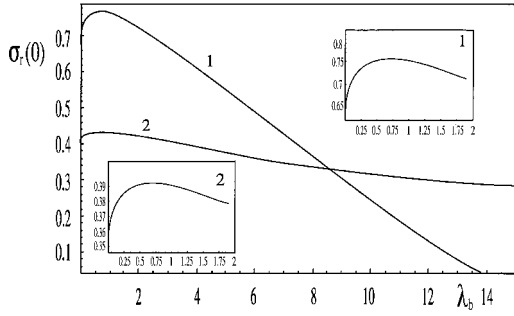
FIG. 2. Ground-state relative magnetization: (1) boson treatment and (2) spin RPA treatment.

Let us concentrate on the behavior for small values of λ_b, which is similar in both cases and represented in insets. The increase of λ_b leads to an increase of the antiferromagnetic ordering, until it reaches a saturation value for $\lambda_b \approx 1$. Then the magnetization begins to decrease, and this is where we encounter two essentially different types of behavior.

It can be seen that within the boson treatment, the long-range order (LRO) at $T=0$ always vanishes for strong intra-cell coupling. (This agrees, in a certain degree with the results of Refs. 4 and 5, where the LRO vanishes for comparatively lower values of λ_b.) On the other hand, within the spin treatment, the LRO never vanishes, but asymptotically tends to zero for very high values of λ_b. This implies that, according to the boson treatment, quantum fluctuations for $\lambda_b \geq 10$ can destroy the in-plane LRO, while, according to the spin treatment, this practically never occurs. The formal reason for such a disagreement lies in the fact that the boson expression represents only the first term in the expansion of the spin result. Matsuda and Hida[4] tried to propose an explanation based on the creation of singlet states consisting of spins belonging to neighboring planes, relating this to the spin-fluctuation mechanism of pair formation in high-T_c superconductors.[11,12] Our results, which do not support singlet formation, do not exclude this mechanism in the superconducting phase, since they are valid only for the AF phase of high-T_c cuprates [$x<0.41$ for (1:2:3)]. As we have mentioned, the curves for two and three dimensions practically coincide, implying that the in-plane quantum fluctuations are dominant.

In the other limiting case, we shall concentrate on the phase transition, where we shall discuss only the results of the RPA treatment, since the boson approximation is not valid in this temperature range, as shown by Irkhin et al.[13] The expression for θ_N within the RPA can be obtained from Eq. (17) in the limit $\sigma \rightarrow 0$:

$$\theta_N = \frac{J}{C_1 + C_2}, \quad C_{1/2} = \frac{2\varepsilon}{N} \sum_{\vec{k}} \frac{1}{\varepsilon^2 - [\gamma(\vec{k}) \pm |\gamma_z|]^2}. \tag{28}$$

We shall first analyze this expression numerically for a set of parameters relevant for high-T_c cuprates [(1:2:3)] frequently stated in the literature.[7,8,14,15,16] It turns out that the essential parameter is the in-plane anisotropy $g = 1 + \eta$. As long as $\eta \neq 0$, for both two- and three-dimensional cases, for J

≈ 100 meV and $\lambda_b = 5 \times 10^{-2}$ we obtain values of $\theta_N \approx 430$ K close to experimental values $\theta_N \approx 415$ K.[7,14] For the three-dimensional case, one can also look at the isotropic system ($g=1$), while keeping the parameters λ_b and λ' finite. The values of θ_N are then highly underestimated. The results are summarized in Table I.

This implies that, contrary to common statements, it is not three dimensionality which is essential for the antiferromagnetic ordering in this system, but in-plane spin anisotropy ($\eta \neq 0$). This is in agreement with the opinion shared by some authors[9,11,12] that two-dimensional spin fluctuations also play an essential role in the superconductive phase. This is also supported by the fact that the AF phase transition, in (1:2:3) for $x=0$, at a temperature of 415 ± 5 K is of second order, with a critical exponent for the staggered magnetization $\beta = 0.25 \pm 0.03$, which is characteristic of a 2D AF system.[7]

It might seem strange that the small finite value of in-plane spin anisotropy (η) influences the value of T_N so drastically. In fact, we can explain this effect starting from the 2D case, where this is rather transparent. Looking back at expression (28) we see that integrals $C_{1/2}$ strongly depend on the in-plane anisotropy. When $g=1$, this term exactly cancels the contribution of $\gamma(\vec{k})$ for $\vec{k} \rightarrow 0$. Thus, it is the part with η that preserves the convergence of the integral (similar to the integral appearing in the proof of Mermin-Wagner theorem[17,18]). The same reasoning can be applied to the 3D case. Here the convergence is preserved for $g=1$, yet the influence of η still remains.

At this point, we wish to demonstrate a problem that occurred frequently in the literature, concerning an important technical detail. In a two-dimensional case, the integration over the first Brillouin zone (IBZ) is usually taken in the limits ($\pm \pi/a$) for k_x and k_y, both for ferromagnet and antiferromagnet with simple quadratic lattice. However, the correct boundaries are dictated by the shape of the IBZ. For an antiferromagnet, each quadrant of the IBZ is a triangle in 2D momentum space, i.e., the boundaries in $k_x, k_y \geq 0$ range are $[0 \leq k_x \leq \pi/a, 0 \leq k_y \leq (\pi/a) - k_x]$. So, not only is the AF IBZ twice smaller, but one also must take into account the variable boundaries. A typical example of this mistreatment is the work by Singh et al.[19] However, we must comment upon this work in more detail. At first sight, the authors reached an extremely good agreement between theory and experimental results, in particular for the transition temperature [for the system (1:2:3)]. We previously showed that no such agreement could be achieved in the absence of spin anisotropy (for $g=1$; see Table I). The agreement is in fact the consequence of the underestimated volume of unit cell appearing in expressions (5) and (6) in Ref. 19, $v_o = a^2 c$ instead of $v_o = 4a^2 c$. This is combined with incorrect integration boundaries, so the proper value of the integral $I(r)$ is about twice as large, and the transition temperature following from their estimates is in fact twice as small.

We now turn our attention to the intermediate region of low, but finite temperatures, and compare the boson and spin expressions for the energy and magnetization. General expressions are summarized in Eqs. (14) and (17) for spins and

TABLE I. Transition temperature dependence on system parameters.

				η				
	10^{-4}					0		
λ_b	λ'	J (meV)	T_N (K)	λ_b	λ'	J (meV)	T_N (K)	
10^{-2}	10^{-6}	80	313.004	10^{-2}	10^{-7}	80	210.964	
10^{-2}	10^{-5}	80	313.383	10^{-2}	10^{-5}	80	253.143	
5×10^{-2}	10^{-5}	80	343.595	5×10^{-2}	10^{-5}	80	272.705	3D
10^{-2}	10^{-6}	100	391.255	10^{-2}	10^{-7}	100	263.70	
10^{-2}	10^{-5}	100	391.728	10^{-2}	10^{-5}	100	316.428	
5×10^{-2}	10^{-5}	100	429.494	5×10^{-2}	10^{-5}	100	340.88	
10^{-2}	10^{-6}	120	469.506	10^{-2}	10^{-7}	120	316.446	
10^{-2}	10^{-5}	120	470.074	10^{-2}	10^{-5}	120	379.714	
5×10^{-2}	10^{-5}	120	515.392	5×10^{-2}	10^{-5}	120	409.057	
10^{-2}	0	80	312.961					
5×10^{-2}	0	80	343.096					
10^{-2}	0	100	391.20					2D
5×10^{-2}	0	100	428.87					
10^{-2}	0	120	469.442					
5×10^{-2}	0	120	514.644					

in Eqs. (22) and (25) for bosons. Here we also comment on some of the results that occurred in the literature.

We have already demonstrated the essential role of magnetic anisotropy. However, before going into any details, let us comment upon different manifestations of anisotropy. Our approach includes two types of anisotropy: one is the anisotropy in spin space (simply put, spin anisotropy) and here it appears as the in-plane anisotropy of xxz type. On the other hand there also appears a so-called "spatial anisotropy"[20] since interlayer and intralayer exchange integrals differ. The distinction between the two types of anisotropy is essential: spatial anisotropy does not influence the existence of the acoustic branch [the Goldstone mode is $\lim_{k\to 0}E(k)=0$], and the energy gap in this branch appears only as a consequence of the spin anisotropy. However, Pratap et al.[6] introduced spatial anisotropy by adding a term depending on the dispersion along the z axis, which can be strictly introduced only for an infinitely extended superlattice in the z direction. It is important to stress that with this kind of interaction they obtained a gap for the acoustic branch in the single bilayer, which is definitely an incorrect result.

Let us first discuss the single bilayer ($\lambda'=0,k_z=0$). The spin-wave dispersion law in the boson case becomes

$$E^B_{1/2}(\vec{k})=\frac{1}{2}\sqrt{(4g+\lambda_b)^2-[\gamma(\vec{k})\pm\lambda_b]^2},\qquad(29)$$

which differs from expression (7) in Ref. 6 only by $g\neq 1$. Due to the spin anisotropy, both branches possess a gap in the long-wavelength limit:

$$\Delta^2_{1/2}=4(g\mp 1)[2(g\pm 1)+\lambda_b].\qquad(30)$$

In the lowest temperature range, i.e., $0<\theta<\Delta_1$, the expression for the magnetization is

$$\Delta\sigma^B(\theta)=-\frac{4g+\lambda_b}{\pi(4+\lambda_b)}\theta\ln(1-e^{-\Delta_1/\theta})+O(e^{-\Delta_2/\theta}).\qquad(31)$$

One should note that Pratap et al.,[6] in the lowest range, obtained (due to an erroneous integration over k_z) a quadratic temperature dependence, characteristic of a three-dimensional antiferromagnet (as will be shown later), while in the next temperature range, the behavior is formally similar to the one that we produce $\theta\ln\theta$; yet the difference is in the origin of the gap. In the next temperature range $\Delta_1<\theta<\Delta_2$ the magnetization has the form

$$\Delta\sigma^B(\theta)=\frac{4g+\lambda_b}{\pi(4+\lambda_b)}\theta\ln\frac{\theta}{\Delta_1}+O(e^{-\Delta_2/\theta}),\qquad(32)$$

while for $\Delta_2<\theta<\theta_N$ we obtain,

$$\Delta\sigma^B(\theta)=\frac{4g+\lambda_b}{\pi(4+\lambda_b)}\theta\ln\frac{\theta}{\Delta_1}+\frac{4g+\lambda_b}{\pi(4-\lambda_b)}\theta\ln\frac{\theta}{\Delta_2}. \quad (33)$$

We shall now analyze the energy of the system for $g=1$ only. This particular case is characterized by the fact that one of the branches (E_1^B) is now gapless (Goldstone mode). One has

$$\langle H\rangle=N\frac{16J\zeta(3)}{\pi(4+\lambda_b)}\theta^3+N\frac{32J\lambda_b}{\pi(4-\lambda_b)}\theta\exp\left(-\frac{2\sqrt{\lambda_b}}{\theta}\right), \quad (34)$$

where $\zeta(3)$ is Rieman's function. Finally let us write down an expression for $C_v=d\langle H\rangle/dT$,

$$C_v=N\frac{48k_B\zeta(3)}{\pi(4+\lambda_b)}\theta^2+NO(e^{-2\sqrt{\lambda_b}/\theta}), \quad (35)$$

where the second term decays exponentially at low temperatures, and this can be neglected. These results obviously differ from the corresponding ones Eqs. (30) and (31) in Ref. 6]. We now proceed to the 3D case, i.e., to a superlattice extended infinitely in the z direction. The excitation energies are given by

$$E_{1/2}^B(\vec{k})=\frac{1}{2}\sqrt{(4g+\lambda_b+\lambda')^2-\{\gamma(\vec{k})\pm[(\lambda_b+\lambda')^2-2\lambda_b\lambda'(1-\cos k_z c_o)]^{1/2}\}^2}, \quad (36)$$

where $c_o=d_1+d_2$ is the lattice constant in the z direction. It is important to note that for a superlattice formed of bilayers, the intralayer (λ_b) and interlayer (λ') interaction terms enter into all expressions in an absolutely symmetrical manner. Further analysis will be based on the isotropic case ($g=1$), where E_1^B is the Goldstone mode while E_2^B possesses a gap. In the lowest temperature range, for $\theta\leq\min[\lambda_b,\lambda']$, expression (27) gives

$$\Delta\sigma^B(\theta)=\frac{1}{6}\sqrt{\frac{\lambda_b+\lambda'}{\varepsilon\lambda_b\lambda'}}\theta^2+O(e^{-\Delta_2/\theta}),\quad \Delta_2=2\sqrt{\lambda_b+\lambda'}. \quad (37)$$

The quadratic temperature dependence of magnetization is a typical AF 3D behavior. Also note that λ_b and λ' enter the expression completely symmetrically. For $\min[\lambda_b,\lambda']\leq\theta\ll\theta_N$ there arises a crossover from three- to two-dimensional behavior:

$$\Delta\sigma^B(\theta)\approx\frac{1}{2\pi}\theta\ln\left[\theta\left(\frac{4(\lambda_b+\lambda')}{\varepsilon\lambda_b\lambda'}\right)^{1/2}\right]. \quad (38)$$

The above example indicates that although there exists a formal symmetry between couplings, when their order of magnitude differs substantially there obviously appears an asymmetry which governs the behavior. For example, in (1:2:3) structures, where $\lambda_b\gg\lambda'(\lambda'\approx10^{-2}\lambda_b)$, we have

$$\Delta\sigma^B(\theta)\approx\frac{1}{2\pi}\theta\ln\left[2\theta\frac{1}{(\varepsilon\lambda')^{1/2}}\right], \quad (39)$$

so the weaker interlayer coupling λ' determines the 2D behavior.

Let us now turn our attention to the results of a RPA treatment. In the presence of in-plane anisotropy ($g\neq1$), both excitation energy branches possess a gap, so that the basic temperature dependence of the magnetization at low temperatures is exponential: $\approx\exp(-\Delta_{1/2}/\theta)$. This case will

not be analyzed in detail. In the isotropic regime ($g=1$), in the lowest temperature range, the expression for $\Delta\sigma(T)$ is equal to

$$\Delta\sigma(\theta)=\frac{1}{3}\sqrt{\frac{\lambda_b+\lambda'}{\varepsilon\lambda_b\lambda'}}\theta^2+O(e^{-\sigma_r(0)\Delta_2/\theta}), \quad (40)$$

which differs from Eq. (37) only by a factor of 2. This difference follows from the different procedure of evaluating the magnetization, since the spin magnetization is determined in a self-consistent way. In the range $\min[\lambda_b,\lambda']\leq\theta\ll\theta_N$, there occurs a crossover, leading to

$$\Delta\sigma_r(\theta)=\frac{\sigma_r(0)}{\pi}\theta\ln\left[\theta\sigma_r(0)\left(\frac{4(\lambda_b+\lambda')}{\varepsilon\lambda_b\lambda'}\right)^{1/2}\right]. \quad (41)$$

This differs from the boson expression [Eq. (38)], not only by a numerical factor (2), but also by the presence of $\sigma_r(0)$ which is again the consequence of self-consistent approximation.

The expressions for the energy of the system will be essentially different due to the presence of a temperature-dependent magnetization in the expressions for the energy [Eqs. (15) and (16)]. Even the correction of the ground-state energy ΔE_o does not vanish for $T\neq0$, but changes in a similar manner as it does for the magnetization. In fact, it is this correction that dictates the low-temperature behavior of the energy, it is a quadratic function of the temperature, so that $C_v\approx\theta$. This behavior is essentially different from the behavior of the energy of a boson system ($\langle H\rangle\sim\theta^4,C_v\sim\theta^3$), and is a consequence of the fact that a more correct treatment of spin statistics (in terms of RPA decoupling) reflects the fermionic nature of spin ($S=\frac{1}{2}$) operators acting at the same site.

VI. CONCLUSION

The aim of this study was to review the similarities and differences in the results obtained by treating a magnetic AF

bilayer in boson and RPA-spin approximations, and at the same time indicate to various misinterpretations occurring in some particular applications. One of the basic achievements of our study is the application to a spin system occurring in (1:2:3) structures, where we have shown that, in the antiferromagnetic phase ($x < 0.4$), the in-plane anisotropy and two-dimensional quantum spin fluctuations both play an important role, much more significant than previously assumed. However, we stress that our results cannot be simply extrapolated to the superconductive phase, although they probably indicate the importance of these fluctuations. Finally, we must stress once more that the Tyablikov (or RPA) approximation for the Heisenberg model, although very simple, conforms to the Mermin-Wagner theorem in all relevant limiting cases.

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