Magnetic dynamics of bilayer cuprate superconductors

Amit Pratap,* Govind, and R. S. Tripathi
Department of Physics, G.B. Pant University of Agriculture and Technology, Pantnagar 263 145, India
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In the present paper, we use the Heisenberg antiferromagnetic model within linear spin-wave theory to study the magnetic dynamics of bilayer antiferromagnets such as $YBa_2Cu_3O_{6+x}$. The Zubarev's double-time Green's-function formalism has been employed in order to evaluate the expressions for spin-wave dispersion, sublattice magnetization, and specific heat. It has been shown that in these systems, the intrabilayer coupling leads towards a ''spin gap.'' The optical mode is found to contribute significantly to the sublattice magnetization only in the high-temperature regime. In the low-temperature regime, the contribution from the acoustic mode is sensitive to the anisotropy term. We observe that the dipolar anisotropy does not produce the three-dimensional (3D) Néel ordering, while the exchange anisotropy is essential to keep 3D Néel ordering in these systems. Further, we observe a crossover from 3D to quasi-2D behavior at a certain temperature. The presence of the optic mode does not seem to alter the quasi-2D behavior of these systems in the higher temperature regime. The specific heat is also found to be dependent on the ratio of intrabilayer to in-plane coupling strength (r). These results are compared with the existing results. [S0163-1829(99)01233-3]

I. INTRODUCTION

It is well established now that in their normal state, compounds such as La_2CuO_4 and $YBa_2Cu_3O_{6+x}$ are layered antiferromagnets and highly anisotropic. It has been observed that upon doping there is a structural transition from the insulating antiferromagnetic (AFM) to the orthorhombic superconducting phase and the magnetic properties become sensitive to the dopant concentration.[1] In $YBa_2Cu_3O_{6+x}$, the Néel temperature (T_N) decreases on increasing the oxygen concentration x and for $x>0.41$, the magnetization vanishes. The magnetic dynamics of quasi-two-dimensional (2D) systems like La_2CuO_4 has widely been studied by various workers. These studies mainly deal with the anisotropic Heisenberg model within the random-phase approximation (RPA),[2–4] linear,[5] nonlinear,[6] and modified spin-wave theory,[7,8] Callen decoupling scheme,[9] and the Schwinger boson approach,[10,11] and are well documented in the review articles by Micnas *et al.*[12] and Monouskis.[13] It has been shown[2,6,14,15] that the exchange coupling strength (J^z) along the z direction is essential to keep the 3D Néel ordering in these systems. In fact, for $K_BT<2J_\parallel\phi_0$ ($\phi_0=J^z/J_\parallel$), the magnetization varies as T^2 while in the limit $K_BT>2J_\parallel\phi_0$, it follows a $T\ln T$ behavior. At $K_BT=2J_\parallel\phi_0$, there is a crossover from 3D to quasi-2D behavior. However, Kopietz[11] has discussed that near T_N, $T\ln T$ behavior breaks down and magnetization varies as $(1-T/T_N)^{1/2}$. Recently, we have studied the role of J^z on the magnetic dynamics of these systems.[6] Within the nonlinear spin-wave theory, we have shown that various properties such as sublattice magnetization, specific heat, parallel and perpendicular susceptibilities, and the thermal expansion are sensitive to the ratio of two coupling strengths as well as to the magnon-magnon interaction.

On the other hand, the experimental studies on $YBa_2Cu_3O_{6+x}$ have confirmed that the system possesses two CuO_2 planes within the single unit cell. The Cu spins of these two layers are strongly coupled antiferromagnetically.[16–19] Most of the above-mentioned works do not incorporate this feature in the magnetic dynamics of $YBa_2Cu_3O_{6+x}$.

By considering the AFM coupling between the layers ($J_\perp$), it has been shown theoretically[16] that the spin-wave spectrum consists of two branches (i) acoustic and (ii) optic. In fact, this leads to a spin gap with minimum energy $2\sqrt{J_\perp J_\parallel}$. The neutron-scattering experiment conducted by Reznik *et al.*[20] has confirmed the presence of the optic mode with minimum energy 65–70 meV in $YBa_2Cu_3O_{6.2}$. Further, the Heisenberg model has itself proved to be an appropriate starting point to investigate the normal-state magnetic properties of these systems. Recently, Millis *et al.*[21] using the Schwinger boson method, calculated the dynamical susceptibility of these bilayer systems. These authors have shown that the intrabilayer coupling does provide a better understanding of the 41 meV peak observed in the neutron-scattering experiments[22] on superconducting $YBa_2Cu_3O_{6+x}$. Du *et al.*[23] have calculated the sublattice magnetization and Néel temperature of bilayer systems using the Green's-function technique within RPA (random-phase approximation). These authors have shown that in the absence of intrabilayer or interbilayer exchange couplings the system does not show the long-range magnetic order and the Néel temperature becomes zero.

In the light of the above facts, it seems plausible to investigate the magnetic dynamics of these bilayer systems. For this purpose, in Sec. II, we consider the Heisenberg AFM model Hamiltonian with in-plane coupling ($J_\parallel$) and the intrabilayer coupling ($J_\perp$). We use Holstein-Primakoff transformation within the linear spin-wave approximation to convert the model Hamiltonian into the boson operator form. The double-time Green's-function formalism has been employed to obtain the expressions for spin-wave dispersion and various correlation functions. In Sec. III, we focus our attention on calculating the contribution from acoustic and optic modes to the sublattice magnetization. It is shown that corresponding to the optic mode, no anisotropy is required

while for the acoustic mode, the magnetization is sustained only in the presence of anisotropy from whatever source. We further consider the examples of two such anisotropy terms (i) the anisotropy in exchange coupling strengths and (ii) the anisotropy due to dipolar interactions. In the possible temperature regions, we discuss the different roles of these anisotropies on the magnetic dynamics of these bilayer systems. Finally, we compare our results with the existing ones and summarize them in Secs. IV and V.

II. THEORETICAL FORMULATION

For a bilayer system, the Heisenberg Hamiltonian may be written as

$$H=J_{\parallel}\sum_{ij} S_i^{\alpha}\cdot S_j^{\alpha}+J_{\perp}\sum_{i} S_i^1\cdot S_i^2, \tag{1}$$

where $\alpha=1,2$ are the layer indices, i,j denote the lattice sites with j being the nearest neighbor of i, $J_{\parallel}$ and $J_{\perp}$ are, respectively, the AFM coupling constants within the plane and between the planes of bilayer.

Besides the interactions considered in Hamiltonian (1), in a real system there may also be an interaction between the two bilayers of different unit cells and that with the Cu-O chains. However, in the present paper, we confine ourselves only to the bilayers within the unit cell and neglect the other interactions.

Next, we consider the four sublattice models and introduce the following Holstein-Primakoff transformations:

$$S_{ai1}^{-}=(2S)^{1/2}[b_{ai1}-(2S)^{-1}b_{ai1}^{+}b_{ai1}b_{ai1}],$$

$$S_{ai1}^{+}=(2S)^{1/2}b_{ai1}^{+},$$

$$S_{ai1}^{z}=-S+b_{ai1}^{+}b_{ai1},$$

$$S_{bj1}^{-}=(2S)^{1/2}[b_{bj1}-(2S)^{-1}b_{bj1}b_{bj1}^{+}b_{bj1}],$$

$$S_{bj1}^{+}=(2S)^{1/2}b_{bj1}^{+},$$

$$S_{bj1}^{z}=S-b_{bj1}^{+}b_{bj1},$$

$$S_{ci2}^{-}=(2S)^{1/2}[b_{ci2}-(2S)^{-1}b_{ci2}b_{ci2}^{+}b_{ci2}],$$

$$S_{ci2}^{+}=(2S)^{1/2}b_{ci2}^{+},$$

$$S_{ci2}^{z}=S-b_{ci2}^{+}b_{ci2},$$

$$S_{dj2}^{-}=(2s)^{1/2}[b_{dj2}-(2S)^{-1}b_{dj2}^{+}b_{dj2}b_{dj2}],$$

$$S_{dj2}^{+}=(2S)^{1/2}b_{dj2}^{+},$$

$$S_{dj2}^{z}=-S+b_{dj2}^{+}b_{dj2}.$$

The Fourier transform b's are given by

$$b_{ai1}=(2/N)^{1/2}\sum_{K} C_{1k}\exp(ik\cdot R_{ai1}),$$

$$b_{ai1}^{+}=(2/N)^{1/2}\sum_{K} C_{1k}^{+}\exp(-ik\cdot R_{ai1}),$$

$$b_{bj1}=(2/N)^{1/2}\sum_{K} d_{1k}\exp(-ik\cdot R_{bj1}),$$

$$b_{bj1}^{+}=(2/N)^{1/2}\sum_{K} d_{1k}^{+}\exp(ik\cdot R_{bj1}),$$

$$b_{ci2}=(2/N)^{1/2}\sum_{K} C_{2k}\exp(ik\cdot R_{ci2}),$$

$$b_{ci2}^{+}=(2/N)^{1/2}\sum_{K} C_{2k}^{+}\exp(-ik\cdot R_{ci2}),$$

$$b_{dj2}=(2/N)^{1/2}\sum_{K} d_{2k}\exp(-ik\cdot R_{dj2}),$$

$$b_{dj2}^{+}=(2/N)^{1/2}\sum_{K} d_{2k}^{+}\exp(ik\cdot R_{dj2}).$$

Thus, within the linear spin-wave approximation, the Hamiltonian (1) is transformed into the boson operator form which reads

$$H=-2NS^2J+J\sum_{K}(C_{1k}^{+}C_{1k}+C_{2k}^{+}C_{2k}+d_{1k}^{+}d_{1k}+d_{2k}^{+}d_{2k})+2SJ_{\parallel}Z_{ab}\sum_{K}\gamma(k)(C_{1k}^{+}d_{1k}^{+}+C_{1k}d_{1k}+C_{2k}^{+}d_{2k}^{+}+C_{2k}d_{2k})$$

$$+2SJ_{\perp}\sum_{K}(C_{1k}^{+}C_{2k}^{+}+C_{1k}C_{2k}+d_{1k}^{+}d_{2k}^{+}+d_{1k}d_{2k}), \tag{2}$$

where N is the total number of lattice sites and

$$J=2SJ_{\parallel}Z_{ab}+2SJ_{\perp},$$

$$\gamma(k)=\frac{1}{Z_{ab}}\sum_{\delta}^{ab}\exp(ik\cdot\delta),$$

where $Z_{ab}=4$ is the number of nearest neighbors with the CuO_2 plane.

We employ the Green's-function formalism[24] to investigate Hamiltonian (2). For this, we define

$$G_{11}=\langle\langle C_{1k};\ C_{1k}^{+}\rangle\rangle,$$

$$G_{21}=\langle\langle d_{1k}^{+};\ C_{1k}^{+}\rangle\rangle,$$

$$G_{31}=\langle\langle C_{2k}^{+};\ C_{1k}^{+}\rangle\rangle,$$

and

$$G_{41}=\langle\langle d_{2k};\ C_{1k}^{+}\rangle\rangle.$$

We obtain the equations of motion for the above Green's functions and in the matrix notation these may be written as

$$Mg=u \tag{3}$$

with

$$M=\begin{bmatrix} \omega-J & -J_{\parallel}(k) & -J_{\perp}' & 0 \\ J_{\parallel}(k) & \omega+J & 0 & J_{\perp}' \\ J_{\perp}' & 0 & \omega+J & J_{\parallel}(k) \\ 0 & J_{\perp}' & -J_{\parallel}(k) & \omega-J \end{bmatrix}, \tag{4}$$

$$g=\begin{bmatrix} G_{11} \\ G_{21} \\ G_{31} \\ G_{41} \end{bmatrix} \text{ and } u=\begin{bmatrix} 1/2\pi \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{5}$$

with $J_{\parallel}(k)=2SJ_{\parallel}Z_{ab}\gamma(k)$ and $J_{\perp}'=2SJ_{\perp}$.

The spin-wave dispersion relation may be obtained easily by solving the equation $\det(M)=0$. This gives the four roots of ω but they are 2×2 equal. In fact, we obtain

$$\omega_{1,2}=[J^2-(J_{\parallel}(k)\pm J_{\perp}')^2]^{1/2}. \tag{6}$$

Substituting the values of $J_{\parallel}(k)$ and $J_{\perp}'$ for the spin-1/2 case ($S=1/2$), Eq. (6) may be simplified as

$$\omega_{1,2}=J_{\parallel}[(4+r)^2-\{2(\cos k_x a+\cos k_y a)\pm r\}^2]^{1/2}, \tag{7}$$

where, $r=J_{\perp}/J_{\parallel}$.

It is important to note that the above equation (7) is similar to that obtained earlier by Reznik *et al.*,[20] where the $(+)$ sign corresponds to the acoustic mode and the $(-)$ sign corresponds to the optic mode. Equation (7) leads to a spin gap with minimum energy

$$\omega_{\text{opt}}=2\sqrt{J_{\perp}J_{\parallel}}. \tag{8}$$

Further, we solve the set of Eq. (3) to evaluate the various Green's functions. By the knowledge of these Green's functions, the corresponding correlations may be obtained. Following the standard procedure,[24] we obtain

$$\langle C_{1k}^{+}C_{1k}\rangle=-1/2+\frac{J}{4\omega_1}\coth(\beta\omega_1/2)+\frac{J}{4\omega_2}\coth(\beta\omega_2/2), \tag{9}$$

$$\langle C_{1k}^{+}d_{1k}^{+}\rangle=\frac{[J_{\parallel}(k)+J_{\perp}']}{4\omega_1}\coth(\beta\omega_1/2)+\frac{[J_{\parallel}(k)-J_{\perp}']}{4\omega_2}\coth(\beta\omega_2/2), \tag{10}$$

and

$$\langle C_{1k}^{+}C_{2k}^{+}\rangle=\frac{(J_{\parallel}(k)+J_{\perp}')}{4\omega_1}\coth(\beta\omega_1/2)-\frac{(J_{\parallel}(k)-J_{\perp}')}{4\omega_2}\coth(\beta\omega_2/2). \tag{11}$$

Further, the symmetry of the system allows us to take

$$\langle C_{1k}^{+}C_{1k}\rangle=\langle C_{2k}^{+}C_{2k}\rangle=\langle d_{1k}^{+}d_{1k}\rangle=\langle d_{2k}^{+}d_{2k}\rangle, \tag{12}$$

$$\langle C_{1k}^{+}d_{1k}^{+}\rangle=\langle C_{2k}^{+}d_{2k}^{+}\rangle=\langle C_{1k}d_{1k}\rangle=\langle C_{2k}d_{2k}\rangle, \tag{13}$$

$$\langle C_{1k}^{+}C_{2k}^{+}\rangle=\langle C_{1k}C_{2k}\rangle=\langle d_{1k}^{+}d_{2k}^{+}\rangle=\langle d_{1k}d_{2k}\rangle, \tag{14}$$

III. MAGNETIZATION AND SPECIFIC HEAT

In this section, we use the results obtained in Sec. II to evaluate the expressions for sublattice magnetization and specific heat.

For sublattice a in layer 1, the magnetization may be obtained as

$$M_1^a(T)=\langle S_{a1}^2\rangle=S-(2/N)\sum_k\langle C_{1k}^{+}C_{1k}\rangle. \tag{15}$$

Substituting the expression of $\langle C_{1k}^{+}C_{1k}\rangle$ from Eq. (9) into Eq. (15), we obtain

$$-\delta M(T)=M_1^a(T)-M_1^a(0)=-N^{-1}\sum_k\left(\frac{J}{\omega_1(e^{\beta\omega_1}-1)}+\frac{J}{\omega_2(e^{\beta\omega_2}-1)}\right) \tag{16}$$

with

$$M_1^a(0)=1/2-N^{-1}\sum_k\left(\frac{J}{\omega_1}+\frac{J}{\omega_2}-1\right). \tag{17}$$

In Sec. II, we have already obtained the expressions for $\omega_{1,2}$ as Eq. (7). For small k values, we approximate $\cos k_x a=1-k_x^2a^2/2$; $\cos k_y a=1-k_y^2a^2/2$ and write $k_x^2a^2+k_y^2a^2=\theta_p^2$. Under this approximation, Eq. (7) may be rewritten as

$$\omega_1=J_{\parallel}[2(4+r)\theta_p^2]^{1/2} \tag{18}$$

and

$$\omega_2=J_{\parallel}[16r+2(4-r)\theta_p^2]^{1/2}. \tag{19}$$

Thus, substituting Eqs. (18) and (19) into Eq. (16), the reduced magnetization may be obtained easily by converting the summation over k values into an integration. In doing so, it can be shown that the first integral in Eq. (16) corresponding to the acoustic mode diverges at $\theta_p=0$ implying the absence of magnetic order in bilayers. We, therefore, conclude that the intrabilayer coupling does not favor the magnetic order and the system still remains two dimensional. A similar conclusion has also been drawn by Du *et al.*[23] for the bilayer systems. Therefore, to obtain the contribution to the sublattice magnetization from the acoustic mode, we must include some anisotropy in Eq. (18). Let the contribution of such a term be incorporated through ϕ so that Eq. (18) reads

$$\omega_1 = J_\parallel [2(4+r)\theta_p^2 + \phi^2]^{1/2}. \quad (20)$$

We would like to emphasize that though ϕ appears in the above equation arbitrarily, it has some microscopic origins. For instance, if the orthorhombic distortions of the system are taken into account, there will be an interlayer exchange coupling (J^z) along the z direction and, therefore, $\phi = \phi_0(1 - \cos k_z c)^{1/2}$, where, $\phi_0 = J^z/J_\parallel$ and k_z is the wave vector along the z direction with lattice constant c.[2,4,6] Further, if we consider the anisotropy due to the dipolar interactions within the CuO_2 plane, in the simplest approximation $\phi \propto W_0/J_\parallel$, where W_0 is the amount of gap produced by the dipolar interactions.[25–30]

In fact, as will be shown below, various anisotropies may play different roles in the magnetic dynamics of these systems. We, therefore, rather than considering it in the model Hamiltonian explicitly, choose this term phenominologically which may originate from any known source.

Before we proceed further, it is important to mention the numerical estimates of various parameters appearing in the present formalism. Based on the neutron-diffraction experiments of Tranquada *et al.*,[1] Singh *et al.*[4] and Ajay *et al.*[9] have calculated $T_N = 450$ K for $YBa_2Cu_3O_{6+x}$. These authors have shown that T_N is sensitive to ϕ_0 which further depends on dopant concentration (x). At $x = 0.41$, ϕ_0 vanishes and hence $T_N \to 0$, while $J_\parallel$ remains unaffected. The ϕ_0 has been estimated to be of the order of 10^{-3}. On the other hand, the dipolar interactions are too weak to be observed experimentally. However, a rough estimate suggests that $W_0/J_\parallel$ is one or two orders weaker than that of ϕ_0.[25–28]

The value of intrabilayer coupling constant ($J_\perp$) may be obtained using Eq. (8). The recent experiment of Reznik *et al.*[20] suggests a minimum energy of the optic mode to be 65–70 meV. Using $J_\parallel = 120$ meV, they have obtained $J_\perp = 10$ meV. Shamoto *et al.*[18] have estimated a lower limit of $J_\perp$ equal to 8 meV by taking $J_\parallel = 120 \pm 20$ meV. The band theory calculations yield 13 meV (Ref. 31) and Millis and Monien[21] have estimated $J_\perp = 14$ meV. Therefore, it is reasonable to consider that the ratio $r = J_\perp/J_\parallel$ is of the order of 10^{-1} in $YBa_2Cu_3O_{6+x}$.

Thus, in the light of the above numerical estimates, we may say that $\phi \ll r$ and therefore, its addition will not affect ω_2 [Eq. (20)] significantly, while for the acoustic mode (ω_1), no matter that how small ϕ is, its addition is necessary to sustain magnetization at any finite temperature.

Now, first of all, we consider the role of exchange coupling anisotropy in the sublattice magnetization. For this, we set $\phi = \phi_0(1 - \cos k_z c)^{1/2}$. Further, we write $k_z c = \theta_z$ and following our previous paper,[6] we convert the summation over the k values in Eq. (16) into an integration and after performing the integral over θ_p, we obtain

$$\delta M(T) = -\frac{1}{(2\pi)^2}\left(\frac{K_B T}{2J_\parallel}\right)\int_{-\pi}^{\pi} \ln[1 - e^{-Y}]\, d\theta_z - \frac{(4+r)}{2(4-r)}\left(\frac{K_B T}{J_\parallel}\right)\ln[1 - e^{-X}] \quad (21)$$

with

$$Y = J_\parallel \phi / K_B T \quad \text{and} \quad X = 4J_\parallel \sqrt{r}/K_B T.$$

Based on the numerical estimate of various parameters, it is important to note that in the limit $K_B T < 4J_\parallel \sqrt{r}$, the last term of Eq. (21) contributes negligibly and, therefore, the major contribution arises only from the acoustic mode. The above equation reduces to

$$\delta M(T) = -\frac{1}{(2\pi)^2}\left(\frac{K_B T}{2J_\parallel}\right)\int_{-\pi}^{\pi} \ln[1 - e^{-Y}]\, d\theta_z \quad (22)$$

and for the exchange anisotropy,

$$Y = J_\parallel \phi_0 (1 - \cos\theta_z)^{1/2}/K_B T. \quad (23)$$

Now, it is easy to solve Eq. (22) in the two temperature regimes (i) $K_B T < 4J_\parallel \phi_0$ and (ii) $4J_\parallel \sqrt{r} > K_B T > 4J_\parallel \phi_0$.

In the regime $K_B T < 4J_\parallel \phi_0$, approximating $Y \approx J_\parallel \phi_0 \theta_z / K_B T \sqrt{2}$, the integral (22) yields

$$\delta M(T) = \frac{\sqrt{2}}{12}\left(\frac{K_B T}{2J_\parallel}\right)\left(\frac{K_B T}{2J_\parallel \phi_0}\right) \quad (24)$$

and in the regime $4J_\parallel \sqrt{r} > K_B T > 4J_\parallel \phi_0$, we approximate $\ln(1 - e^{-Y}) \approx \ln Y$ and therefore, the integral (22) gives

$$\delta M(T) = \frac{1}{4\pi}\left(\frac{K_B T}{2J_\parallel}\right)\ln\left(\frac{K_B T \sqrt{2}}{J_\parallel \phi_0}\right). \quad (25)$$

Thus in the limit $K_B T < 4J_\parallel \sqrt{r}$, there further exist two temperature regimes. In the low-temperature regime ($K_B T < 4J_\parallel \phi_0$) magnetization follows a T^2 behavior, while for temperature $4J_\parallel \sqrt{r} > K_B T > 4J_\parallel \phi_0$ it follows a $T \ln T$ behavior.

Moreover, we note that expressions (24) and (25) differ from the previous results only by some numerical factor. The difference in our results with those of Refs. 2 and 6 is due to the fact that in the present paper we have considered only the functional form of anisotropy ϕ. Because of this, the contribution of a numerical term ($Z_c = 2$) which denotes the number of nearest neighbors along the z axis could not be incorporated. Therefore, the discrepancy in the results may be easily removed by considering the anisotropy explicitly in the model Hamiltonian. However, it is evident that the inclusion of Z_c do not change the qualitative nature of the results.

Further, in the limit $K_B T > 4J_\parallel \sqrt{r}$, the second term of Eq. (21) also contributes significantly. In this limit, it is easy to show that both the terms in Eq. (21) follow a $T \ln T$ behavior and if $r \to 0$, the logarithmic term approaches infinity and it is not possible to obtain the magnetization at any finite temperature.

The above analysis leads us to conclude that in the high-temperature region $K_B T > 4J_\parallel \sqrt{r}$, magnetization follows a quasi-2D behavior while in the low-temperature regime the T^2 dependence of magnetization is consistent with the 3D behavior. The presence of the optic mode in the high-temperature region does not seem to change the quasi-2D behavior of the system.

Now, we briefly outline the effects of dipolar anisotropy in these systems. Pich *et al.* [27] have studied the effect of dipolar interaction in 2D isotropic Heisenberg antiferromagnets. These authors have shown that the dipolar interaction produces two branches and for $k \to 0$ there is a gap W_0 in the excitation spectrum. However, the two branches can be re-

solved only when the ratio of dipolar interaction and the exchange coupling is sufficiently large. For a realistic ratio (10^{-3}) the two magnon branches practically coincide and for small k values the excitation energy may be written as

$$\omega_k = \sqrt{8J_\parallel^2\theta_p^2 + W_0^2}.$$

Such a gap due to dipole-dipole interaction in the spin-wave excitation spectrum has been experimentally confirmed by Borovik-Romanov *et al.*[30] in the case of easy-plane antiferromagnets with weak ferromagnetism. Thus for such an anisotropy, in our formalism we may set $\phi = W_0/J_\parallel$.[29] It is important to note that ϕ is independent of k_z and hence in expression (16) we convert the summation over k values into an integration only over k_x and k_y. Finally, integrating over θ_p as previously, we obtain

$$\delta M(T) = -\frac{1}{(2\pi)}\left(\frac{K_BT}{2J_\parallel}\right)\ln[1-e^{-Y}] - \frac{(4+r)}{4\pi(4-r)}\left(\frac{K_BT}{J_\parallel}\right)\ln[1-e^{-X}] \tag{26}$$

with $Y = J_\parallel\phi/K_BT$, $X = 4J_{\parallel\sqrt{}}r/K_BT$, and $\phi = W_0/J_\parallel$.

Clearly, if the $K_BT > 4J_{\parallel\sqrt{}}r$, both terms follow a $T\ln T$ behavior while in the low-temperature limit, T^2 behavior may not be obtained. This leads us to conclude that though the dipolar interactions do establish the AFM long-range order in 2D systems, they do not seem to produce 3D Néel ordering at low temperatures as observed in $YBa_2Cu_3O_{6+x}$.[14] However, expression (26) may be useful to estimate the strength of dipolar interaction in these systems.

IV. SPECIFIC HEAT

Now, we calculated the specific heat which may be obtained from

$$C = dE/dT, \tag{27}$$

where E is the internal energy of the system and may be obtained by thermally averaging the Hamiltonian (2). Thus, we get

$$E = E_0 + 2\sum_k \left(\frac{[J^2+\{J_\parallel(k)+J'_\perp\}^2]}{\omega_1(e^{\beta\omega_1}-1)} + \frac{[J^2+\{J_\parallel(k)-J'_\perp\}^2]}{\omega_2(e^{\beta\omega_2}-1)}\right) \tag{28}$$

with

$$E_0 = -2NS^2J - 2J + \sum_k \left(\frac{[J^2+\{J_\parallel(k)+J'_\perp\}^2]}{\omega_1} + \frac{[J^2+\{J_\parallel(k)-J'_\perp\}^2]}{\omega_2}\right). \tag{29}$$

Further, the summation over k values are converted into an integration and for the 2D case in the low-temperature limit, the solution yields

$$E = E_0 + \frac{2NJ_\parallel}{\pi}\left(\frac{K_BT}{2J_\parallel}\right)^3 + \frac{NJ_\parallel}{\pi(4-r)}\left(\frac{K_BT}{2J_\parallel}\right)^3. \tag{30}$$

Using Eqs. (27) and (30), the expression for specific heat may be obtained which reads

$$C = \frac{3NK_B}{2\pi}\frac{(12-r)}{(16-r^2)}\left(\frac{K_BT}{J_\parallel}\right)^2. \tag{31}$$

Thus, the specific heat of these systems follows a T^2 behavior.

V. CONCLUSION

We have performed a study of magnetic dynamics of bilayer antiferromagnets within the framework of the usual spin-wave theory. It is shown that in the presence of the intrabilayer coupling ($J_\perp$), the spin-wave spectrum consists of acoustic and optic modes. The minimum energy gap is found to be $2\sqrt{J_\perp J_\parallel}$. This result is similar to the previous theoretical predictions[16] as well as experimental observation.[20]

Further, we have investigated the role of intrabilayer coupling in the sublattice magnetization of $YBa_2Cu_3O_{6+x}$. It is shown that corresponding to the optic mode no extra anisotropy term is required to sustain magnetization at finite temperatures while for the acoustic mode, in the absence of anisotropy the magnetization vanishes. To obtain the contribution from the acoustic mode, we introduce the anisotropy term phenomenologically and show that anisotropy terms, such as dipolar interactions, only establish the AFM long-range order in 2D systems, while the z-direction coupling (J^z) is necessary to keep the observed 3D Néel ordering in these systems.

Moreover, in the low-temperature regime, magnetization follows a T^2 behavior which is characteristic of a 3D system and in the high-temperature regime the contributions from both the modes (acoustic and optic) give a $T\ln T$ behavior which is characteristic of a quasi-2D system. Thus, over the entire temperature range, 3D to quasi-2D crossover is expected at $K_BT = 2J_\parallel\phi_0$ in these systems. Further, in the absence of r, it is not possible to sustain the magnetization. This suggests that besides ϕ_0, r also plays an important role in the magnetic dynamics of bilayer systems.

The specific heat of these systems has no linear term in the expression. This is in accordance with the previous theoretical calculations[5,6] and the experimental observations of Kumagai *et al.*[32]

Finally, we emphasize that in the present formalism we have not considered the effects of magnon-magnon interaction. In fact, it has been shown by us[6] that the effect of $(1+\alpha)$, where α is the manifestation of magnon-magnon interaction, is more pronounced in quasi-2D systems than that of the 3D case. Therefore, it will be fruitful to incorporate the role of such interactions in the magnetic dynamics of these bilayer systems.

*Present address: 250, National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi 12, India.

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