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Magnetic bilayer coupling in $YBa_2Cu_3O_7$

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The spin-fluctuation spectrum of an extended t-J model appropriate to bilayer Y-Ba-Cu-O is investigated within a renormalized-mean-field approach. Strong antiferromagnetic correlation between bilayers is found for realistic values of the interplane coupling in a regime where the in-plane susceptibility is strongly exchange enhanced even though the antiferromagnetic correlation length is short. The influence of spin pairing on the spin-fluctuation spectrum, in this case via a d-wave order parameter, is included. The model predicts a strong energy dependence of the modulation in the vicinity of the characteristic energy for spin fluctuations.

Puzzling features of the interlayer correlations in cuprate superconductors became apparent shortly after the discovery of these materials. At the single-particle level, normal-state c-axis transport measurements show an unusual semiconducting behavior for underdoped material versus a metallic behavior for overdoped material.[1] The superconducting transition temperatures correlate with c-axis coupling strength in different materials, suggesting a role for two-electron tunneling processes in determining T_c.[2] Less celebrated but equally unusual are the interplane magnetic (particle-hole) correlations. Several groups[3–5] performing inelastic-neutron-scattering experiments have reported pronounced modulations in the scattered intensity as a function of q_z at the planar antiferromagnetic wave vector $\mathbf{Q} = (\pi, \pi)$, an effect which is characteristic of strong antiferromagnetic (AFM) correlation between layers. While this can be readily understood in magnetically ordered $YBa_2Cu_3O_6$, it is surprising that this correlation persists in a metal ($YBa_2Cu_3O_7$) whose AFM correlation length is as short as one lattice constant.[4] Indeed, partly motivated by these experiments and partly by NMR, some authors have argued that the interplane Heisenberg AFM exchange may be strong enough to induce local interplane singlet formation.[6]

Recently it has been observed that a semiquantitive account of the spin-fluctuation spectrum in optimally or overdoped cuprates can be obtained by combining a q-dependent Heisenberg exchange enhancement with a "realistic" CuO-plane electronic structure.[7] These models account for the observed commensurate AFM response for $Tl_2Ba_2CuO_{6+x}$-like band structures, and the incommensurate response for $La_{2-x}Sr_xCuO_4$.[8] Here we extend this picture to investigate bilayer correlations in metallic Y-Ba-Cu-O. Following Refs. 9 and 10 we employed a tight-binding model with parameters chosen to reproduce the bonding and antibonding Fermi surfaces found in local-density-approximation band-structure calculations.[11] The value of the interplane hopping matrix element $t_\perp$ which results from this procedure is $0.35t$, where the near-neighbor hopping is $t = 0.52$ eV. Exchange constants corresponding to $J = 0.35t$ and $J^\perp = 0.03t$ were obtained by Rossat-Mignod *et al.*[4] from spin-wave analysis of the $YBa_2Cu_3O_6$ material. Following the renormalized mean-field theory of the t-J model of Ref. 12 we can define inter- and intraband susceptibilities $\chi_0^{(\alpha\beta)}$ in terms of renormalized "spinon" quasiparticle bands $\xi_{\mathbf{k}}^\alpha = \epsilon_{\mathbf{k}}^\alpha - \mu$ (α, β refer to bonding or antibonding bands). The intraplane and interplane susceptibilities can in turn be expressed as $\chi_0^{\rm intra} = \frac{1}{4}\sum_{\alpha\beta}\chi^{(\alpha\beta)}$ and $\chi_0^{\rm inter} = \frac{1}{4}\sum_{\alpha\beta}(2\delta_{\alpha\beta} - 1)\chi^{(\alpha\beta)}$, respectively.

The effects of the near-neighbor intra- and interplane exchange interactions can be included via $\mathbf{q}$-dependent Stoner-type correction factors which enhance the response in the vicinity of the AFM wave vector $\mathbf{Q}$. The full responses in the bilayer model are found to be

$$\chi^{\rm intra}(\mathbf{q},\omega) = \frac{\chi_0^{\rm intra}(1 + J_{\mathbf{q}}\chi_0^{\rm intra}) - J_{\mathbf{q}}(\chi_0^{\rm inter})^2}{(1 + J_{\mathbf{q}}\chi_0^{\rm intra} + \frac{J^\perp}{2}\chi_0^{\rm inter})^2 - (\frac{J^\perp}{2}\chi_0^{\rm intra} + J_{\mathbf{q}}\chi_0^{\rm inter})^2}\,, \tag{1a}$$

$$\chi^{\rm inter}(\mathbf{q},\omega) = \frac{\chi_0^{\rm inter}(1 + \frac{J^\perp}{2}\chi_0^{\rm inter}) - \frac{J^\perp}{2}(\chi_0^{\rm intra})^2}{(1 + J_{\mathbf{q}}\chi_0^{\rm intra} + \frac{J^\perp}{2}\chi_0^{\rm inter})^2 - (\frac{J^\perp}{2}\chi_0^{\rm intra} + J_{\mathbf{q}}\chi_0^{\rm inter})^2}\,. \tag{1b}$$

Here we define $J_{\mathbf{q}} \equiv J(\cos q_x + \cos q_y)$. The full q_z-dependent response can be expressed as $\chi(\mathbf{q}, q_z, \omega) = \chi^{\rm intra}(\mathbf{q},\omega) + \cos(q_z d)\chi^{\rm inter}(\mathbf{q},\omega)$, where d is the layer spacing. It is now clear that the q_z modulation measures the *ratio of inter- and intraplane susceptibilities.*

Expressions (1a) and (1b) predict an AFM instability at a critical doping level $\delta_c(T)$, corresponding to the zero of the denominator which occurs at wave vector $\mathbf{Q}$ and zero frequency. Precisely at this point, it follows from Eqs. (1b) and (1a) that $\chi^{\rm inter} \to -\chi^{\rm intra}$. Therefore, at wave vector **Q**, the low-frequency bilayer modulation becomes significant near the instability. The negative sign, corresponding to AFM coupling, gives the observed phase shift.[3–5]

Since the O_7 material is in fact a high-temperature superconductor, with a spin gap of order 40 meV, a meaningful comparison with experiment requires that we include spin pairing in the model. Following earlier work on t-J and related models,[9] we do this via a d-wave[13] order parameter, which is favored by the exchange interaction. The magnitude of the gap function $\Delta_{\mathbf{k}} = \Delta_d(\cos k_x - \cos k_y)$ can be computed self-consistently using a mean-field uncoupling of the Heisenberg term. We have not included an interplane d-wave order parameter as its magnitude is small compared to the intraplane contribution.

The bare spin susceptibilties per Cu site in this model are (generalizing slightly from Ref. 14)

$$\chi_0^{(\alpha\beta)} = \frac{1}{4N}\sum_{\mathbf{k}}\left(1+\frac{\xi^\alpha_{\mathbf{k}}\xi^\beta_{\mathbf{k+q}}+\Delta_{\mathbf{k}}\Delta_{\mathbf{k+q}}}{E^\alpha_{\mathbf{k}}E^\beta_{\mathbf{k+q}}}\right)\left[\frac{f(E^\beta_{\mathbf{k+q}})-f(E^\alpha_{\mathbf{k}})}{\omega+E^\alpha_{\mathbf{k}}-E^\beta_{\mathbf{k+q}}+i\Gamma}+\frac{f(E^\alpha_{\mathbf{k}})-f(E^\beta_{\mathbf{k+q}})}{\omega-E^\alpha_{\mathbf{k}}+E^\beta_{\mathbf{k+q}}+i\Gamma}\right]$$
$$+\frac{1}{4N}\sum_{\mathbf{k}}\left(1-\frac{\xi^\alpha_{\mathbf{k}}\xi^\beta_{\mathbf{k+q}}+\Delta_{\mathbf{k}}\Delta_{\mathbf{k+q}}}{E^\alpha_{\mathbf{k}}E^\beta_{\mathbf{k+q}}}\right)\left[\frac{f(E^\alpha_{\mathbf{k}})+f(E^\beta_{\mathbf{k+q}})-1}{\omega-E^\alpha_{\mathbf{k}}-E^\beta_{\mathbf{k+q}}+i\Gamma}+\frac{1-f(E^\alpha_{\mathbf{k}})-f(E^\beta_{\mathbf{k+q}})}{\omega+E^\alpha_{\mathbf{k}}+E^\beta_{\mathbf{k+q}}+i\Gamma}\right], \quad (2)$$

where $E^\alpha_{\mathbf{k}} \equiv \sqrt{(\xi^\alpha_{\mathbf{k}})^2+\Delta^2_{\mathbf{k}}}$, f is the Fermi function, and Γ is a positive infinitesimal number. d-wave pairing leads to a suppression of the low-frequency susceptibilities near zero wave vector (Knight shift) but in most circumstances has a small effect on the response near $\mathbf{Q} = (\pi,\pi)$. Equation (2) completes the description of the magnetic fluctuation spectrum.

Figure 1 shows the mean-field phase diagram. Figure 2 shows the in-plane response $\mathrm{Im}\chi^{\mathrm{intra}}(\mathbf{Q},\omega)$ and the modulation parameter $\mathrm{Im}\chi^{\mathrm{inter}}(\mathbf{Q},\omega)/\mathrm{Im}\chi^{\mathrm{intra}}(\mathbf{Q},\omega)$ as the AFM transition is approached. Notice that the modulation parameter reaches unity as the instability is approached. The influence of the gap is clearly seen in the low-frequency response, leading to a peak in the modulation parameter at a frequency of order the gap. Figure 3 shows the behavior of the magnetic correlation length [now defined as the inverse width of the AFM peak in the quantity $\mathrm{Re}\chi^{\mathrm{intra}}(\mathbf{q},\omega=0)$]. Notice that the bilayer modulation can be appreciable even when ξ is of order a lattice constant. The reason for this surprising behavior can be traced to the fact that the susceptibility is large but weakly $\mathbf{q}$-dependent in the vicinity of (π,π); this behavior is a feature of a primarily exchange driven instability and would not occur in models with nested Fermi surfaces. The bilayer modulation is mostly determined by $J_\perp$; very similar curves are obtained setting $t_\perp = 0$.

It is tempting to associate the 41-meV peak observed in Refs. 4 and 5 with the characteristic scale for AFM

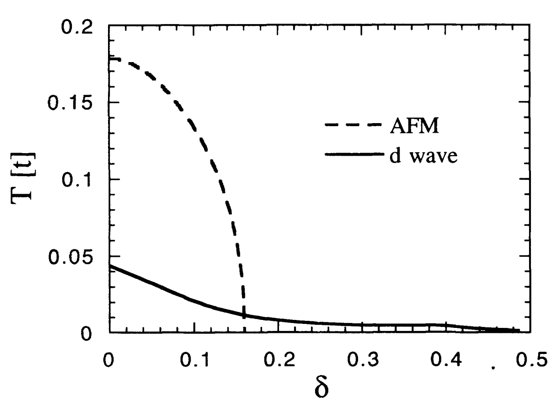

FIG. 1. Mean-field phase diagram for bilayer Y-Ba-Cu-O. The tight-binding model used included a nearest-neighbor hopping $t = 0.52$ eV, a next-nearest-neighbor hopping $t' = -0.45t$, a second-next-neighbor hopping $t'' = 0.16t$, and an interplane hopping $t^\perp = 0.35t$. Uniform resonating valence bond intra- and interplane order parameters, and intraplane d-wave pairing were computed self-consistently. Spin pairing has only a minor effect on the antiferromagnetic instability which dominates at low doping.

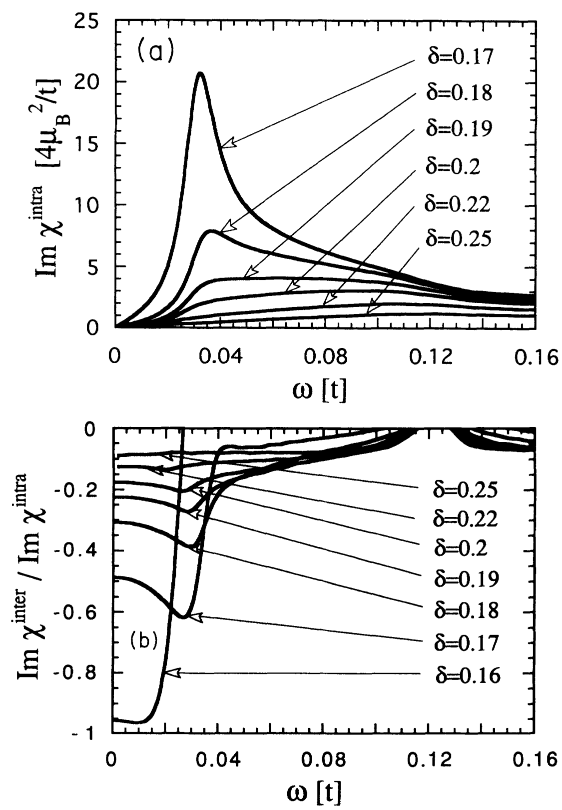

FIG. 2. Frequency dependence of the imaginary part of the response $\chi^{\mathrm{intra}}(\mathbf{Q},\omega) \equiv \langle S^+_{\mathbf{Q},\omega}S^-_{-\mathbf{Q},\omega}\rangle$ (a) and the modulation parameter $\mathrm{Im}\chi^{\mathrm{inter}}/\mathrm{Im}\chi^{\mathrm{intra}}$ (b) at the AFM wave vector $\mathbf{Q} = (\pi,\pi)$ and temperature $T = 0.005t$. The doping $\delta = 0.2$ corresponds to a gap parameter $\Delta_d = 0.008t$.

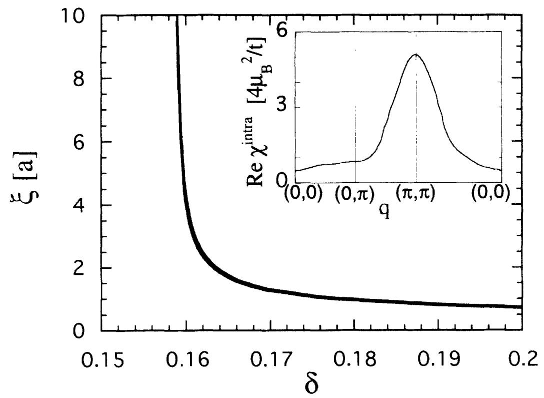

FIG. 3. Doping dependence of the AFM correlation length ξ, defined as the inverse width of the AFM peak in $\mathrm{Re}\chi^{\mathrm{intra}}(\mathbf{q},\omega=0)$ (plotted along the symmetry lines for $T=0.005t$, $\delta=0.2$ in the inset). Near the AFM instability, the correlation length diverges as $(\delta-\delta_c)^{-\frac{1}{2}}$.

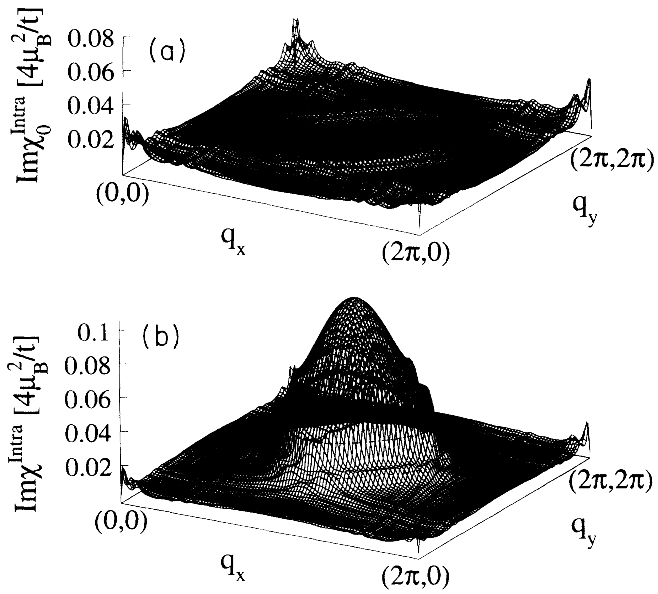

FIG. 4. q dependence of the bare and exchange enhanced intraplane response $\mathrm{Im}\chi_0^{\mathrm{intra}}$ (a) and $\mathrm{Im}\chi^{\mathrm{intra}}$ (b) at $\delta=0.2$, $\omega=0.005t$, and $T=0.005t$ with gap parameter $\Delta_d=0.008t$.

spin fluctuations corresponding to the low-energy peak of Fig. 2(a) in the vicinity of δ_c. (Although the peak in Fig. 2 corresponds to only about 20 meV, this shifts to higher energy if a larger pair coupling is chosen.[9]) A key prediction of the model is then that the modulation parameter is strongly energy dependent, with a maximum which coincides with the peak in the intraplane susceptibility. Some evidence for this seems to be present in the unpolarized neutron-scattering experiments of Ref. 4.

Finally Fig. 4(a) shows the *bare* q-dependent response χ_0^{intra} in the spin paired state. It was pointed out by Lu[15] that scattering between nodal points on the Fermi surface should dominate the response when $\omega \ll \Delta_d$. However, this effect is very weak in our Y-Ba-Cu-O model for two reasons. First, the various internode scattering wave vectors are not close to nesting wave vectors of the underlying Fermi surface as in the example of Ref. 15. Second, exchange enhancement leads to an AFM peak even in the d-wave state which dominates all other features in the vicinity of δ_c, as can be seen by comparing Figs. 4(a) and 4(b).

In conclusion we have shown that the observed bilayer correlation in Y-Ba-Cu-O may be consistent with proximity of this system to an AFM instability, in the sense that the AFM enhancement is large. A long correlation length is not required to explain these features. An obvious difficulty with this explanation is the absence of any observed AFM instability in underdoped metallic Y-Ba-Cu-O. However, in Ref. 6 it was argued that thermal fluctuations in the presence of weak three-dimensional couplings may be sufficient to suppress AFM long-range order in this system in favor of superconductivity.

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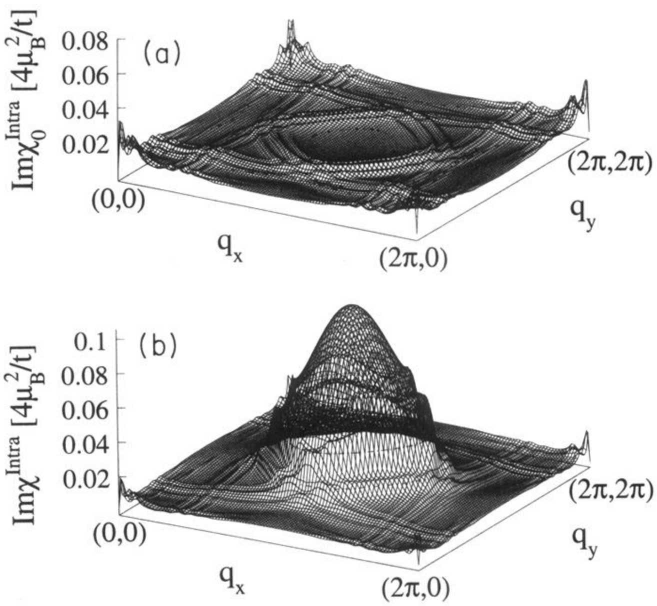

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