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Antiferromagnetic excitations and van Hove singularities in $YBa_2Cu_3O_{6+x}$

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We show that in quasi-two-dimensional d-wave superconductors van Hove singularities close to the Fermi surface lead to magnetic quasiparticle excitations. We calculate the temperature and doping dependence of dynamical magnetic susceptibility for $YBa_2Cu_3O_{6+x}$ and show that the proposed excitations are in agreement with inelastic-neutron-scattering experiments. In addition, the values of the gap parameter and in-plane antiferromagnetic coupling are much smaller than usually believed.

The spin dynamics of the cuprate superconductors is still a subject of controversy. The spin-spin correlation function $\chi_{Ph}(\mathbf{q},q_z,\omega)\equiv\chi'+i\chi''$, $\mathbf{q}\equiv(q_x,q_y)$, usually probed by NMR, magnetic Raman scattering or, more directly, by inelastic neutron scattering (INS) experiments, is still not well understood. INS measurements on $YBa_2Cu_3O_{6+x}$ (YBCO) have been performed by a number of groups[1–3] and have led to a consistent picture of the measured physical susceptibility $\chi_{Ph}(\mathbf{q},q_z,\omega)$ for $\mathbf{q}$ near the antiferromagnetic (AF) wave vector $\mathbf{Q}\equiv(\pi,\pi)$. It has been found that the dynamical AF spin fluctuations persist over the whole range of doping $(0.4\leqslant x\leqslant 1)$ and the following remarkable features have been reported:

(a) In the superconducting (SC) state $\chi''_{Ph}(\mathbf{Q},q_z,\omega)$ is limited by an energy gap, E_g (Ref. 3). In heavily doped regime $(0.65\leqslant x\leqslant 0.92)$ E_g is roughly proportional to the SC transition temperature T_c, that is $E_g\approx 3.4k_BT_c$. In the weakly doped regime E_g is very small and it is a much stronger function of T_c (Ref. 4).

(b) In addition, in highly doped YBCO the spin excitation spectrum is characterized by a sharp peak at some energy $E_r>E_g$, e.g., for optimally doped $YBa_2Cu_3O_{6.92}$, $E_r=41$ meV (Refs. 5–7). For underdoped samples a broad resonance has been observed at $20<E_r<40$ meV (Refs. 2,4). The resonance excitation is localized in both energy and wave vector and has $\chi''_{Ph}(\mathbf{Q},q_z,E_r)\propto\sin^2(q_zd/2)$ modulation, where d is the distance between two adjacent CuO_2-planes in the unit cell of YBCO.

(c) At $\omega\approx 50$ meV there is a high energy cut off, i.e., the intensity sharply decreases, regardless of the doping level.

(d) In the normal state $\chi''_{Ph}(\mathbf{Q},q_z,\omega)$ is characterized by a broad feature, spread practically over the whole energy range, with a characteristic energy $\omega\sim 30$ meV, approximately independent of the oxygen concentration.

There have been a number of theoretical proposals for the explanation of features (a)–(d). It has been shown by Lu[8] that for d-wave SC state $\chi''(\mathbf{q},q_z,\omega)$ should exhibit anomalous resonance peaks in $\mathbf{q}$ space. Feature (b) has been treated in terms of spin-flip excitations across the SC gap[9–18] or as collective mode excitations in the particle-particle channel.[19]

In this paper we show that the YBCO bilayer structure and two-dimensional (2D) band topology, renormalized for AF interactions, with d-wave SC order parameter, leads to magnetic quasi-particle excitations which explain all of the features (a)–(d), observed in INS.

We start by calculating $\chi''_{Ph}(\mathbf{q},q_z,\omega)$ for YBCO: we consider a system of two 2D planes, corresponding to the Cu_2O_4 bilayer in a unit cell of YBCO, with an effective band dispersion: $\xi^{(i)}_{\mathbf{k}}=-2t[\cos(k_x)+\cos(k_y)]-4t'\cos(k_x)\cos(k_y)-2t''[\cos(2k_x)+\cos(2k_y)]\pm t_\perp-\mu$. Here index (i) corresponds to the electron bands with *odd* (o) and *even* (e) wave functions with respect to the mirror plane between the adjacent planes. We choose the parameters t, t', t'', $t_\perp$ and μ by requiring that the shape and depth of the band and the size of the Fermi surface (FS) are approximately equal to those observed in ARPES measurements. According to Ref. 20, the *even* band is nearly half filled regardless of the oxygen content, while at optimal doping the *odd* band is shifted upwards by $2t_\perp\approx 100$ meV and thus it is far away from half filling. This yields band parameters $t=115$ meV, $t'/t=-0.2$, $t''/t=0.25$, and $\mu=-228$ meV (density of electrons $n^{(o)}=0.55$ and $n^{(e)}=0.9$). Although one usually interprets the parameters t, t', and t'' in terms of tight-binding overlap integrals, here they should be regarded as results of our fits to the experimental data and as such, they should include some of the effects of mass renormalization. The *odd* band has a *bifurcated saddle point* at $\mathbf{q}=(\pi,0)$, with $\xi^{(o)}_{\pi,0}=30$ meV and

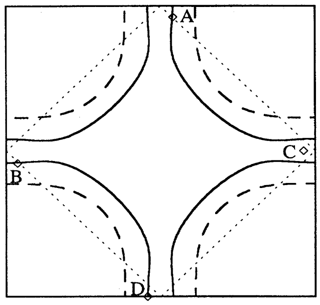

FIG. 1. Fermi surfaces of odd (solid line) and even bands (dashed line) in YBCO. The parameters are given in the text. The dash-dotted line shows the magnetic Brillouin zone. Points A and B (C and D) can be connected by the AF wave vector $\mathbf{Q}\equiv(\pi,\pi)$ and correspond to E_g (E_r) resonances observed in INS measurements (see text).

$\xi^{(o)}_{0.7\pi,0}=10$ meV (Ref. 21); however, none of our conclusions are altered if one assumes an extended Van Hove singularity (VHS) instead. The FS of the *odd* and *even* bands are shown in Fig. 1.

In BCS theory the 2D Fermi liquid spin susceptibility is given by[22,23]

$$\chi_0^{(ij)}(\mathbf{q},\omega)=\sum_{\mathbf{k}} l^{(ij)2}_{\mathbf{k+q},\mathbf{k}} E^{(ij)}_{-}(\mathbf{k},\mathbf{q}) \frac{f(E^{(i)}_{\mathbf{k+q}})-f(E^{(j)}_{\mathbf{k}})}{E^{(ij)2}_{-}-(\omega-i\Gamma)^2} + \sum_{\mathbf{k}} p^{(ij)2}_{\mathbf{k+q},\mathbf{k}} E^{(ij)}_{+}(\mathbf{k},\mathbf{q}) \frac{1-f(E^{(i)}_{\mathbf{k+q}})-f(E^{(j)}_{\mathbf{k}})}{E^{(ij)2}_{+}-(\omega-i\Gamma)^2}, \tag{1}$$

where $E^{(ij)}_{\pm}=E^{(j)}_{\mathbf{k}}\pm E^{(i)}_{\mathbf{k+q}}$, $E^{(i)}_{\mathbf{k}}=\sqrt{\xi^{(i)2}_{\mathbf{k}}+\Delta^{(i)2}_{\mathbf{k}}}$ is the quasiparticle dispersion law in the SC state, $f(E^{(i)}_{\mathbf{k}})=1/[\exp(E^{(i)}_{\mathbf{k}}/T)+1]$ is the Fermi function and the coherence factors are given by

$$p^{(ij)2}_{\mathbf{k+q},\mathbf{k}}=\frac{1}{2}\left(1-\frac{\xi^{(i)}_{\mathbf{k+q}}\xi^{(j)}_{\mathbf{k}}+\Delta^{(i)}_{\mathbf{k+q}}\Delta^{(j)}_{\mathbf{k}}}{E^{(i)}_{\mathbf{k+q}}E^{(j)}_{\mathbf{k}}}\right),$$

$$l^{(ij)2}_{\mathbf{k+q},\mathbf{k}}=\frac{1}{2}\left(1+\frac{\xi^{(i)}_{\mathbf{k+q}}\xi^{(j)}_{\mathbf{k}}+\Delta^{(i)}_{\mathbf{k+q}}\Delta^{(j)}_{\mathbf{k}}}{E^{(i)}_{\mathbf{k+q}}E^{(j)}_{\mathbf{k}}}\right). \tag{2}$$

We assume that the SC gap parameter $\Delta^{(i)}_{\mathbf{k}}$ has a simple form $\Delta^{(i)}_{\mathbf{k}}=\Delta^{(i)}_{max}[\cos(k_x)-\cos(k_y)]/2$, although self-consistent numerical solutions of the gap equation suggest that $\Delta^{(i)}_{\mathbf{k}}$ may have a somewhat different shape.[24] In Eq. (1) Γ is the phenomenological damping parameter. Accounting for the interaction between the susceptibility bubbles, we calculate the spin susceptibility renormalized in the RPA manner:[13–15,23,26]

$$\chi^{(i,j)}(\mathbf{q},\omega)=\chi_0^{(i,j)}(\mathbf{q},\omega)/[1+J^{(i,j)}(\mathbf{q})\chi_0^{(i,j)}(\mathbf{q},\omega)], \tag{3}$$

where $J^{(e,e)}(\mathbf{q})=J_{\parallel}+J_{\perp}$, $J^{(o,o)}(\mathbf{q})=J_{\parallel}-J_{\perp}$, $J^{(e,o)}(\mathbf{q})=J^{(o,e)}(\mathbf{q})=0$, $J_{\parallel}(\mathbf{q})$ is the in-plane magnetic interaction and $J_{\perp}(\mathbf{q})$ is the interplane magnetic coupling. We do not take into account the vertex and self-energy corrections which would further renormalize $\chi^{(i,j)}(\mathbf{q},\omega)$.

For the bilayer case the physical susceptibility, proportional to the INS measured intensity, is given by $\Sigma_{m,n}\exp[iq_z(z_m-z_n)]\chi^{(m,n)}(\mathbf{q},\omega)$ (Ref. 25), where m and n are layer indexes. If coherence is preserved within, but not between the bilayers, this expression can be rewritten:

$$\chi_{Ph}(\mathbf{q},q_z,\omega)=2[\chi^{(e,e)}(\mathbf{q},\omega)\cos^2(q_zd/2) + \chi^{(o,o)}(\mathbf{q},\omega)\sin^2(q_zd/2)]. \tag{4}$$

It is clear from Eq. (4) that the experimentally observed $\sin^2(q_zd/2)$ modulation of the INS (b) must originate from the *odd* band, provided the coupling between bilayers is incoherent.

For fixed $\mathbf{q}$ the quantity $E^{(i,i)}_{+}(\mathbf{k},\mathbf{q})$ is a function of 2D vector $\mathbf{k}$ and we denote its minima and saddle points by $E^{(i,i)}_{\min}(\mathbf{q})$ and $E^{(i,i)}_{\rm sp}(\mathbf{q})$, respectively. In a 2D system and in the $\Gamma,T\to0$ limit these extrema produce logarithmic singularities in either $\chi_0'^{(i,i)}(\mathbf{q},\omega)$ or $\chi_0''^{(i,i)}(\mathbf{q},\omega)$ [see Eq. (1)]. For example, for $p^{(i,i)2}_{\mathbf{k+q}}\neq0$, $\chi_0'^{(i,i)}(\mathbf{q},\omega)$ diverges at $\omega\approx E^{(i,i)}_{\min}(\mathbf{q})$, while $\chi_0''^{(i,i)}(\mathbf{q},\omega)$ behaves like a step function. Alternatively, $\chi_0''(\mathbf{q},\omega)$ diverges at the saddle point energies, $E^{(i,i)}_{\rm sp}(\mathbf{q})$, while $\chi_0'^{(i,i)}(\mathbf{q},\omega)$ has a "kink."[18] Provided that $J_{\parallel}$ and $J_{\perp}$ are not too large, the renormalized susceptibility (3) has poles (resonances) at ω close to both $E^{(i,i)}_{\min}(\mathbf{q})$ and $E^{(i,i)}_{\rm sp}(\mathbf{q})$. Physically, these poles in $\chi^{(i,i)}(\mathbf{q},\omega)$ describe spin-flip quasiparticle excitations (magnons). The self-energy corrections shift the position of the poles to the complex plane, producing the finite lifetime of the excitations, and more importantly, the logarithmic divergences become finite peaks, introducing a minimal value of $J^{(i,i)}(\mathbf{q})$ for the creation of a quasiparticle. For quasi-2D system the resonances become broader due to the weak interaction between the bilayers.

Low energy excitations at $\mathbf{q}=\mathbf{Q}$ correspond to particles and holes near the intercepts of the FS and the magnetic Brillouin zone (e.g., points A and B in Fig. 1). The SC gap at these points $\Delta^{(o)}_{\mathbf{k_A}}$ $(=\Delta^{(o)}_{\mathbf{k_B}})$ is close to $\Delta^{(o)}_{\max}$, and thus the *lowest* energy excitation [feature (a) in INS] is $E_g=\Delta^{(o)}_{\mathbf{k_A}}+\Delta^{(o)}_{\mathbf{k_B}}=E^{(o,o)}_{\min}(\mathbf{Q})$. On the other hand, holes near VHS's and particles above the SC gap produce $E^{(o,o)}_{\rm sp}(\mathbf{q})$ resonances. At $\mathbf{q}=\mathbf{Q}$ this yields the excitation energy $E_r=E^{(o,o)}_{\rm sp}(\mathbf{Q})=\Delta^{(o)}_{\mathbf{k}_D}+E^{(o)}_{\mathbf{k}_C}$, where C and D are points depicted in Fig. 1 [feature (b)]. In Fig. 2 we present the energy dispersion of the quasiparticles, originating from both $E^{(o,o)}_{\min}(\mathbf{q})$ and $E^{(o,o)}_{\rm sp}(\mathbf{q})$, for $\mathbf{q}$ along the high symmetry lines leading to $\mathbf{Q}$, and assuming $\Delta^{(o)}_{\max}=15$ meV. Away from $\mathbf{Q}$ the excitations clearly split into several bands, whose dispersion depends on the shape of VHS's, and $E^{(o,o)}_{\rm sp}(\mathbf{q})$ reaches approximately 0.3 eV near the magnetic Brillouin zone boundary. Of course, the excitations (resonances) shown in Fig. 2 may have very different lifetimes as well as intensities, depending not only on the FS geometry, but also on the appropriate coherence factors.

Returning to the INS results, both E_g and E_r can be observed experimentally only if damping is sufficiently small. We calculated the single electron (hole) magnetic relaxation rate $\tau^{-1}_{\mathbf{k}}$[see Eq. (9b) in Ref. 26] and found that in the SC

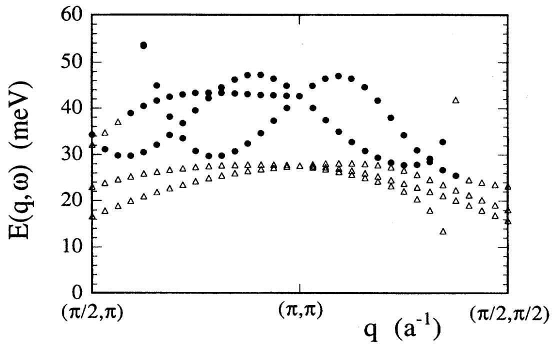

FIG. 2. Magnetic quasi-particle dispersion for **q** along lines of high symmetry, in the vicinity of **Q**. The values are obtained from the minima (triangles) and saddle points (solid circles) of the particle-hole energy $E_{+}^{(o,o)}(\mathbf{k},\mathbf{q})$ [see Eq. (1)] at fixed momentum transfer **q**.

state the relaxation is negligible for **k** near $(\pi,0)$ and energies below $\sim 2.4\Delta_{\max}$, in contrast with ordinary superconductors where $\tau_{\mathbf{k}}^{-1}(\omega,T)$ vanishes for $\omega<3\Delta$ (Ref. 22). As a result, any spin-flip excitation in $\chi''^{(i,i)}(\mathbf{Q},\omega)$, will not be damped for ω smaller than approximately $3.4\Delta_{\max}$ even in d-wave superconductors. Thus, both E_g and $E_r=\Delta_{\mathbf{k}_D}^{(o)}+E_{\mathbf{k}_C}^{(o)}$ *should* be observed experimentally. On the other hand, in the normal state the E_r excitation becomes heavily damped and is sometimes referred to as the *spin pseudogap*. We note that for the *even* band the saddle point energy lies far below the FS and the corresponding resonance excitation is overdamped even in the SC state and contributes only to a structureless background.

The temperature dependence of the calculated *odd* band susceptibility $\chi''^{(o,o)}(\mathbf{Q},\omega)$ is presented in Fig. 3(a). We assume a BCS temperature dependence of the gap parameter, although, admittedly, $\Delta_{\max}^{(o)}(T)$ can be regarded as a fitting parameter in order to match the experimental INS spectra.[4–7] Single band fits to NMR Knight shift suggest a larger value of SC gap parameter[27] than that we use here ($\Delta_{\max}^{(o)}=15$ meV at $T=0$). In the bilayer case only *even* band contributes to $\chi'_{Ph}(0,0,0)$ (Ref. 28), i.e., $\Delta_{\max}^{(e)}$ may be larger than $\Delta_{\max}^{(o)}$ (Ref. 23). In addition, a different form of $\Delta_{\mathbf{k}}^{(i)}$ may alter $\Delta_{\max}^{(i)}$ necessary to fit experiments. We assume $J^{(o,o)}(\mathbf{Q})=-120$ meV. The calculated spectra reproduce all of the observed INS features in the SC state: the gap originating from the SC gap parameter (a); the sharp resonance peak at 41 meV at low temperatures, due to spin-flip quasiparticle excitations related to the VHS in the band structure (b); the sharp drop of the signal above 45 meV, also due to the band topology and the effect of renormalization (c). The overall enhancement of $\chi''^{(o,o)}(\mathbf{Q},\omega)$ is due to the nonvanishing coherence factor $p_{\mathbf{k}_A,\mathbf{k}_B}^{(o,o)2}$, present in d-wave superconductors[8,12] $(\Delta_{\mathbf{k}_A}^{(i)}\Delta_{\mathbf{k}_B}^{(i)}<0)$. At temperatures above T_c the magnetic scattering is depressed. However, in agreement with the experimental data (*d*), a broad peak at $\omega\approx 20-30$ meV remains (*spin pseudogap*). Its origin is the same as that of E_r resonance in the SC state (VHS); its position is shifted due to the SC gap vanishing.

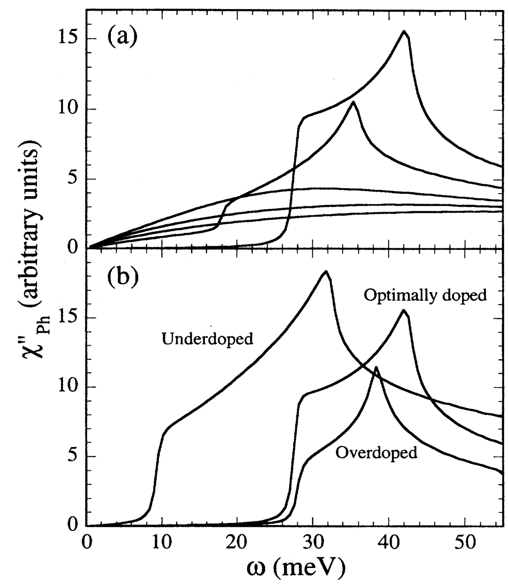

FIG. 3. The *odd* band susceptibility $\chi''^{(o,o)}(\mathbf{Q},\omega)$, defined in Eq. (3) and proportional to the INS measured intensity, as a function of energy. No finite lifetime effects are included (in both normal and SC state $\Gamma=0.5$ meV). $\chi''^{(o,o)}(\mathbf{Q},\omega)$ is gaped in the SC state and has a peak at $E_{sp}^{(o,o)}(\mathbf{q})$ (see text) due to the VHS below the FS. (a) The results for optimally doped YBCO corresponding to $T=0$, 80, 100, 200, 300 K (top to bottom). (b) The results for different doping levels and at $T=0$ K.

The doping dependence of $\chi''^{(o,o)}(\mathbf{Q},\omega)$ is shown in Fig. 3(b). For the underdoped case we applied the same criteria as for the optimally doped, i.e., the band parameters are chosen in accordance with ARPES measurements[20] which show that the VHS at $(\pi,0)$ remains approximately at the same energy below the FS, yet the filling is, obviously, much smaller. Therefore, in order to fit the experimental data we assumed, for the underdoped case, that $t=106$ meV, $t'/t=-0.18$, $t''/t=0.18$ and $\mu=-125$ meV ($n^{(o)}=0.7$), with $\Delta_{max}^{(o)}=5$ meV and $J^{(o,o)}(\mathbf{Q})=-200$ meV, and for the overdoped case we assumed $t=124$ meV, $t'/t=-0.22$, $t''/t=0.24$, and $\mu=-204$ meV ($n^{(o)}=0.5$) with $\Delta_{\max}^{(o)}$ equal to that in the optimally doped case and $J^{(o,o)}(\mathbf{Q})=0$. The calculated result is qualitatively similar to the experimental one.[4] Most importantly, since the value of $\Delta_{\max}^{(o)}$ is smaller for the underdoped materials, but the distance from the VHS at $\mathbf{q}=(\pi,0)$ to the FS remains the same as in the optimally doped case,[20] the resonance E_r must become broad at some doping level when this distance is approximately equal to $2.4\Delta_{\max}^{(o)}$, and this is what the experiment suggests.

In conclusion, we have shown that the Van Hove singularities, observed in ARPES at approximately 30 meV below the Fermi level, lead to well-defined magnetic quasiparticle excitations in the SC state, for quasi-2D systems and d-wave gap symmetry. Our model calculations of $\chi''_{Ph}(\mathbf{Q},q_z,\omega)$ are consistent with *all* major features observed in INS experiments. The model suggests a relatively small value for $\Delta_{\max}^{(o)}\approx 1.9k_BT_c$, and a relatively weak Heisenberg interaction for the *odd* band of optimally doped YBCO. In addition, our results show that the comparison of INS data and other magnetic probes, such as NMR, where both *odd* and *even* bands must be taken into account, may not be as straightforward as previously believed.

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