Interlayer pair tunneling and gap anisotropy in YBa$_2$Cu$_3$O$_{7−\delta}$

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Recent ARPES measurement observed a large ab-axis gap anisotropy, $\Delta(0, \pi)/\Delta(\pi, 0) = 1.5$, in clean YBa$_2$Cu$_3$O$_{7−\delta}$. This indicates that some sub-dominant component may exist in the $d_{x^2−y^2}$-wave dominant gap. We propose that the interlayer pairing tunneling contribution can be determined through the investigation of the order parameter anisotropy. Their potentially observable features in transport and spin dynamics are also studied.

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The symmetry of the order parameter continues to be a fundamental issue in the studies of high-$T_c$ cuprate superconductors. While the order parameter of cuprates is extensively believed to be dominated by $d_{x^2−y^2}$-wave, whether there exists a sub-dominant component remains an open question \[1\]. Recent angle-resolved photoemission spectroscopy (ARPES) measurement \[2\] has revealed a significant superconducting gap anisotropy in clean untwinned YBa$_2$Cu$_3$O$_{7−\delta}$ (YBCO). The excitation gap along the $k_y$ axis is found to be 50% more than that along the $k_x$ axis. This strongly suggests in YBCO that some sub-dominant component is involved in the $d_{x^2−y^2}$-wave dominant order parameter. It is important to ask what the symmetry and the mechanism of the sub-dominant component are.

In terms of structure and electronic properties, YBCO differs from La$_2$Sr$_2$CuO$_4$ (LSCO) or Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) in one crucial aspect. Due to the existence of one-dimensional (1D) CuO chain, the system is orthorhombic rather than tetragonal. The perfect $D_{4h}$ symmetry is broken which accounts naturally for the additional symmetry mixed in the order parameter. In this case, the most favorable order parameter is the so-called $d+s$ model, $\Delta_k \sim \cos(2\phi) + s [\phi$ is the azimuthal angle of $k$ on the Fermi surface (FS)], which arises providing that the in-plane pairing interaction is given by a separable $g(k, k') = -V f(k) f(k')$ with $V > 0$ and $f(k) = \cos(2\phi) + s$. The nodal lines of this gap are deviated from the usual diagonals $(k_x = \pm k_y)$ and consequently the gap magnitude is anisotropic between the $k_x$ and $k_y$ axes. The ARPES data, $\Delta(0, \pi)/\Delta(\pi, 0) = 1.5$, would correspond to $s = -0.2$ in this simple $d+s$ model.

Another complication occurs in YBCO (and also in BSCCO) because it involves more than one conducting layer within a unit cell. This enables the interlayer Cooper pair tunneling in the superconducting state. Following Chakravarty et al. \[3\], a superconducting bilayer is considered to be an interlayer pairing interaction term. Here the index 1 (2) denotes for layer 1 (2) and $T_J(k)$ is the interlayer Josephson pair tunneling coupling. The momentum-conserved interlayer pairing term \[4\] can be generated from the interlayer single-particle hopping $\sim \sum_k t_{ij}(k) a_{i,k}^\dagger a_{j,2k+}$, where the hopping integral $t_{ij}(k)$ can be determined from the band structure \[3\]. Thus $T_J(k) = t_{ij}(k)^2/t$ is usually assumed with $t$ the nearest-neighbor hopping. As pointed out by Chakravarty and Anderson \[3\], due to the highly non-Fermi liquid nature of cuprates, the coherent interlayer single-particle hopping is blocked, which nevertheless gives rise to the interlayer pair tunneling.

Combining \[3\] and the intralayer pairing term, one can write down the BCS gap equation for layer 1 (or 2)

$$\Delta_{kl} = -\sum_{k'} g(k, k') \langle a_{i-k',j} a_{i,k'} \rangle + T_J(k) \langle a_{i-j} a_{i,k} \rangle, \quad (2)$$

where $j \neq i$ and the angular bracket denotes the anomalous mean-field average. It should be stressed that the two (CuO$_2$ plane) layers considered here for YBCO are mediated and renormalized by the third CuO chain layer and appear to be orthorhombic instead of tetragonal. The issue is then how the interlayer pair tunneling plays the role between the two orthorhombic CuO$_2$ layers. For two identical layers, we assume $\langle a_{1-k,1} a_{1,k} \rangle = \langle a_{2-k,2} a_{2,k} \rangle = (\Delta_k^2/2E_k) \tanh(E_k/2T)$ by symmetry, where $E_k = [\xi_k^2 + \Delta_k^2]^{1/2}$ is the quasiparticle excitation spectrum with $\xi_k$ the particle band energy and $\Delta_k$ the overall gap self-consistently determined by \[3\]. At $T = 0$, Eq. \[3\] is reduced to (layer index is redundant)

$$\Delta_k = \Delta_0 f(k) + \Delta_k T_J(k)/2E_k, \quad (3)$$

where $\Delta_0 \equiv V \sum_k \omega_k \Delta_k f(k)/2E_k$ with $\omega_k$ an appropriate BCS cutoff frequency. At or near the FS ($|k| \simeq k_F$), $E_k \simeq |\Delta_k|$ and \[3\] is further reduced to

$$\Delta_k = \Delta_0 f(k) + T_J(k)/2 \text{sgn}[\Delta_k]. \quad (4)$$

Due to the term $\text{sgn}[\Delta_k]$, it sets a constraint in \[4\] that physical solutions of $\Delta_k$ arise only when $T_J(k)$ preserves the symmetry of $f(k)$ which in turn is determined by the nature of the layer pairing interaction. When the
symmetry of $T_J(k)$ is different from that of $f(k)$, the overall gap could exhibit a discontinuous phase on the FS. This would imply a physically unstable state. To fulfill the symmetry requirement, we thus argue that $t_{\perp}(k) \propto (\cos(2\phi) + s)^2$ and $T_J(k) \propto [\cos(2\phi) + s]s$ for the present superconducting orthorhombic bilayer. More precisely, the overall gap function in (4) is given by

$$\Delta_k = \Delta_0 [\cos(2\phi) + s] + \frac{T_J}{2} [\cos(2\phi) + s]^4 sgn[\cos(2\phi) + s],$$

(5)

where $T_J$ denotes the strength of the interlayer pair tunneling. Eq. (5) shows that not only the orthorhombicity $s$, but also the pair tunneling strength $T_J$ can be determined through the investigation of the gap function. It is worth emphasizing that when $s$ is small, the $ab$-axis gap anisotropy could still be large, as long as $T_J$ is significant.

The band structure calculation [3–5] and experimental evidences [6–8] usually assume $t_{\perp}(k) \propto (\cos k_x - \cos k_y)^2$ or $\propto \cos^2(2\phi)$ in the continuum limit for high-$T_c$ cuprates in a square lattice of perfectly tetragonal symmetry. This justifies our proposal $t_{\perp}(k) \propto [\cos(2\phi) + s]^2$ in the tetragonal limit ($s = 0$).

Fig. 3 shows the gap magnitude as a function of $\phi$ for two extreme cases: $s = -0.2, T_J = 0$ and $s = -0.06, T_J = 7.6\Delta_0$. (In fact, $\Delta_0$ is a function of $T_J$ through the self-consistent gap equation.) These two cases all give $\Delta(90^\circ)/\Delta(0^\circ) = 1.5$ in regard to the ARPES result. Several important features are noted for the anisotropic gap. The nodal angle, deviated from the diagonals, is now determined by

$$\phi_{\text{node}} = \frac{1}{2} \arccos(-s) \simeq \frac{\pi}{4} + \frac{s}{2} \quad (\text{for small } s)$$

(6)

in the first quadrant of the FS. Measurement of the nodal angle thus reveals the value of $s$. With the knowledge of $s$, one can then compare the gap magnitude between the two antinodes

$$\frac{|\Delta(90^\circ)|}{|\Delta(0^\circ)|} = \frac{(1 - s)[1 + r(1 - s)^3]}{(1 + s)[1 + r(1 + s)^3]}, \quad r = \frac{T_J}{2\Delta_0}$$

(7)

to obtain the value of $T_J$ (in unit of $\Delta_0$). Alternatively one can also study the gap slope near the nodes

$$\left| \frac{\partial|\Delta(\phi)/\Delta(0^\circ)|}{\partial\phi} \right|_{\phi = \phi_{\text{node}}} = \frac{2\sqrt{1 - s^2}}{(1 + s)[1 + r(1 + s)^3]},$$

(8)

which is 2 for a pure $d_{x^2-y^2}$-wave gap ($s = T_J = 0$).

If the instrumental resolution is fine enough, ARPES would be the best probe to explore $T_J$ and $s$ through the direct measurement of gap anisotropy. In the following, we study longitudinal ultrasonic attenuation and inelastic neutron scattering spectra which are also useful probes on these issues.

**Longitudinal Ultrasonic Attenuation** — Ultrasound attenuation is a directional probe and thus powerful to study the gap anisotropy. It has been successfully used to study the order parameter symmetry in superconducting heavy-fermion UPt$_3$ [9] and high-$T_c$ analog Sr$_2$RuO$_4$ compounds [10]. In clean YBCO where the scattering is in the ballistic limit [11], the longitudinal ultrasonic attenuation in the superconducting state is proportional to [12]

$$\alpha_s(q, T) \propto \sum_k \left[ \frac{\partial f(E_k)}{\partial E_k} \right] \xi_k^2 E_k \times \delta \left( \xi_k \frac{\partial \xi_k}{\partial k} \cdot q + \Delta_k \frac{\partial \Delta_k}{\partial k} \cdot q \right),$$

(9)

where $q$ is the wavevector of the propagating phonon and $f$ is the Fermi distribution function. We shall calculate (6) for one single-layer with the input of the interlayer pair tunneling gap in (3). This is sufficient if no other coupling or vertex correction is considered within the two layers. Inspection of (6) shows that $\alpha_s$ is governed by a delta function, weighted by the FS sum according to how small the gap is. For an isotropic s-wave superconductor, the second term in the delta function vanishes, i.e., only the portion of the FS perpendicular to $q$ contributes. For unconventional superconductors such as YBCO, the second term does contribute but is typically small ($\propto \Delta/\epsilon_F$ with $\Delta$ the maximum gap and $\epsilon_F$ the Fermi energy). By ignoring the second term in the delta function, Eq. (6) is simplified to

$$\frac{\alpha_s}{\alpha_n} = \frac{2\delta(k_F \cdot q)|f(|\Delta_k|)|}{\delta(k_F \cdot q)}$$

(10)

between the superconducting and normal states, where the angular bracket denotes the FS average. Since only two points on the (two-dimensional) FS satisfy $k_F \cdot q = 0$, Eq. (10) is simply solved to be $\alpha_s/\alpha_n = 2f(|\Delta_k|) = 2/\exp(|\Delta_k|/T) + 1]$, where $\theta$ is related to $\phi_q$ (the angle of $q$) by $\theta - \phi_q = \pi/2$. 

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**FIG. 1.** The gap magnitude as a function of the azimuthal angle on the FS for a superconducting orthorhombic bilayer with interlayer pair tunneling [using (6)].
In Fig. 2, \( \alpha_s/\alpha_n \) vs. \( \phi_q \) are shown at different temperatures for those two cases in Fig. 1. We have assumed \( 2\Delta(0^+)/T_c = 3.52 \) and the gap magnitude remains roughly the same for \( T \leq 0.5T_c \). [Of course, the exact \( T \) dependence of gap can be worked out through (2), which is not done in this paper.] The maximum \( \alpha_s/\alpha_n \) appear at a specific angle \( \phi_q \) at

\[
\phi_{\text{max}} = \frac{\pi}{2} - \phi_{\text{node}},
\]

where the nodal angle \( \phi_{\text{node}} \) is given in (3) and we limit \( 0 \leq \phi_{\text{max}}, \phi_{\text{node}} \leq \pi/2 \). Since \( \phi_{\text{node}} \) depends on the value of \( s \), determination of \( \phi_{\text{max}} \) in \( \alpha_s/\alpha_n \) thus determines \( s \). In addition, the ratio at \( \phi_q = 0 \) to \( \pi/2 \),

\[
\begin{align*}
\frac{\alpha_s/\alpha_n(\phi_q = 0)}{\alpha_s/\alpha_n(\phi_q = \pi/2)} &= 1 + \exp \left[ \frac{\Delta_0}{\Delta(0)} \left( \frac{1 + s}{1 + r(1 + s)^3} \right) \right] \\
&\quad \cdot \left( 1 + \exp \left[ \frac{\Delta_0}{\Delta(0)} \left( \frac{1 - s}{1 + r(1 - s)^3} \right) \right] \right),
\end{align*}
\]

(12)

allows one to extract the strength of \( T_J \). Furthermore, near the critical value, the slope

\[
\left| \frac{\partial(\alpha_s/\alpha_n)}{\partial \phi_q} \right|_{\phi_q \approx \phi_{\text{max}}} = \frac{\Delta_0}{T} \frac{\sqrt{1 - s^2}}{(1 + s)[1 + r(1 + s)^3]},
\]

(13)

which gives one more way to look into \( T_J \) and \( s \), as well as \( \Delta_0 \).

Spin Excitation Spectra — Recent inelastic neutron scattering (INS) experiments have reported many interesting results for high-\( T_c \) cuprates regarding the commensurate and incommensurate (IC) peaks at or near the antiferromagnetic (AF) wavevector \( \mathbf{Q}_{\text{AF}} = (\pi, \pi) \) [14]. For YBCO or BSCCO, the appearance of the commensurate peaks are likely due to some kind of resonance, while the IC peaks are associated with the dynamical local nesting effect of the band structures [13, 17].

Theoretically the INS spectra is proportional to the imaginary part of the spin susceptibility and, for simplicity, we study the irreducible BCS spin susceptibility \( \chi_0^s(\mathbf{q}, \omega) \) for one single-layer. In Fig. 3, \( \text{Im}\chi_0^s \) are calculated at \( T = 0 \) for some fixed frequency \( \omega \) and momentum \( \mathbf{q} \) scanned along the direction shown in the inset. The primary interest is to see how the gap (3) affects the INS spectra. To study the IC peaks, a tight-binding band \( \xi_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu \) is inevitably used, where \( t \) and \( t' \) are respectively the nearest-neighbor and next-nearest-neighbor hopping and \( \mu \) is the chemical potential. Typical values of \( t' = -0.25t \) and \( \mu = -0.65t \) are employed. For the gap, \( \cos(2\phi) \) in (3) is replaced by \( (\cos k_y - \cos k_x)/2 \) in the present lattice case and we assume the gap magnitude at \( k_x \)-axis, \( \Delta(0) = 0.3t. \) The same two cases in Figs. 1 and 3 are studied. For the \( T_J = 0 \) (larger \( s \)) case, the nodes are shifted away from the diagonals and consequently the nesting effect is highly anisotropic: the IC peak parallel...
to $q_y$ axis (along the $q$ scan route chosen) is more intense than the one parallel to $q_x$ axis. At lower frequency, the latter could completely disappear before the nesting effect can set in. For the strong $T_J$ (small $s$) case, in contrast, the nodes remain closer to the diagonals and, as a result, the nesting effect is roughly isotropic. The IC peaks are nearly symmetric along the $q$ route, regardless the change of frequency. These are the key features which can be used to distinguish the strong and weak $T_J$ (or small and large $s$) cases.

When the commensurate peaks are also considered, the Random phase approximation (RPA) corrected spin susceptibility $\chi^s(q, \omega) = \chi^s_0(q, \omega)/[1 - V(q)\chi^s_0(q, \omega)]$ is often studied, where $V(q)$ is usually modeled by an “AF” interaction $V(q) = -J(\cos q_x + \cos q_y)/2$ ($J > 0$). Since here we are only interested in the IC peaks which appear beyond the AF resonant regime, it’s adequate to study $\chi^s_0$. The line shape in $\text{Im} \chi^s(q, \omega)$ will be very similar to those in $\chi^s_0(q, \omega)$, apart from different intensity.

Mook et al. [18,19] have recently reported the 1D nature for the IC peaks in underdoped YBa$_2$Cu$_3$O$_{6.6}$. The IC peak intensity at $(\pi - \delta, \pi)$ is found to be stronger than that at $(\pi, \pi - \delta)$. While the results are referred to favor the formation of the dynamical stripes for that particular doping [18], an alternative explanation to these data is to take into account the in-plane gap anisotropy associated with a homogeneous Fermi liquid [18]. The data of Mook et al. seems indicating an intermediate value of $T_J$ (and an intermediate and positive $s$) on YBa$_2$Cu$_3$O$_{6.6}$, when comparing to the results in Fig. 3. It is important to have INS performed at different frequencies in order to clarify the gap anisotropy.

In summary, we propose that the long-thought interlayer pair tunneling effect can be explored through the detailed studies of the gap anisotropy in YBa$_2$Cu$_3$O$_{6.6}$. Considering an orthorhombic superconducting bilayer with interlayer pair tunneling, one can simultaneously determine the in-plane orthorhombicity and the strength of the pair tunneling. For probable probes, we study longitudinal ultrasonic attenuation and inelastic neutron scattering.

Finally, we comment on the effect of pair tunneling on the collective modes. For a superconducting bilayer coupled by the pair tunneling, apart from the gap renormalization, the system will exhibit the characteristic in-phase and out-of-phase phase modes associated with the order parameters on the two layers. The in-phase Anderson-Bogoliubov phase mode has a phonon dispersion, $\omega^2 = v_F^2 q^2/2$, which is lifted to plasmon mode when long-range Coulomb potential is included. These in-phase modes, which are intrinsic characteristics of a superconductor, are independent of $T_J$. In contrast, the out-of-phase phase mode has an optical phonon dispersion $\omega^2 = \omega_0^2 + v_F^2 q^2/2$, where $\omega_0$ depends on the relative size of planar pair interaction $V$ and $T_J$ [20]. It is also interesting to study $T_J$ through the search of the out-of-phase phase modes, such as those recently observed in SmLa$_{0.8}$Sr$_{0.2}$CuO$_{4-\delta}$ with two different Josephson couplings [21].

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