Quasiparticle bands and superconductivity in bilayer cuprates.

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We analyze the generic features of the energy spectrum for two coupled CuO$_2$ layers with a realistic extended Hubbard model. The quasiparticle bands exhibit flat regions near X(Y) points in the Brillouin zone with a large reduction of the bonding-antibonding splitting, and pinning of extended van-Hove singularity to the Fermi level, which is more efficient for a bi-layers than for a single layer. In contrast to the results with simpler models, the superconducting temperature for $d_{x^2-y^2}$ pairing is not lowered by the bi-layer hopping.

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The role of multiple layers in the high-temperature superconductors continues to be one of the most intriguing puzzles, with many conflicting proposals and interpretations. One proposal is that superconductivity is enhanced by electronic correlations which are argued to greatly reduce single-particle hopping between layers while allowing pair-tunneling. Angle-resolved photoemission (ARPES) studies of the energy spectrum near the Fermi energy for bi-layer materials can in principal answer the questions of the nature of the bonding and antibonding bands near the Fermi level. However, one recent ARPES experiment resolved only one CuO$_2$ band at the Fermi surface in BSCO-2212, supporting the idea of a greatly reduced interlayer hopping, whereas another measurement reports two Fermi sheets, in general agreement with the predictions of band structure calculations. In addition, there is evidence for important effects of coupling between the layers in bilayer systems. Neutron scattering experiments see maximum intensity for wave vectors the $q_z \sim \pi/L$, where L is the interlayer spacing, for both the antiferromagnetic insulator and in the superconductor.

A generic feature which has emerged from the ARPES experiments is a “flat-band” or “extended van-Hove singularity” which is “pinned” to the Fermi level for different hole dopings. Bifurcated saddle points very close to the Fermi level had, in fact, been predicted by LDA calculations for YBCO-123 and caused by dimpling of the CuO$_2$ planes. The flat band observed by ARPES has also been attributed to many-body effects, and a number of studies have been done for correlated electronic states in a single CuO$_2$ plane. The flat region in the quasiparticle spectrum has been proposed to be a “fermion condensate”, or a non-Fermi liquid area formed in $(\mathbf{q}, \omega)$ space near two-dimensional van-Hove singularity. The one-band and three-band Hubbard models as well as t-J model show a flat quasiparticle band just below the Fermi energy, which has an “extended” van-Hove singularity near the X(π,0)-point, due to antiferromagnetic spin fluctuations. The same antiferromagnetic fluctuations at $\mathbf{q} \approx (\pi, \pi)$ lead to $d_{x^2-y^2}$ superconductivity with a relatively high transition temperature. For the two-plane Hubbard model with a simple tight-binding spectrum a reduction of superconducting correlations was found due to the interlayer coupling.

In this paper we study the bi-layer Hubbard model with realistic LDA derived hopping integrals. Combination of this realistic tight-binding (TB) model with many-body effects accounts for anomalous properties of cuprate superconductors. Thus in the normal state of our BSCO model, many body effects strongly reduce the splitting between the bonding and antibonding bands in the regions in the $\mathbf{k}$-space where the one-body splitting is large, leading to flat bands near the chemical potential to within an energy of order room temperature. On the other hand, in the regions where the many-body effects are small, there is also little splitting in the one-particle spectrum, due to geometry of the bi-layer bonding in the cuprates. We analyze the pinning of the chemical potential to these van-Hove singularities in the case of a mono- and bi-layer model for different hole dopings. A calculation of the superconducting transition temperature shows robust stability of the $d_{x^2-y^2}$ state in the “three-dimensional” bi-layer case.

Let us start with the Hubbard hamiltonian for a bilayer CuO$_2$ model:

$$H = \sum_{\alpha \sigma} \epsilon_\alpha c^\dagger_\alpha \sigma c^{}_{\alpha \sigma} + U \sum_{\alpha} n_{\alpha \uparrow} n_{\alpha \downarrow} - \mu \sum_{\alpha} n_{\alpha \sigma},$$

Here $t_{i\alpha,j\beta}$ are the hopping integrals which gives the energy bands $\epsilon_\alpha(\mathbf{k})$, $i,j$ are the site indices inside the plane and $\alpha(\beta)$ are the plane indices, U is the on-site Coulomb repulsion and $\mu$ is the chemical potential. Due to the mirror plane symmetry for the bilayer we can define bonding ($+$) and antibonding ($-$) electron bands $\epsilon_+(\mathbf{k})$ and $\epsilon_-(\mathbf{k})$, where $\mathbf{k}$ is a vector in the two dimensional Brillouin zone. This symmetry also holds for the quasiparticle excitation spectrum of the full interacting system. For our studies we have used different schemes which range from the simplest model (only nearest-neighbor
hopping in-plane and between planes) to realistic four-and eight-band models, obtained by integrating out the high-energy degrees of freedom from the full LDA calculations for cuprate superconductors [16].

For BSCO bi-layer materials we use a four-band Hamiltonian [17], which includes the standard Cu-3dₓ²₋ᵧ², and O-pₓ+pᵧ orbitals, plus the “Cu-s” orbital which has also some Cu-dₓ²-zy character. The last band is needed because the standard 3-band model does not give an adequate description of the valence band and the Fermi surface [17]. The Cu-s orbital provide the 2nd and 3rd nearest neighbor (t’ and t”) intra-plane hopping integrals, as well as the hoping between the CuO₂ planes in the low-energy Hamiltonian H. Diagonalization of its first term yields the (simplified) “LDA bands”:

\[ \varepsilon_\pm(k) = -2t(\cos k_x + \cos k_y) - 4t’ \cos k_x \cos k_y - 2t''(2k_x + \cos k_y) \mp t_\perp (\cos k_x - \cos k_y)^2 / 4. \]

Note that the interlayer hopping is anisotropic with the maximum splitting of \( \varepsilon_+ (k) \) and \( \varepsilon_- (k) \) at the X(\( \pi, 0 \)) and Y(\( 0, \pi \)) points and no splitting in the direction from \( \Gamma(0, 0) \) to M(\( \pi, \pi \)). We chose values of the tight-binding parameters for BSCO: \( t = 0.5 \text{ eV}, \ t’ / t = -0.3, \ t'' / t’ = 0.2 \) and \( t_\perp = 0.15 \text{ eV} \), close to the LDA parameters [17]. The total band width is \( 6t = 4 \text{ eV} \) and the bonding-antibonding splitting at the X-point is \( 2t_\perp = 0.3 \text{ eV} \). The screened electron-electron interaction parameter for Cuₓ orbitals obtained in the constrained LDA calculations for cuprate is \( 7-8 \text{ eV} \) [18]. Since the Cu_s character at the Fermi surface is approximately 65% [17] the effective \( U \) is reduced by 0.65² and we used in the present study \( U = 3.2 \text{ eV} \). This is a bit less than the band width, but general results are not very sensitive to the real \( U \)-values. Note that most many-body Monte-Carlo calculations [14,15] use only a simple tight-binding model: single - \( t \) parameter and isotropic \( t_\perp \). We believe that in the cuprate system both many body effects and the band dispersion play a crucial role.

We used the conserving fluctuation-exchange (FLEX) approximation [19], which gives an energy spectrum for CuO₂ plane almost identical to Quantum Monte Carlo results [14]. We calculate the self-consistent one-electron Green’s function in the normal state:

\[ G_\pm(k, \omega_n) = \frac{1}{i\omega_n - \varepsilon_\pm(k) - \mu - \Sigma_\pm(k, \omega_n)}, \]

where \( \Sigma_\pm(k, \omega_n) \) are bonding and antibonding self-energies and \( \omega_n = (2n+1)\pi T \) are the fermion Matsubara frequencies with \( n \) an integer and \( T \) the system temperature. It is convenient to introduce the simple notation: \( k = (k, \omega_n) \) and \( \sum_k = \frac{1}{N} \sum_k \omega_n \), where \( N \) is the total number of momentum points. The straightforward generalization of the FLEX approximation [19] to the case of a bilayer two-band Hubbard model gives the following equation for the self-energy:

\[ \Sigma_\pm(k) = \sum_q [V_+(q)G_\pm(k - q) + V_-(q)G_\mp(k - q)], \]

where the contribution to effective potential \( V_\pm(q) = V_\pm^s(q) + V_\pm^c(q) \) from spin and charge fluctuation are:

\[ V_\pm^s = \frac{3}{2} \frac{U^2 \chi_\pm}{1 - U \chi_\pm} - V_\pm^{dc}, \quad V_\pm^c = \frac{1}{2} \frac{U^2 \chi_\pm}{1 + U \chi_\pm} - V_\pm^{dc}, \]

here \( V_\pm^{dc} = \frac{1}{2} U^2 \chi_\pm \) is the double counted contribution and \( V_\pm(q) \) is defined self-consistently thorough particle-hole susceptibility for bi-layer:

\[ \chi_\pm(q) = - \sum_k [G_+(k)G_\pm(k + q) + G_-(k)G_\mp(k + q)]. \]

We solve the nonlinear integral FLEX-equations using the fast Fourier transform (FFT) method [20] on the discrete mesh of 64×64 momenta in the two dimensional Brillouin zone and 600-900 Matsubara frequencies with the cutoff of 20-30 eV (which corresponds to the temperature range of 80-200K). Analytical continuation on the real axes was done by Padé approximation. The calculations have been carried out for different hole concentrations: \( \delta = 0.1 - 0.4 \) per plane.

![FIG. 1. The bi-layer spectral function for different directions in the Brillouin zone (\( \delta = 0.25, T=150 \text{ K} \)).](image)

The spectral function \( A(k, \omega) = -1 / \pi Im(G_+(k, \omega) + G_-(k, \omega)) \) for hole doping \( \delta = 0.25 \) per CuO₂ and \( T=150 \text{ K} \) is shown in Fig.1 for \( \Gamma-X-M \) directions. One sees that there is only a single peak with a “non-Lorentzian” behavior crossing the Fermi level. In fact there are two bands with the large renormalization of the interlayer splitting from 300 meV to 40 meV, and there is large broadening at the actual temperature of the measurement in the normal state.
FIG. 2. Energy spectrum for $U=0$ (TB) and $U\neq 0$ (QP) for the antibonding (top) and bonding (bottom) bands.

This is illustrated in Fig. 2, which shows a comparison of the pure tight-binding spectrum ($U=0$) and the quasiparticle spectrum (QP) for $\delta = 0.25$ for the bonding (b) and antibonding (a) bands together with corresponding Fermi-surface (zero-energy contour). The quasiparticle dispersion $\varepsilon_{\pm}(k)$ have been determined through the maximum in the spectral function $A_{\pm}(k, \omega)$. Note that already the TB (or LDA) bands differ substantially from the simple model with only one hopping $-t$: the position of the saddle points at the X and Y points is lower (for “$t$-model” they are located at the middle of the band i.e. at $1 \text{ eV}$ in Fig. 2). This TB-spectrum changes the topology of the Fermi surface, and makes the hole doped and the electron doped situations quite different (as it should be experimentally) and suppresses the nesting near half-filling. The last effect increases the width of a susceptibility peak near M($\pi, \pi$) point and reduces the antiferromagnetic spin-correlation length from $\approx 3$ to $\approx 1$ one lattice spacing. This leads to the suppression of the “shadow bands” in the quasiparticle spectrum which occur in the simpler model with $t' = t'' = 0$ and small doping $\delta \approx 0.1$.

A more important consequence of $t'$ and $t''$ is related to the increased flatness of the van-Hove singularities in the direction towards $\Gamma$, which leads to a larger phase space for the spin and charge excitations. This results in a drastic renormalization of the energy spectrum (Fig. 2), mainly due to spin-fluctuation effects. The quasiparticle bands exhibit flat regions near X(Y) points in the Brillouin zone with a large reduction of the bonding-antibonding splitting. Note that the susceptibility for anti-ferromagnetic coupling across the bi-layer $\chi_{-}(q)$ exceeds that $\chi_{+}(q)$, for ferromagnetic coupling and near $q = (\pi, \pi)$ the difference could be even an order of magnitude for $t' = t'' = 0$, reflecting the enhancement of the antiferromagnetic fluctuations between the layer. The Fermi surface is similar to the LDA, but the large flattening of the quasiparticle bands and the broadening of the spectral function is not properly described in LDA.

We plot in Fig. 3 the “temperature” smeared Fermi surface ($\mu = \pm T$ for $T = 150K$) and constant occupation number contours: $n(k) = \sum_n A(k, \omega_n)$ with $n_0=0.5$ corresponding to the Fermi surface. Note the extensive regions of nearly equal occupation $\approx 0.5$ near the X and Y points. It is clear that the difference between the bonding and antibonding Fermi surface sheets for the BSCO model is very small and hard to detect experimentally. We believe that the “shadow band” obtained in the recent ARPES experiment is related to the large dark region near X(Y)-point for the antibonding bands. This flat region of the quasiparticle spectrum within the room temperature scale from the Fermi level gives the anomalous linear dependence of the self energy on temperature and frequency, just from the “phase-space” argument detected numerically near X and Y points.

In order to show more clearly the formation of the flat quasiparticle band in the bi-layer system we plot in the Fig. 4 the TB and QP spectrum for $\delta = 0.35$ where the Fermi level is approximately between bonding and antibonding bands at X. While the Fermi-level crossing-points are nearly the same in the TB and QP bands, the bonding and antibonding QP bands are “pinned” to the Fermi level within room temperature scale. In other words, the system has increased the spin and charge fluctuations by pinning the saddle points to the Fermi level and forming the extended van-Hove singularities instead of the standard renormalization of the spectrum only in the small region near the Fermi surface.
We have analyzed the effect of the saddle-points pinning to chemical potential for the monolayer \( (t_\perp = 0) \) and the bilayer models. The energy position of the saddle-point at \( X \) with respect to the Fermi level for the TB- and QP-spectrum as functions of the hole doping shown in the Fig.4. The antibonding QP-band for the bi-layer model \( (\text{Bi-a}) \) stays within the \( \pm 5 \) meV for large hole concentration range \( 0.1 < \delta < 0.3 \) per CuO\(_2\). Such a pinning effect is less pronounced in the monolayer (Fig.3).

We have repeated the calculations for the YBCO eight-band TB-model and found that the "bifurcated" saddle points in the TB-spectrum helps to create the extended anisotropic van-Hove singularity. In the YBCO model interlayer splitting is reduced by only a factor of two and could be in principle detected by ARPES measurements.

In conclusion, we have shown that the generic feature of bi-layer as well as mono-layer cuprate is the formation of extended van-Hove singularities near the chemical potential on the scale of the temperature, which occurs more readily in bi-layers. This leads to large areas of the Brillouin zone with nearly constant occupation \( \approx 0.5 \), which can explain the anomalous normal state properties and lead to enhanced \( d_{x^2-y^2} \) superconductivity.

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[1] S. Chakravarty, A. Sudbø, P.W. Anderson, and S. Strong, Science, 261, 337 (1993)
[2] Z.-X. Shen et al., Science, 267, 343 (1995).
[3] H.Ding et al., Phys. Rev. Lett. 74, 2784 (1995); H.Ding, A.F. Bellman et al., preprint.
[4] J.M. Tranquada et al., Phys. Rev. B 46, 5561 (1992).
[5] O.K. Andersen et al., Physica C185-189, 147 (1991).
[6] O.K.Andersen et al., Phys. Rev. B 49, 4145 (1994).
[7] N. Bulut et al., Phys. Rev. B 50, 7215 (1994).
[8] E. Dagotto et al., Phys. Rev. Lett. 73, 728 (1994).
[9] R. Preuss et al., Phys. Rev. Lett. 75, 1344 (1995).
[10] V.A. Khodel et al., JETP Lett. 51, 553 (1990).
[11] P. Nozieres, J. Phys. 2, 443, 1992.
[12] I.E. Dzyaloshinskii, Sov. Phys. JETP 66, 848, 1987.
[13] R. Putz, R. Preuss et al., preprint.
[14] D.J. Scalapino, Physics Reports. 251, 1 (1994).
[15] N. Bulut et al., Phys. Rev. B 45, 5577 (1992).
[16] R.T. Scalettar et al., Phys. Rev. B 50, 13419 (1994).
[17] O.K. Andersen et al., J. Phys. Chem. Solids, (1995).
[18] A.K. Mcmahon et al., Phys. Rev. B 38, 6650 (1988).
[19] N.E. Bickers et al., Annals of Physics, 193, 206 (1989).
[20] J.W. Serene et al., Phys. Rev. B 44, 3391 (1991).
[21] A.P. Kampf et al., Phys. Rev. B 42, 7967 (1990).
[22] M. Langer, J. Schmalian et al., preprint.
[23] M. Randeria et al., Phys. Rev. Lett. 74, 4951 (1995)
[24] S. Gopalan et al., Phys. Rev. B46, 11798 (1992).
[25] P. Monthoux et al., Phys. Rev. Lett. 72, 1874 (1994).
[26] P.A. Lee and N. Read, Phys. Rev. Lett. 25, 2691, 1987.