Proximity Effects and Quantum Dissipation in the Chains of \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \)

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We argue that the results of recent scanning tunneling microscopy, angle-resolved photoemission and infrared spectroscopy experiments on the CuO chains of \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \) (YBCO) and how the onset of planar superconductivity affects the electronic degrees of freedom in the chains. The observation of a superfluid component in the chains below the planar temperature \( T \) is consistent with recent scanning tunneling microscopy (STM) experiments which reported a large gap ∼ 15−25 meV in the chain density of states (CDOS) below \( T_c \). Additional information comes from angle-resolved photoemission (ARPES) experiments which observed a sharp peak as well as a large incoherent "hump" in the chain spectral function, \( A_c \).

In this Letter we show that the above-cited results of IS, STM and ARPES experiments are consistently explained within a proximity model by the interplay of a coherent chain-plane (CP) and an incoherent interchain (IC) coupling \( \tilde{t}_{1\perp} \). We demonstrate that the coherent/incoherent nature of these couplings causes the CuO₂ planes to be an ohmic heat bath for the electronic degrees of freedom in the chains. As a result, the chains exhibit a substantial quantum dissipation, similar to the case of a two-level system coupled to set of harmonic oscillators \( \tilde{t}_{1\perp} \). With the onset of planar superconductivity a frequency gap opens in the dissipative heat bath, and a Fermi-gas like peak appears in the chain spectral function. Simultaneously, charge excitations in the chains acquire a universal superconducting (SC) gap whose phase and magnitude are momentum dependent. We predict that the magnitude of this gap varies non-monotonically with the hole concentration in the chains.

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Little is known about the coupling of the CuO₂ planes and CuO chains in \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \) (YBCO) and how the onset of planar superconductivity affects the electronic degrees of freedom in the chains. The observation of a superfluid component in the chains below the planar temperature \( T \) is consistent with recent scanning tunneling microscopy (STM) experiments [2,3] which reported a large gap ∼ 15−25 meV in the chain density of states (CDOS) below \( T_c \). Additional information comes from angle-resolved photoemission (ARPES) experiments which observed a sharp peak as well as a large incoherent "hump" in the chain spectral function, \( A_c \).

In this Letter we show that the above-cited results of IS, STM and ARPES experiments are consistently explained within a proximity model by the interplay of a coherent chain-plane (CP) and an incoherent interchain (IC) coupling \( \tilde{t}_{1\perp} \). We demonstrate that the coherent/incoherent nature of these couplings causes the CuO₂ planes to be an ohmic heat bath for the electronic degrees of freedom in the chains. As a result, the chains exhibit a substantial quantum dissipation, similar to the case of a two-level system coupled to set of harmonic oscillators \( \tilde{t}_{1\perp} \). With the onset of planar superconductivity a frequency gap opens in the dissipative heat bath, and a Fermi-gas like peak appears in the chain spectral function. Simultaneously, charge excitations in the chains acquire a universal superconducting (SC) gap whose phase and magnitude are momentum dependent. We predict that the magnitude of this gap varies non-monotonically with the hole concentration in the chains.

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For the calculation of the CDOS and spectral function, measured in surface sensitive ARPES and STM experiments, we consider an infinite array of CuO-chains which is aligned along the x-axis and coupled to a single CuO₂-plane via a hopping term \( \tilde{t}_{1\perp} \). We neglect the second CuO₂-plane in the bilayer unit cell since the planes are only weakly coupled \( \tilde{t}_{1\perp} \). We assume that the superconducting pairing interaction resides solely in the plane, and describe the planar electrons by a mean-field BCS-hamiltonian. The hamiltonian for the chain-plane system is thus given by

\[
\mathcal{H} = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k} \left( \Delta_{k} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c. \right) \\
+ \sum_{k,\sigma} \zeta_k d_{k,\sigma}^\dagger d_{k,\sigma} - t_{1\perp} \sum_{k,\sigma} \left( c_{k,\sigma}^\dagger d_{k,\sigma}^\dagger + h.c. \right) \quad (1)
\]

where \( c_{k,\sigma}^\dagger, d_{k,\sigma}^\dagger \) are the fermionic creation operators in the plane and chain, respectively. The tight-binding dispersions for the plane and chain electrons, \( \varepsilon_k \) and \( \zeta_k \), are given by

\[
\varepsilon_k = -2t_p \left( \cos(k_x) + \cos(k_y) \right) - 4t_p' \cos(k_x) \cos(k_y) - \mu_p \ ,
\]

\[
\zeta_k = -2t_{1\perp} \cos(k_x) - \mu_c .
\]

Here, \( t_p, t_p' (t_{1\perp}) \) are the planar (chain) hopping elements between nearest and next-nearest neighbors, respectively, and \( \mu_p (\mu_c) \) is the planar (chain) chemical potential. The planar SC gap is given by \( \Delta_k = \Delta_{SC} \left( \cos(k_x) - \cos(k_y) \right)/2 \).

An effective action for the chain electrons, \( S_c \), is obtained by integrating out the planar electronic degrees of freedom. One obtains

\[
S = \sum_{\omega_n, l,m} \int dk_x d_l^\dagger \tilde{G}_c^{-1}(\omega_n, k_x, l, m) \tilde{d}_l \quad (3)
\]

where \( l, m \) are chain indices, and

\[
\tilde{d}_l^\dagger = (d_{l\uparrow}^\dagger(k_x, \omega_n), d_{l\downarrow}^\dagger(-k_x, -\omega_n)) . \quad (4)
\]

For the matrix \( \tilde{G}_c^{-1} \) one has

\[
\tilde{G}_c^{-1} = \begin{pmatrix} G_{00}^{-1}(k_x, \omega_n) & F_{00}^{-1}(k_x, \omega_n) \\ F_{00}^{-1}(k_x, \omega_n) & -G_{00}^{-1}(-k_x, -\omega_n) \end{pmatrix} , \quad (5)
\]
ments on YBCO [4] and a planar SC gap, $\Delta_{SC}$. One evaluates Eq.(3) using the ansatz $A(k,\omega)$ $= 1$ $+ e^{i\omega_{\parallel}(l-m)}$; hence no superconducting correlations are present in the chains, in disagreement with the results of IS experiments [1]. We thus conclude that the experimental STM and IS data provide strong evidence for an incoherent interchain and coherent chain-plane coupling in YBCO.

Before we can address the physical origin of the different CDOS for coherent and incoherent IC coupling, it is necessary to study the spectral function, $A_c(k,\omega)$, for incoherent IC coupling, in more detail. In Fig. 2 we present our numerical results for $A_c$ at $k_c = 0.25\pi$. For comparison with ARPES measurements we have multiplied $A_c$ with the Fermi distribution function $n_F = \left(\exp(\omega/k_BT) + 1\right)^{-1}$, which shifts the peak in $A_c$ to lower energies. In the normal state (dashed line) the spectral function exhibits a broad peak, indicating a strong quasiparticle damping. The source of the quasiparticle dissipation is best understood by analytically evaluating the integrals on the r.h.s. of Eq.(3). One obtains for the retarded chain Greens function at momentum $k_x$.
where $\alpha = \frac{t_1^2}{v} \bar{v} = (\partial \epsilon_k / \partial k_n) |_{p_0}$, and $p_0$ is a momentum on the planar Fermi surface (FS) with $p_0^2 = k_x$ (see inset of Fig. 2). Due to the coupling, $t_{\perp}$, the chain electrons can decay into a continuum of planar states perpendicular to the chain direction. The planes thus represent a dissipative environment which gives rise to a frequency independent quasiparticle damping, $\alpha$. This form of dissipation is analogous to the “ohmic case” discussed by Leggett et al. 3 for a two-level system coupled to a set of one-dimensional harmonic oscillators, which constitute a similar dissipative “heat bath”. Thus, $\alpha$ does not arise from a Coulomb-type interaction, but from the different dimensionality of the chain and plane system.

With the onset of superconductivity, the planar heat bath acquires a gap and the frequency dependence of $A_c$ (solid line in Fig. 2) changes dramatically. At low frequencies, the damping of the chain electrons is strongly reduced and a Fermi-gas-like low-frequency quasiparticle peak (LFQP) appears. The suppression of the quasiparticle damping arises from a kinematic constraint since a chain electron can only decay into the continuum of planar states if its frequency exceeds the necessary energy, $\Delta(k_x) = |\Delta(p_0)|$, to break a Cooper-pair. Hence, one recovers a substantial quasiparticle damping only for $\omega > \Delta(k_x)$. Moreover, the LFQP is shifted downward in energy from the position of the broad peak at $\omega = 0$ in the normal state (cf. solid line), indicating the presence of a gap for electronic excitations in the chains. This gap arises from a virtual hopping of a chain electron into the planar continuum states, a process which lowers the electronic ground state energy; hence, one expects the gap to be of order $t_{\perp}^2 / v_F$. Moreover, an analysis of $F_0$, Eq. (3), shows that the phase of the induced gap is momentum dependent and changes at $k_n$, where $K_{\text{node}} = (k_n, k_n)$ is the momentum of the planar SC nodes. The separation of the LFQP and the incoherent background by a dip in Fig. 2 is reminiscent of planar ARPES data 15 where a decrease of the fermionic damping in the SC state due to the opening of a spin gap gives also rise to a “peak-dip-hump” structure in the spectral function.

In order to better understand the momentum dependence of $A_c$ below $T_c$, it is necessary to analytically study the retarded chain Greens function, $G_c^R$, in Eq. (1). One obtains

$$G_c^R(k_x, \omega) = \frac{1}{\omega - \zeta_k + i \delta},$$

where $\zeta_k = \frac{\alpha \omega}{\sqrt{\Delta^2 - \omega^2}},$ and $\omega = \omega + i \delta$. The dispersion, $\zeta_k$, of the LFQP is determined by $\text{Re} B(\omega = \zeta_k) = 0$. In the limit $\alpha^2 + \zeta_k^2 \ll \Delta^2$, i.e., close to the chain Fermi points, one has

$$\chi_k = \pm \sqrt{\alpha + \zeta_k^2},$$

where $\alpha$ is the universal SC chain gap, which is independent of the planar gap, $\Delta_{\text{SC}}$. In the opposite limit, $\alpha^2 + \zeta_k^2 \gg \Delta^2$, one obtains

$$\chi_k = \pm \Delta \left[1 - \frac{2 \alpha^2 \Delta^2}{(\alpha^2 + \zeta_k^2)^2}\right],$$

and the LFQP is thus confined to frequencies $|\omega| < |\Delta|$ for all $k_x$. In addition, one finds a high-frequency quasiparticle peak (HFQP) whose dispersion is given by $\phi_k = \pm \sqrt{\zeta_k^2 + \alpha^2}$. Since $\phi_k > |\Delta|$, the HFQP is overdamped with

$$A_c(k_x, \omega = \phi_k) = \sqrt{\phi_k^2 - \Delta^2} \frac{\phi_k + \zeta_k}{\alpha \phi_k^2} \sim \alpha^{-1}. \quad (13)$$

In the limit $\zeta_k \gg \max\{\Delta, \alpha\}$, the HFQP follows the dispersion of the free chain electrons, $\phi_k = \zeta_k$, with a momentum independent intensity, $A_c = \alpha^{-1}$.

In Fig. 3 we present our numerical results for $A_c$ in the SC state for several momenta around $k_F$. For momenta much below $k_F$ ($k_x = 0.19\pi$, solid line; $k_x = 0.22\pi$, dashed line) $A_c$ possesses a HFQP and a LFQP, which both move to higher energies as $k_x$ approaches $k_F$. The dispersion of the LFQP is much weaker than that of the HFQP, since the LFQP is located close to $\Delta(k_x)$ which changes only weakly with momentum while the HFQP’s dispersion is given by $\zeta_k$. Note the momentum independence of the HFQP’s intensity. At the Fermi momentum, $k_F = 0.25\pi$, the HFQP has disappeared and only a
broad incoherent background remains with a maximum close to its onset frequency $\Delta \approx -17$ meV. For momenta above $k_F^\perp$, $(k_x = 0.27\pi$, dashed-dotted line) the LFQP shifts again to lower energies, while its intensity and that of the incoherent background decreases rapidly. An increased CP coupling ($t_{\perp} = 0.4t_p$) leaves $A_c$ qualitatively unchanged, albeit with a much broader HFQP. The momentum and frequency dependence of $A_c$ shown in Fig. 3 is in qualitative agreement with recent ARPES experiments by Schabel et al. in the SC state of YBa$_2$Cu$_3$O$_{6.95}$. They also report a broad dispersing peak for momenta $k_x \ll k_F^\perp$, while for $k_x \approx k_F^\perp$, $A_c$ exhibits a hump and a sharper quasi-particle peak (cf. Fig. 7d in Ref. 3).

The gap induced in the CDOS for incoherent IC coupling varies strongly with the hole concentration, $x$, in the chains, as shown in Fig. 4. For $t_{\perp} = 0.4t_p$, one finds $\alpha > \Delta(k_F^\perp)$ and hence the frequency of the gap edges in the CDOS is determined by $\Delta(k_F^\perp)$ (cf. Eq(12)). Since $\Delta(k_F^\perp)$ decreases as the hole concentration is reduced from $x=50\%$ to $x=40\%$ (see inset of Fig. 4), the magnitude of the induced gap also decreases, in agreement with our results in Fig. 4. The gap in the CDOS is the smallest for $x=22\%$, since here $k_F^\perp = k_n$ and $\Delta(k_F^\perp) = 0$. We thus predict that the gap in the CDOS varies non-monotonically with $x$: as $x$ is decreased from $x=50\%$ the induced gap first decreases, exhibits a minimum at $x=22\%$ and then increases again for even smaller hole concentrations. Moreover, for small frequencies we find $N(\omega) \sim \omega$ which is a direct consequence of the linear momentum dependence of $\Delta_k$ in the vicinity of the nodes. In contrast, the chain DOS in the normal state (dashed line) is only weakly frequency and doping dependent.

The origin of the qualitatively different CDOS for coherent and incoherent IC coupling is twofold. First, for coherent IC coupling, the chain states are described by a two-dimensional momentum, $k$, and the dimensionality of the coherent chain array and the CuO$_2$ planes is the same. Thus, the CuO$_2$ planes do not constitute a dissipative environment for the electronic degrees of freedom in the chains. Second, the changes which occur in the CDOS for a given frequency, $\omega$, upon entering the SC state arise from those electronic states which can reduce their ground state energy by a virtual hopping process into the planes. It follows from Eqs.(12) and that in the case of coherent IC coupling these states must satisfy $t_{\perp}^2 \gg \omega^2 - k_F^2 - \Delta_k^2$. Simple phase space counting shows that the number of states which undergo a shift in the ground state energy is much smaller for coherent than for incoherent IC coupling. As a result, the CDOS for incoherent IC coupling exhibits a much larger SC gap than that for coherent IC coupling.

Two explanations for the absence of a coherent IC coupling in YBCO are possible. First, STM experiments have provided evidence for inhomogeneous doping in the chains. The resulting distribution of Fermi momenta likely prevents the coherent coupling between momenta in the vicinity of $k_F$, and thus renders the coupling incoherent. Second, a series of experimental probes have reported charge and spin inhomogeneities (stripes) in the CuO$_2$ planes which are aligned parallel to the chains. Since planar electrons are likely scattered by these inhomogeneities, a coherent coupling only exists between those chains which can be connected by an electron path that is not intersected by a stripe. This scenario can be tested in the underdoped YBCO compounds where the stripe-stripe distance increases and coherent IC coupling between an increasing number of chains is expected.

Recently, there has been an extensive discussion on the relative strength of incoherent versus coherent hopping of carriers between the planes. Since the CP hopping is a part of the hopping process between the bilayers in YBCO, our results support the notion that coherent hopping is a crucial part of the communication of electrons between the planes. Though the CP hopping, $t_{\perp}$, in the bulk is likely somewhat reduced from the value extracted above (the distance between the surface chain layer and the next CuO$_2$ layer is smaller than the corresponding separation in the bulk) we expect it to remain coherent.

Finally, the phase of the induced SC gap as well as its non-monotonic doping dependence, Fig. 4, are salient features of the PSC state which distinguish it from other possible ground states, e.g., a charge-density-wave. We thus propose phase-sensitive Josephson tunneling or Josephson STM experiments as a crucial test for our above scenario.

In summary, we propose a scenario in which the results of recent IS, STM and ARPES experiments on the chains of YBCO can consistently be explained by the interplay of a coherent chain-plane coupling and an incoherent interchain coupling. We show that the CuO$_2$ planes act as a dissipative environment for the electronic
degrees of freedom in the chains and induce a substantial quantum dissipation. We find that the chains exhibit superconducting correlations and a universal gap below $T_c$, and predict that the magnitude of this gap varies non-monotonically with the hole concentration in the chains.

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