# Impurities and Quantum Interference in the Chains of $YBa_2Cu_3O_{6+x}$

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Motivated by recent experiments, we study the electronic structure near impurities in the chains of $YBa_2Cu_3O_{6+x}$. Using a model of proximity induced chain superconductivity, we show that a resonance state in the chain density of states is induced only by a magnetic impurity. The spatial form of the resonance reflects the particle-hole nature of chain superconductivity and therefore distinguishes it from other broken symmetry phases. Because of quantum interference effects between impurities, the chains can undergo a quantum phase transition into a polarized state.

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The electronic structure near impurities in the $CuO_2$ planes of the high-temperature superconductors has attracted considerable experimental [1] and theoretical [2–4] attention over the last few years. The physical origin of the experimentally observed resonances in the local density of states near the impurities was attributed to electronic scattering off classical impurities [2] or to the Kondo effect [3]. Since the spatial and frequency dependence of these resonances is determined by the electronic correlations of the host system, they provide important insight into the microscopic origin of high-temperature superconductivity. Recently Derro *et al.* [5], using scanning tunneling microscopy (STM), studied the electronic structure of the CuO chains in $YBa_2Cu_3O_{6+x}$ (YBCO). They observed that below the planar $T_c$, the chain density of states (CDOS) exhibits (a) a large gap, consistent with proximity induced superconductivity, and (b) resonances whose amplitudes exhibit strong spatial oscillations. Moreover, [1] Derro *et al.* identified *four* resonance peaks, whose origins are still unclear, inside the gap in the CDOS. Because of the chain-plane coupling, these results also provide significant information on the planes' electronic correlations—a key to our understanding of high-temperature superconductivity. Much theoretical work [6] focused on this coupling and its implications for a large range of experiments [7–12].

In this Letter, we argue that the resonances observed by Derro *et al.* arise from the presence of impurities in the chains. Our starting point is a model [13] in which the coupling to the $CuO_2$ planes leads to proximity induced chain superconductivity below $T_c$. This model correctly describes the large gap in the experimentally observed CDOS [5] and predicts an $s$-wave symmetry of the superconducting (SC) state in the chains. Because of this symmetry, only magnetic impurities induce scattering resonances that are accompanied by two peaks in the CDOS. Their spatial oscillations directly reflect the particle-hole nature of chain superconductivity and therefore distinguishes it from other broken symmetry states proposed to exist in the chains [11]. We argue that the presence of four resonance peaks in the CDOS arises from quantum interference of electronic waves that scattered by two magnetic impurities. We predict that as the distance between the impurities is decreased, the SC chains undergo a quantum phase transition in which their spin polarization changes from $\langle s_z \rangle = 0$ to $\langle s_z \rangle = 1/2$.

Our starting point is a BCS Hamiltonian of the chain-plane system [6,13] given by

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_{\mathbf{k}} c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_k (\Delta_k c^\dagger_{k,\uparrow} c^\dagger_{k,\downarrow} + \text{H.c.}) + \sum_{k,\sigma} \zeta_{\mathbf{k}} d^\dagger_{k,\sigma} d_{k,\sigma} - t_\perp \sum_{k,\sigma} (c^\dagger_{k,\sigma} d_{k,\sigma} + \text{H.c.}), \quad (1)$$

where $c^\dagger_k, d^\dagger_k$ are the fermionic creation operators in the planes and chains, respectively. The normal state tight-binding dispersions of the planes, $\epsilon_{\mathbf{k}}$, and chains, $\zeta_{\mathbf{k}}$, are

$$\epsilon_{\mathbf{k}} = -2t_p[\cos(k_x) + \cos(k_y)] - 4t'_p \cos(k_x)\cos(k_y) - \mu_p, \qquad (2)$$
$$\zeta_{\mathbf{k}} = -2t_c \cos(k_x) - \mu_c.$$

Here, $k_x$ is the momentum along the chains, $t_p = 300$ meV, $t'_p = -0.22t_p$, $\mu_p = -0.812t_p$ are the planar hopping elements and chemical potential [9], and $\Delta_{\mathbf{k}} = \Delta_0[\cos(k_x) - \cos(k_y)]/2$ is the planar SC gap with $\Delta_0 \approx 40$ meV [14]. The chain Fermi momentum, $k^c_F \approx 0.25\pi$ [7,10], yields $\mu_c = -1.41t_c$, with chain hopping element $t_c \approx 200$ meV [9], and we take $t_\perp = 0.4t_p$ [13]. After integrating out the planar fermions, the chain Greens function $\hat{G}_0 = -\langle \mathcal{T} \Psi_{k_x,l}(\tau) \Psi^\dagger_{k_x,m}(\tau') \rangle$ with $\Psi^\dagger_{k_x,l} = (d^\dagger_{k_x,l,\uparrow}, d^\dagger_{k_x,l,\downarrow}, d_{-k_x,l,\uparrow}, d_{-k_x,l,\downarrow})$, and chain indices $m, l$, is given by

$$\hat{G}_0^{-1} = \begin{pmatrix} B(k_x, \omega_n)\hat{\sigma}_0 & C(k_x, \omega_n)\hat{\sigma}_0 \\ C(k_x, \omega_n)\hat{\sigma}_0 & -B(-k_x, -\omega_n)\hat{\sigma}_0 \end{pmatrix}, \qquad (3)$$

where $\hat{\sigma}_0$ is the unit matrix in spin space, and

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$$B = (i\omega_n - \zeta_{\mathbf{k}})\delta_{l,m} - t_\perp^2 N^{-1} \sum_{k_y} \frac{i\omega_n + \epsilon_{\mathbf{k}}}{(i\omega_n)^2 - (\epsilon_{\mathbf{k}})^2 - \Delta_k^2} e^{ik_y(l-m)}; \quad (4)$$
$$C = -t_\perp^2 N^{-1} \sum_{k_y} \frac{\Delta_k}{(i\omega_n)^2 - (\epsilon_{\mathbf{k}})^2 - \Delta_k^2} e^{ik_y(l-m)}.$$

We showed in Ref. [13] that the experimentally observed CDOS in a clean, i.e., impurity free, system can be explained only if one assumes that *coherent* correlations between the chains are absent, e.g., due to the presence of planar stripes and/or doping inhomogeneities in the chains. This assumption implies that we approximate the chain Greens function in Eq. (3) by $\hat{G}_0^{-1}(k_x, l, m,) = \hat{G}_0^{-1}(k_x)\delta_{l,m}$. In this case, the chains possess only two $k_F$ points (see Fig. 1), and the symmetry of their SC state is $s$ wave, i.e., $\Delta(k_F^c) = \Delta_c(-k_F^c)$.

We consider an impurity with spin $S$ whose interaction with the chain electrons is described by the Hamiltonian $\mathcal{H}_{sc} = \sum_{k_x,k_x',m} \Psi_{k_x,m}^\dagger \hat{V} \Psi_{k_x',m}$. Here, $\hat{V} = \hat{\tau}_3(U_0\hat{\sigma}_0 - J\mathbf{S}\hat{\sigma})$, $J(U_0)$ is the magnetic (potential) scattering strength, and $\tau_i, \sigma_i$ are the Pauli matrices in Nambu and spin space, respectively. To describe the effects of impurities, we employ the $\hat{T}$-matrix formalism [15], which treats the impurity spins as classical, static variables, corresponding to the limit $JS = \text{const}$ and $S \to \infty$. This approach is in general valid if the possibility for a Kondo effect can be precluded, which we believe applies to the chain system in the SC state. In particular, we showed in Ref. [13] that the superconducting CDOS in the clean system scales as $N(\omega) \sim |\omega|$ at small frequencies. The criteria for the occurrence of a Kondo effect in systems with $N(\omega) \sim |\omega|$, such as the high-temperature superconductors, were in detail studied in Ref. [16]. It was shown that (a) no Kondo effect occurs if the system is particle-hole symmetric and (b) that for particle-hole asymmetric systems, a Kondo effect occurs only if $J$ exceeds a critical value, $J_c$. While $J_c$ strongly depends on the particular asymmetry of the system, it is always of the order, or larger than the electronic bandwidth, $D$. We therefore consider values of $J$, which are much smaller than the bandwidth of the chains, $D = 800$ meV, thus eliminating the possibility of a Kondo effect (work is currently under way to study whether a Kondo effect can occur in the chains for $J > D$). The $\hat{T}$-matrix formalism [15] is then valid, and the impurity spin is static on electronic time scales. This conclusion is also supported by the experimentally measured CDOS [5] which shows no evidence for a Kondo effect below $T_c$.

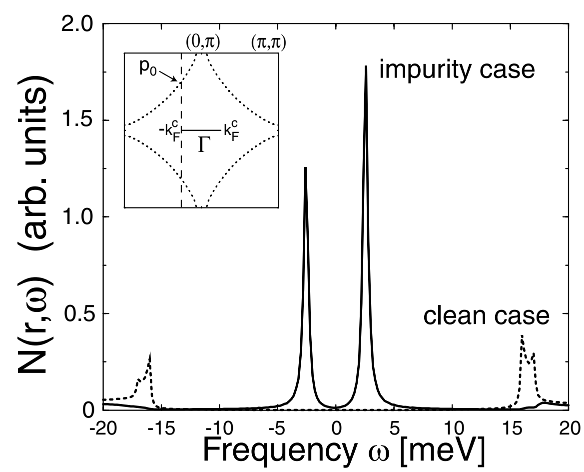


FIG. 1. CDOS in the SC state for the clean case (dashed line) and at the site of a magnetic impurity with $\beta = 200$ meV and $U_0 = 0$ (solid line). We set the lattice constant $a_0 = 1$. Inset: Fermi sea of the chain (solid line) and Fermi surface of the plane (dotted line).

Within the $\hat{T}$-matrix approach, one has for the full Greens function [with $\hat{G}_0$ from Eq. (3)]

$$\hat{G}(\mathbf{r}, \mathbf{r}', i\omega_n) = \hat{G}_0(\mathbf{r} - \mathbf{r}', i\omega_n) + \hat{G}_0(\mathbf{r}, i\omega_n)\hat{T}(i\omega_n)\hat{G}_0(-\mathbf{r}', i\omega_n), \quad (5)$$

where $\hat{T}(i\omega_n) = [1 - \hat{V}\hat{G}_0(r_x = 0, i\omega_n)]^{-1}\hat{V}$. The CDOS follows from Eq. (5) with $N(\mathbf{r}, \omega) = A_{11} + A_{22}$, where $A_{ii}(\mathbf{r}, \omega) = -\text{Im}\hat{G}_{ii}(\mathbf{r}, \omega + i\delta)/\pi$, and $\delta = 0.1$ meV.

We first consider a purely magnetic impurity with $U_0 = 0$ and $J \neq 0$, which induces a resonance in the CDOS. Assuming for definiteness $J > 0$, this resonance consists of a holelike ($|h, \uparrow\rangle$) and a particlelike ($|p, \downarrow\rangle$) contribution, corresponding to two peaks in the CDOS at $\pm\omega_{res}$ ($\uparrow, \downarrow$ denotes the quasiparticle spin along the $\pm z$ direction). The resonance frequency, $\omega_{res}$, is given by

$$\frac{\omega_{res}}{\alpha\bar{\Delta}}[\sqrt{\bar{\Delta}^2 - \omega_{res}^2} + \alpha] = \frac{1 - \gamma^2}{1 + \gamma^2}, \quad (6)$$

where $\gamma = \beta/v_F^c$, $v_F^c$ is the chain Fermi velocity, and $\beta = JS/2$. Moreover, $\alpha = t_\perp^2/\bar{v}$, $\bar{v} = (\partial\epsilon_{\mathbf{k}}/\partial k_y)|_{\mathbf{p}_0}$, where $\mathbf{p}_0$ is the momentum on the planar Fermi surface with $p_0^x = k_F^c$ (see the inset of Fig. 1) and $\bar{\Delta} = |\Delta(\mathbf{p}_0)|$. While in the limit $\gamma \ll 1$, $\omega_{res}$ is close to $\bar{\Delta}$, it shifts to lower energies with increasing $\gamma$. At $\gamma_c = 1$, i.e., $\beta_c = v_F^c$, the two peaks in the CDOS cross at $\omega_{res} = 0$, which changes their particle/hole nature, i.e., $|h, \uparrow\rangle \to |p, \uparrow\rangle$ and $|p, \downarrow\rangle \to |h, \downarrow\rangle$. This indicates that the impurity breaks a Cooper pair and forms a bound state with the pair's spin-down electron [17,18]. As a result, the SC chains undergo a quantum phase transition in which their total spin polarization changes from $\langle s_z\rangle = 0$ for $\gamma < \gamma_c$ to $\langle s_z\rangle = 1/2$ for $\gamma > \gamma_c$. Note that this type of phase transition [17,18] is not a collective, but a single impurity effect.

In Fig. 1 we present the superconducting CDOS, obtained from a numerical evaluation of Eq. (5) at the site of a magnetic impurity with $\beta = 200$ meV and $U_0 = 0$. A comparison with the clean CDOS shows the emergence of two resonance peaks at $\pm 2.6$ meV and a suppression of the coherence (gap edge) peaks at $\omega_{cp} = \pm 16.0$ meV. The impurity induces spatial oscillations in the CDOS, which we plot in Fig. 2 for the resonance peaks and the coherence peaks (see inset). The oscillations of the resonance peaks are determined by a broad range of wave vectors with $|k_{osc}| \leq 1.45$, which, together with the presence of the SC gap, lead to the rapid decay of the oscillations' amplitude with distance from the impurity. The decay length, $\xi_d \approx 10a_0$, is consistent with the experimentally obtained value of 40 Å [5]. Note that the oscillations at $\pm\omega_{res}$ are out of phase, such that a maximum in the DOS for $+\omega_{res}$ coincides with a minimum for $-\omega_{res}$. This complementary intensity pattern in real space reflects the particle-hole nature of Bogoliubov quasiparticles [1,19]. It is thus a characteristic feature of chain superconductivity and distinguishes it from other broken symmetry states, such as a charge-density wave [11], that were proposed to exist in the chains. In contrast, the spatial oscillations of the coherence peaks at $\pm\omega_{cp}$ (see inset) are in phase. Their amplitude decays slowly with distance from the impurity site since their wave vectors are centered in a narrow range, $\Delta k \approx 0.02$, around $k_{osc} = 0.81$. We find that the wavelength, $\lambda$, of the oscillations in the CDOS exhibits an asymmetric frequency dependence with $\lambda(-\omega_0) > \lambda(\omega_0)$ for $\omega_0 > 0$ and a minimum at $\omega_0 \approx 0$, in agreement with STM experiments [5]. The amplitude of the CDOS oscillations increases in the SC state, leading to larger variations in the electron density, consistent with the observed broadening of the Cu(1) nuclear quadrupole resonance line in the SC state [11,12].

Since the two $k_F$ points in the chains possess the *same* SC phase, we expect that a nonmagnetic impurity ($J = 0$, $U_0 \neq 0$) does not induce a scattering resonance. This conclusion is supported by our numerical evaluation of Eq. (5) which shows no sign of a resonance peak in the CDOS, but again large spatial oscillations at $\pm\omega_{cp}$.

We next study a general impurity with $J, U_0 \neq 0$ and present in Fig. 3 the CDOS at the impurity site for $\beta = 200$ meV and three values of $U_0$. With increasing $U_0$, $\omega_{res}$ shifts up in energy from $\omega_{res} = 2.6$ meV for $U_0 = 0$ to $\omega_{res} = 9.5$ meV for $U_0 = 200$ meV, and spectral weight is transferred from the particlelike to the holelike peak (while the spatially integrated weight of the particlelike peak is 1.43 times larger than that of the holelike peak for $U_0 = 0$, the ratio is 0.77 for $U_0 = 200$ meV). This shift in $\omega_{res}$ implies that the value of $\gamma_c$ at which the SC chains undergo a quantum phase transition into a spin-polarized state increases, similar to the case of a two-dimensional $s$-wave superconductor [18].

We showed above that a single magnetic impurity induces two peaks in the CDOS. This result suggests that the experimentally observed four resonance peaks [5] arise from quantum interference of electronic waves that are scattered by two impurities. To study this scenario we generalize the $\hat{T}$-matrix formalism to two impurities [18] and obtain for the full Greens function

$$\hat{G}(\mathbf{r}, \mathbf{r}', \omega_n) = \hat{G}_0(\mathbf{r}, \mathbf{r}', \omega_n) + \sum_{i,j=1}^{2} \hat{G}_0(\mathbf{r}, \mathbf{r}_i, \omega_n)\hat{T}(\mathbf{r}_i, \mathbf{r}_j, \omega_n)\hat{G}_0(\mathbf{r}_j, \mathbf{r}', \omega_n), \tag{7}$$

where $\mathbf{r}_{1,2}$ are the positions of the impurities, and $\hat{T}$ obeys the Bethe-Salpeter equation

$$\hat{T}(\mathbf{r}_m, \mathbf{r}_n, \omega_n) = \hat{V}\delta_{r_m, r_n} + \hat{V}\sum_{l=1}^{2} \hat{G}_0(\mathbf{r}_m, \mathbf{r}_l, \omega_n)\hat{T}(\mathbf{r}_l, \mathbf{r}_n, \omega_n). \tag{8}$$

For definiteness, we consider two identical impurities with parallel spins. In general, we expect that the CDOS for two impurities is similar to that of a single impurity for $\Delta r = |\mathbf{r}_2 - \mathbf{r}_1| > 2\xi_d$, where $\xi_d$ is the above introduced single impurity decay length. In contrast, for $\Delta r < 2\xi_d$ significant interference effects from multiple scattering processes should occur. This intuitive picture

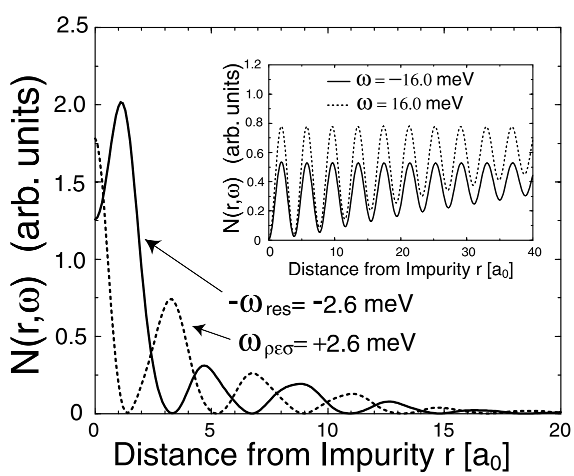


FIG. 2. CDOS as a function of distance from the impurity site for the resonance states at $\pm\omega_{res}$ and (see inset) for the coherence peaks at the gap edges, $\pm\omega_{cp}$.

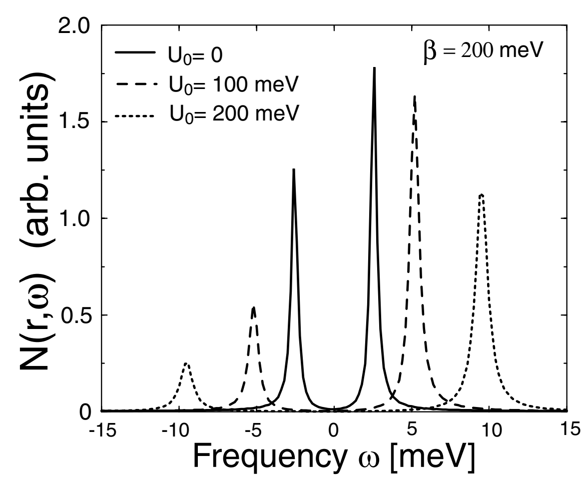


FIG. 3. Frequency dependence of the CDOS at the impurity site for $\beta = 200$ meV and $U_0 = 0$ (solid line), $U_0 = 100$ meV (dashed line), and $U_0 = 200$ meV (dotted line).

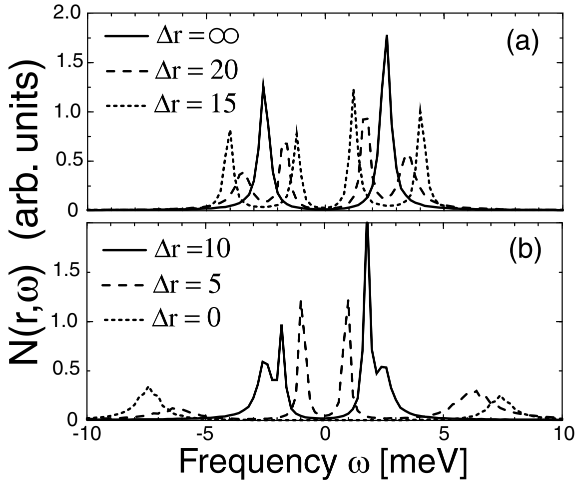


FIG. 4. Frequency dependence of the CDOS for two identical impurities with parallel spins at one of the impurity sites with $\beta = 200$ meV, $U_0 = 0$ and (a) $\Delta r = \infty$ (solid line), $\Delta r = 20$ (dashed line), and $\Delta r = 15$ (dotted line) and (b) $\Delta r = 10$ (solid line), $\Delta r = 5$ (dashed line), and $\Delta r = 0$ (dotted line).

is confirmed by the numerically obtained CDOS, shown in Fig. 4 at one of the two-impurity sites. For $\Delta r = \infty$ [Fig. 4(a)] the CDOS is as expected that for a single impurity with two resonance peaks at $\pm 2.6$ meV. As $\Delta r$ decreases ($\Delta r = 20$), interference effects between scattered electrons lead to the formation of bonding and antibonding resonances states, and thus to a splitting of the two resonance peaks into four (note that for antiparallel aligned impurity spins, the resonance states possess different quantum numbers, and no splitting of the peaks occurs). This splitting, which first becomes discernible for $\Delta r \approx 2\xi_d$, provides an explanation for the experimentally observed four resonance peaks in the CDOS [5]. The splitting increases further for $\Delta r = 15$, but for $\Delta r = 10$ [Fig. 4(b)], the peaks begin to recombine and spectral weight is transferred to new resonance peaks at higher energies ($\Delta r = 5$). In the limit $\Delta r \to 0$, only two resonance peaks remain at $\pm 7.5$ meV, as the two impurities now effectively behave as a single impurity with scattering strength, $\tilde{\beta} = 2\beta$. Since for $\Delta r = \infty$, we have $\beta < \beta_c$ for the single impurity, but for $\Delta r = 0$ we have $\tilde{\beta} > \beta_c$, the SC chains undergo a quantum phase transition from an unpolarized to a polarized state as the distance between the two impurities is varied. Thus, this quantum phase transition is a two-impurity effect.

In conclusion we presented a model in which the CuO chains of YBCO are SC below $T_c$ due to proximity coupling to the $CuO_2$ planes. We studied the electronic structure near impurities in the chains and showed that a resonance state is induced only by a magnetic impurity. The spatial oscillations of the corresponding peaks in the CDOS reflect the particle-hole nature of chain superconductivity and therefore distinguishes it from other broken symmetry phases. Quantum interference between scattered electrons leads to a splitting of the resonance peaks, thus providing an explanation for the four resonance peaks observed in Ref.[5]. As the distance between the impurities is varied, the chains undergo a quantum phase transition, in which the spin polarization of their SC ground state changes from $\langle s_z \rangle = 0$ to $\langle s_z \rangle = 1/2$.

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