Quantum interference between nonmagnetic impurities in $d_{x^2-y^2}$-wave superconductors

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We study quantum interference of electronic waves that are scattered by multiple nonmagnetic impurities in a $d_{x^2-y^2}$-wave superconductor. We show that the number of resonance states in the density of states, as well as their frequency and spatial dependence change significantly as the distance between the impurities or their orientation relative to the crystal lattice is varied. Since the latter effect arises from the momentum dependence of the superconducting gap, we argue that quantum interference is a tool to identify the symmetry of unconventional superconductors.

Over the last few years, the study of impurities in unconventional superconductors has attracted considerable theoretical[1–4] and experimental[5–7] attention. In particular, a series of groundbreaking scanning tunneling microscopy (STM) experiments has provided detailed information on the density of states (DOS) near single nonmagnetic[5] and magnetic[6] impurities in $Bi_2Sr_2CaCu_2O_{8+\delta}$, a high-temperature superconductor (HTSC). Of particular interest is the experimentally observed emergence of resonance states near the impurities. Several theoretical scenarios have been proposed that ascribe the origin of these resonances to electronic scattering off classical impurities with magnetic and nonmagnetic scattering potentials,[1–3] or to the Kondo screening of a local spin polarization that is induced by nonmagnetic impurities.[4] At the same time, a different line of experiments studied quantum interference of electronic waves that are scattered by multiple impurities. In particular, Manoharan *et al.*[8] demonstrated that quantum interference in a corral of magnetic impurities arranged on the surface of a metallic host leads to the focusing of electronic waves into a quantum image; a result that has recently been addressed in several theoretical studies.[9] Similar quantum interference experiments using unconventional superconductors can be expected in the future. First evidence for quantum interference in the HTSC was recently reported by Derro *et al.*[7] in the one-dimensional chains of $YBa_2Cu_3O_{6+x}$.

Motivated by the experimental progress in this field, we present in this paper a theoretical model that combines the study of impurities in unconventional superconductors with that of quantum interference effects. In particular, generalizing the formalism presented in Refs. 1,2,10, we investigate the electronic structure in the vicinity of two nonmagnetic impurities in a $d_{x^2-y^2}$-wave superconductor. We show that quantum interference due to the presence of a second impurity dramatically changes the DOS obtained near a single impurity. In particular, we demonstrate that the number of resonance states in the DOS, as well as their frequency and spatial dependence, change significantly as the distance between the impurities or their orientation relative to the crystal lattice is varied. Since the latter effect arises from the momentum dependence of the superconducting gap, we argue that quantum interference is a tool to identify the symmetry of unconventional superconductors. This result might be of particular importance for Sr_2RuO_4, an unconventional super-

conductor whose symmetry is still a topic of controversy.[11] While the study of quantum interference is not only of fundamental importance for our understanding of complex impurity structures, it can also clarify the origin of the resonances observed in the HTSC. In particular, we expect that the form of the resonances arising from Kondo screening of two magnetic impurities is different from those discussed below; work is currently under way to verify this conjecture.[12]

The starting point for our calculations is the $\hat{T}$-matrix formalism[13] that we extended to treat scattering off multiple impurities[1,10] in a $d_{x^2-y^2}$-wave superconductor. Quantum interference in s-wave superconductors was recently discussed in Refs. 14,15. For simplicity, we restrict our considerations to two nonmagnetic impurities; our formalism, however, allows the study of an arbitrary, but finite number of impurities. The study of more complex impurity structures, as well as that of magnetic impurities, will be the focus of future work.[12] Within the Nambu formalism and for Matsubara frequencies ω_n, the electronic Green's function in the presence of N impurities is given by

$$\hat{G}(r,r',\omega_n) = \hat{G}_0(r,r',\omega_n) + \sum_{i,j=1}^{N} \hat{G}_0(r,r_i,\omega_n)$$
$$\times \hat{T}(r_i,r_j,\omega_n)\hat{G}_0(r_j,r',\omega_n), \qquad (1)$$

where the $\hat{T}$ matrix is obtained from the Bethe-Salpeter equation,

$$\hat{T}(r_i,r_j,\omega_n) = \hat{V}_{r_i}\delta_{r_i,r_j} + \hat{V}_{r_i}\sum_{l=1}^{N} \hat{G}_0(r_i,r_l,\omega_n)\hat{T}(r_l,r_j,\omega_n). \qquad (2)$$

For two nonmagnetic impurities located at $\mathbf{r}_i$ ($i=1,2$) with $\Delta r = |\mathbf{r}_2 - \mathbf{r}_1|$, the scattering matrices are given by $\hat{V}_{r_i} = U_i \tau_3/2$ with U_i being the nonmagnetic scattering potential and τ is the Pauli matrices in Nambu space. The Green's function of the unperturbed (clean) system in momentum space is given by

$$\hat{G}_0^{-1}(\mathbf{k},i\omega_n) = i\omega_n\tau_0 - \epsilon_{\mathbf{k}}\tau_3 - \Delta_{\mathbf{k}}\tau_1. \qquad (3)$$

For the electronic excitation spectrum in the normal state, we take a form that is characteristic of an optimally doped HTSC (Refs. 16–18) and given by

$$\epsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] - 4t'\cos(k_x)\cos(k_y) - \mu, \quad (4)$$

with $t = 300$ meV, $t'/t = -0.4$ as the nearest and next-nearest-neighbor hopping integrals, respectively, and a chemical potential $\mu/t = -1.18$, corresponding to 14% hole doping. Moreover, the superconducting gap with $d_{x^2-y^2}$ symmetry is given by $\Delta_{\mathbf{k}} = \Delta_0[\cos k_x - \cos k_y]/2$ with $\Delta_0 = 25$ meV.[17] Our results presented below are qualitatively robust against changes in the form of $\epsilon_{\mathbf{k}}$, or the size of Δ_0. We obtain the DOS, $N(\mathbf{r}, \omega)$, from a numerical evaluation of Eqs. (1)–(3) with $N(\mathbf{r}, \omega) = A_{11} + A_{22}$ and $A_{ii}(\mathbf{r}, \omega) = -\mathrm{Im}\hat{G}_{ii}(\mathbf{r}, \omega + i\delta)/\pi$.

We briefly review some important features in the DOS near a single nonmagnetic impurity in a $d_{x^2-y^2}$-wave superconductor.[1,2] The resulting diagonal $\hat{T}$ matrix

$$\hat{T}_{11,22} = \frac{\pm U_0}{1 - U_0 G_0(r=0, \pm\omega)}, \quad (5)$$

where the upper (lower) sign applies to $\hat{T}_{11}(\hat{T}_{22})$ and $G_0 = [\hat{G}_0]_{11}$, exhibits a particlelike ($\omega_{res} < 0$) and holelike ($\omega_{res} > 0$) resonance. These resonances give rise to sharp peaks in the DOS only in the unitary limit ($|\omega_{res}|/\Delta_0 \ll 1$), where $U_0^{-1} = \mathrm{Re}G_0(0, \pm\omega_{res})$.

In the presence of two impurities, the $\hat{T}$ matrix, [Eq. (2)], is rather complex. However, in the limit $F_0(\Delta r, \omega) \ll G_0(\Delta r, \omega)$, where $F_0 = [\hat{G}_0]_{12}$ and for identical impurities with $U_{1,2} = U_0$, the $\hat{T}$ matrix simplifies considerably and is again diagonal. Defining

$$S_{\pm}(\omega) = \{1 - U_0[G_0(0, \omega) \pm G_0(\Delta r, \omega)]\}^{-1}, \quad (6)$$

one obtains ($i \neq j$)

$$\hat{T}_{11,22}(r_i, r_i) = U_0[S_+(\pm\omega) + S_-(\pm\omega)]/2,$$
$$\hat{T}_{11,22}(r_i, r_j) = \frac{U_0 G_0(\Delta r, \pm\omega)}{1 - U_0 G_0(0, \pm\omega)}\hat{T}_{11,22}(r_i, r_i), \quad (7)$$

where the upper (lower) sign applies to $\hat{T}_{11}(\hat{T}_{22})$. By comparing the $\hat{T}$ matrices in Eqs. (5) and (7), we find that the presence of a second impurity splits the resonances of the single-impurity case by $U_0 G_0(\Delta r, \omega)$. Note that $G_0(\Delta r, \omega)$ does not only change with varying Δr, but also with the angle α between $\mathbf{r}_2 - \mathbf{r}_1$ and the crystal $\hat{x}$ axis, due to the momentum dependence of the superconducting gap. Consequently, the energy and lifetime of the resonances depend on Δr and α. While all four $S_{\pm}$ terms in Eq. (7) can possess resonances, those that are shifted to higher energies are highly overdamped and give rise only to oscillations in the DOS without the signature of a sharp peak.

In what follows, we consider two identical impurities with scattering potential $U_{1,2} = U_0 = 700$ meV, corresponding to the unitary limit, in agreement with Refs. 1,2. While the
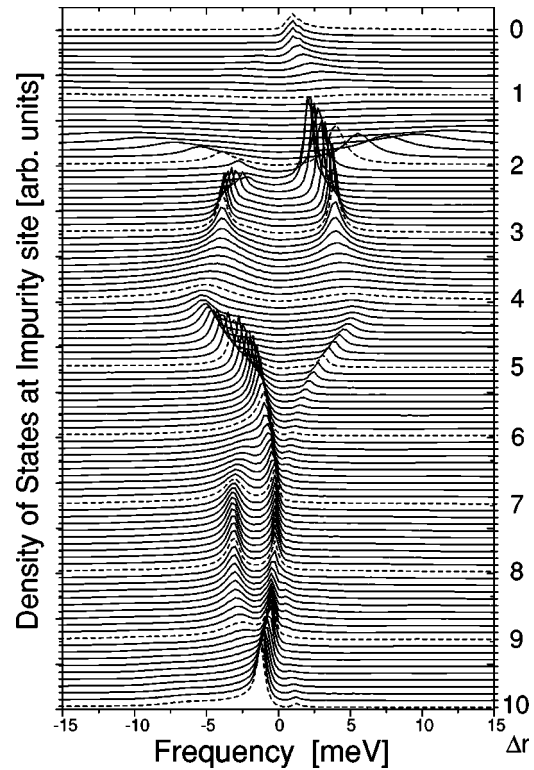

FIG. 1. DOS at $\mathbf{R} = (0,0)$ as a function of Δr for two identical impurities with $U_0 = 700$ meV located at $\mathbf{r}_1 = (0,0)$ and $\mathbf{r}_2 = (\Delta r, 0)$. The lattice constant is set to $a_0 = 1$.

specific form of the DOS changes with U_0, its qualitative features remain unchanged. To study the effects of α and Δr on the DOS separately, we first consider for definiteness two impurities located along the crystal $\hat{x}$ axis at $\mathbf{r}_1 = (0,0)$ and $\mathbf{r}_2 = (\Delta r, 0)$ with $\alpha = 0$. In Fig. 1, we present the DOS at $\mathbf{R} = (0,0)$, i.e., at one of the impurity sites, as a function of Δr. For comparison, we note that for a single impurity with $U_0 = 700$ meV, the resonances are located at $\omega_{res} = \pm 1.5$ meV. As Δr is varied, the DOS undergoes strong modifications. In particular, the frequency of the resonances oscillates and at the same time, their energy width, or lifetime, changes. For a single impurity, the resonance frequency and width are correlated, such that as $|\omega_{res}|$ decreases, the frequency width decreases as well.[1,2] In the case of two impurities, we find that $|\omega_{res}|$ and the lifetime of the resonances are not necessarily correlated. For example, the resonance frequencies for both $\Delta r = 2.0$ and $\Delta r = 3.5$ are $\omega_{res} = \pm 4.0$ meV, but the width of the resonances are considerably larger in the second case. Moreover, for some values of Δr, *all* resonances are very weak and, e.g., for $\Delta r \approx 1$ disappear almost completely. Note, that even for rather large values of $\Delta r \approx 10$, the DOS at $\mathbf{R} = (0,0)$ is still affected by quantum interference and thus different from that obtained in the single-impurity case. This result bears important implications for the interpretation of recent STM experiments,[5–7] since it implies that the DOS near impurities in the two-dimensional HTSC can only be described within the single-impurity framework if the impurity concentration is well below 1%.
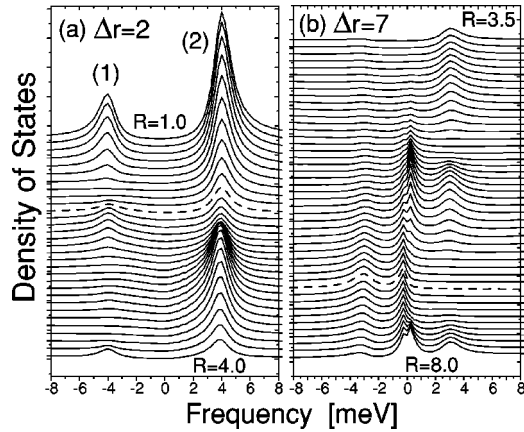
FIG. 2. DOS as a function of spatial position $\mathbf{R}=(R,0)$ for two impurities with $U_0=700$ meV located at $\mathbf{r}_1=(0,0)$ and $\mathbf{r}_2=(\Delta r,0)$ with (a) $\Delta r=2$ and (b) $\Delta r=7$.
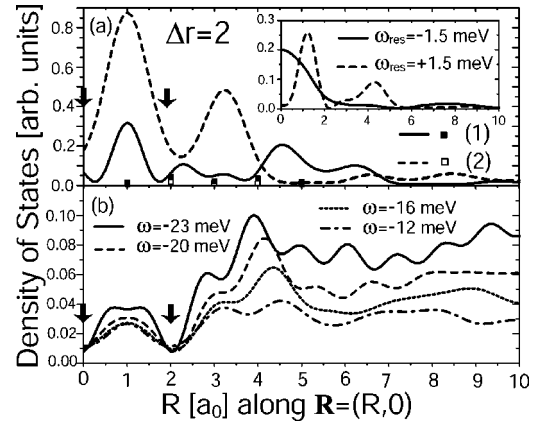

FIG. 3. DOS along $\mathbf{R}=(R,0)$ for the same impurity arrangement as in Fig. 2(a). The positions of the impurities are indicated by arrows. (a) DOS at $\omega_{res}=\pm4$ meV. The open and filled squares present the DOS at $\omega_{res}=\pm4$ meV along the lattice diagonal with $\mathbf{R}=(R,R)$. Inset: DOS along $\mathbf{R}=(R,0)$ for a single impurity at its resonance frequency $\omega_{res}=\pm1.5$ meV. (b) DOS at frequencies $|\omega_{res}|<|\omega|<\Delta_0$.

An additional important result of Fig. 1 is that the number of observable low-energy resonances changes with Δr. In particular, for $\Delta r \lesssim 6$, only two sharp low-energy resonances can be clearly identified. This effect becomes particularly evident when one considers the spatial dependence of the DOS for fixed Δr, as shown in Fig. 2. Here, we plot the DOS as a function of $\mathbf{R}=(R,0)$ for two impurities located at $\mathbf{r}_1=(0,0)$ and $\mathbf{r}_2=(\Delta r,0)$. The uppermost curve corresponds to the midpoint between the two impurities, the dashed line represents the DOS at $\mathbf{r}_2$. For $\Delta r=2$ [Fig. 2(a)], there exist only two low-energy resonances at $\omega_{res}\pm4$ meV. In contrast, for $\Delta r=7$ [Fig. 2(b)], we find two broader resonances at $\omega_{res}=\pm3$ meV and two sharper resonances at $\omega_{res}=\pm0.25$ meV. Note, that the resonances for $\Delta r=2$ at $\omega_{res}\pm4$ meV have a considerably larger amplitude than those for $\Delta r=7$ at $\omega_{res}=\pm3$ meV. This result again differs from the single-impurity case, where the resonance with the smaller $|\omega_{res}|$ always possesses a larger amplitude in the DOS.

While sharp resonances can only be identified for $\omega_{res}\ll\Delta_0$, oscillations in the DOS exist for basically all energies, $|\omega|\lesssim\Delta_0$. To study these oscillations in more detail, we present in Fig. 3 the DOS along $\mathbf{R}=(R,0)$ for various frequencies and the same impurity arrangement as in Fig. 2(a); the locations of the impurities are indicated by arrows. The solid and dashed lines in Fig. 3(a) represent the DOS at $\omega_{res}=\pm4$ meV, corresponding to peak 1 and 2 in Fig. 2(a). The DOS at $|\omega_{res}|$ but along the lattice diagonal, i.e., for $\mathbf{R}=(R,R)$, is shown as open and filled squares. Similar to the single-impurity case, the amplitude of the resonances is much weaker along the direction of the superconducting gap nodes, than along the antinodal direction. The inset shows the DOS along $\mathbf{R}=(R,0)$ for a single impurity with $U_0=700$ meV and resonance energy $\omega_{res}=\pm1.5$ meV. A comparison shows that the amplitude of the DOS oscillations induced by the two impurities is much larger than those induced by a single impurity (the overall scale in the inset is three times smaller than in the main figure). Moreover, in the two-impurity case, the DOS exhibits significant oscillations at much larger distances from the impurities than in the

single-impurity case. This is particularly evident when comparing the particlelike resonances, where in the two-impurity case, the amplitude of the oscillations is still large at a distance to the nearest impurity r_n of about $r_n\approx4$–5; while in the single-impurity case, the oscillations are already substantially reduced at $r_n\approx2$. In Fig. 3(b), we present the
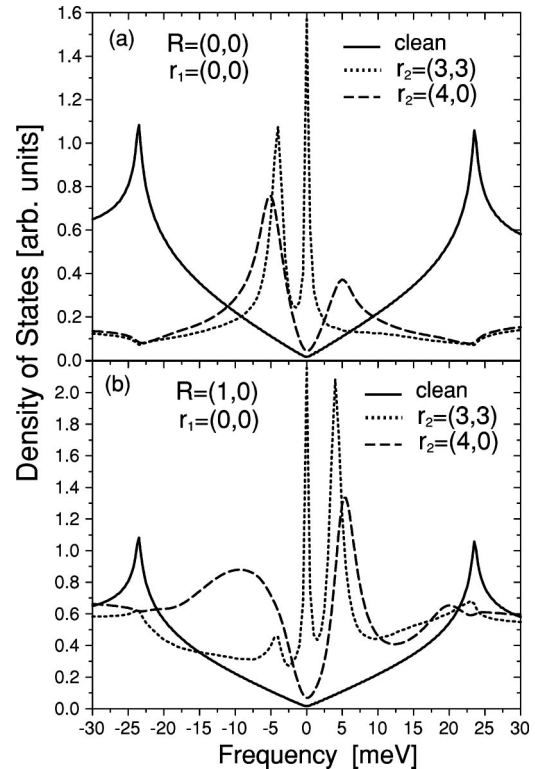

FIG. 4. DOS at (a) $\mathbf{R}=(0,0)$ and (b) $\mathbf{R}=(1,0)$ for two impurities with $U_0=700$ meV. One impurity is located at $\mathbf{r}_1=(0,0)$, the other one either at $\mathbf{r}_2=(3,3)$ (dotted line) or at $\mathbf{r}_2=(4,0)$ (dashed line).

DOS along $\mathbf{R}=(R,0)$ for several frequencies with $|\omega_{res}|<|\omega|<\Delta_0$. While there exist no evidence for a resonance at higher energies, we still find considerable oscillations in the DOS. As $|\omega|$ decreases, the wave vectors of these oscillations also decrease, as can be clearly seen from the shift of the peaks around $R=3$ and 4. Thus, the DOS oscillations exhibit a dispersion, similar to the results obtained in Ref. 7

Due to the momentum dependence of the superconducting $d_{x^2-y^2}$ gap, the DOS changes when the orientation of the two impurities with respect to the crystal lattice is varied. In particular, since the gap vanishes along the lattice diagonal, we expect the largest deviations from the results for $\alpha=0$ shown in Figs. 1–3 when the impurities are located along the lattice diagonal, i.e., for $\alpha=\pi/4$. To study the changes in the DOS due to variations in α and to eliminate effects due to a varying Δr, we chose two different impurity arrangements that can be realized experimentally, and possess almost identical values for Δr. In the first case, the impurities are located along the lattice diagonal ($\alpha=\pi/4$) at $\mathbf{r}_1=(0,0)$ and $\mathbf{r}_2=(3,3)$ (dotted line, $\Delta r\approx4.2$). In the second arrangement, the impurities are aligned along the crystal $\hat{x}$ axis ($\alpha=0$) at $\mathbf{r}_1=(0,0)$ and $\mathbf{r}_2=(4,0)$ (dashed line, $\Delta r=4$). We verified that the DOS for $\mathbf{r}_2=(4.2,0)$, which would yield identical values of Δr, but is experimentally not realizable, differs only slightly from that for $\mathbf{r}_2=(4,0)$. The DOS at $\mathbf{R}=(0,0)$

and $\mathbf{R}=(1,0)$ are shown in Fig. 4. While the DOS for $\alpha=\pi/4$ possesses three distinct resonances, only two resonance peaks are observable for $\alpha=0$. Moreover, for $\alpha=0$, the resonance states are located at higher frequencies and are much broader. The qualitative differences in the DOS between these two different impurity arrangements can be directly traced back to the vanishing of $F(\Delta r,\omega)$ for $\alpha=\pi/4$, and its finite, complex value for $\alpha=0$. Thus, the symmetry of the superconducting gap is directly reflected in the changes that the DOS undergoes when the orientation of the impurities relative to the crystal lattice is varied. This dependence provides a new tool to identify the symmetry of unconventional superconductors.

In summary, we studied quantum interference of electronic waves that are scattered by two nonmagnetic impurities in a $d_{x^2-y^2}$-wave superconductor. We show that the number of resonance states in the DOS, as well as their frequency and spatial dependence, changes significantly as the distance between the impurities or their orientation relative to the crystal lattice is varied. The latter result provides a tool to identify the symmetry of unconventional superconductors, such as Sr_2RuO_4, where the symmetry of the superconducting state is still a topic of controversy.

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