Quantum interference between non-magnetic 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 non-magnetic impurities in a $d_{x^2-y^2}$-wave superconductor. We show that the number of resonance states in the density-of-states (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 novel tool to identify the symmetry of unconventional superconductors.

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Over the last few years, the study of impurities in unconventional superconductors has attracted considerable theoretical and experimental attention. In particular, a series of groundbreaking scanning tunneling microscopy (STM) experiments has provided detailed information on the density-of-states (DOS) near single non-magnetic and magnetic impurities in Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$, 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 attribute the origin of these resonances to electronic scattering off classical impurities with magnetic and non-magnetic scattering potentials, or to the Kondo-screening of a local spin polarization that is induced by non-magnetic impurities. At the same time, a different line of beautiful experiments studied quantum interference of electronic waves that are scattered by multiple impurities. In particular, Manoharan et al. 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. 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. in the one-dimensional chains of YBa$_2$Cu$_3$O$_{6+δ}$.

Motivated by the experimental progress in this field, we present in this article a theoretical model which combines the study of impurities in unconventional superconductors with that of quantum interference effects. In particular, generalizing the formalism presented in Ref. 5, we investigate the electronic structure in the vicinity of two non-magnetic 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 novel tool to identify the symmetry of unconventional superconductors. This result might be of particular importance for Sr$_2$RuO$_4$, an unconventional superconductor whose symmetry is still a topic of controversy.

Starting point for our calculations is the $T$-matrix formalism which we extended to treat scattering off multiple impurities in a $d_{x^2-y^2}$-wave superconductor. Quantum interference in $d_{x^2-y^2}$-wave superconductors was recently discussed in Refs. 5, 14, 15. For simplicity we restrict our considerations to two non-magnetic 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. Within the Nambu-formalism and for Matsubara frequencies, $ω_n$, the electronic Greens function in the presence of $N$ impurities is given by

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

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

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

For two non-magnetic impurities located at $r_i$ ($i = 1,2$) with $Δr = |r_2 - r_1|$, the scattering matrices are given by $\hat{V}_{r_i} = U_{r_i}\tau_3/2$ with $U_{r_i}$ being the non-magnetic scattering potential and $τ$ the Pauli-matrices in Nambu-space.
The Greens function of the unperturbed (clean) system in momentum space is given by
\[ G_0^{-1}(k, i\omega_n) = [i\omega_n\tau_0 - \epsilon_k\tau_3] - \Delta_k\tau_1. \] (3)

For the electronic excitation spectrum in the normal state we take a form that is characteristic of an optimally doped HTSC [\textsuperscript{3,4}] and given by
\[ \epsilon_k = -2t \left[ \cos(k_x) + \cos(k_y) \right] - 4t' \cos(k_x) \cos(k_y) - \mu, \] (4)

with \( t = 300 \text{ meV}, t'/t = -0.4 \) 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 \( \Delta_k = \Delta_0 [\cos k_x - \cos k_y]/2 \) with \( \Delta_0 = 25 \text{ meV} \). Our results presented below are qualitatively robust against changes in the form of \( \epsilon_k \), or the size of \( \Delta_0 \). We obtain the DOS, \( N(r, \omega) \), from a numerical evaluation of Eqs. (3)-(6) with \( N(r, \omega) = A_{11} + A_{22} \) and \( A_{inil}(r, \omega) = -\text{Im} \hat{G}_{iil}(r, \omega + i\delta)/\pi \).

We briefly review some important features in the DOS near a single non-magnetic impurity in a \( d_{x^2-y^2} \)-wave superconductor. The resulting diagonal \( T \)-matrix
\[ \hat{T}_{11,22} = \pm \frac{U_0}{1 - U_0 G_0(r = 0, \pm \omega)}, \] (5)

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

In the presence of two impurities, the \( T \)-matrix, Eq. (5), is rather complex. However, in the limit \( F_0(\Delta r, \omega) \ll G_0(\Delta r, \omega) \), where \( F_0 = [G_0]_{12} \) and for identical impurities with \( U_{1,2} = U_0 \), the \( T \)-matrix simplifies considerably and is again diagonal. Defining
\[ S_{\pm}(\omega) = \{1 - U_0 [G_0(0, \omega) \pm G_0(\Delta r, \omega)]\}^{-1} \] (6)

one obtains (\( i \neq j \))
\[ \hat{T}_{12,22}(r_i, r_j) = \frac{U_0 G_0(\Delta r, \pm \omega)}{1 - U_0 G_0(0, \pm \omega)} \hat{T}_{11,22}(r_i, r_i). \] (7)

where the upper (lower) sign applies to \( \hat{T}_{11}(\hat{T}_{22}) \). By comparing the \( T \)-matrices in Eqs. (7) and (6), 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 \( \Delta r \), but also with the angle, \( \alpha \), between \( r_2 - r_1 \) 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 \( \Delta r \) and \( \alpha \). While all four \( S_{\pm} \)-terms in Eq. (6) 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 \( U_{1,2} = U_0 = 700 \text{ meV} \), corresponding to the unitary limit, in agreement with Refs. [3,4]. While the specific form of the DOS changes with \( U_0 \), its qualitative features remain unchanged. To study the effects of \( \alpha \) and \( \Delta r \) on the DOS separately, we first consider for definiteness two impurities located along the crystal \( \hat{x} \)-axis at \( r_1 = (0,0) \) and \( r_2 = (\Delta r, 0) \) with \( \alpha = 0 \). In Fig. 1, we present the DOS at \( R = (0,0) \), i.e., at one of the impurity sites, as a function of \( \Delta r \). For comparison, we note that for a single impurity with \( U_0 = 700 \text{ meV} \), the resonances are located \( \omega_{\text{res}} = \pm 1.5 \text{ meV} \). As \( \Delta r \) 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 \( |\omega_{\text{res}}| \) decreases, the frequency width decreases as well [3,4]. In the case of two impurities, we find that \( |\omega_{\text{res}}| \) 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 \( \omega_{\text{res}} = \pm 4.0 \text{ meV} \), but the width of the resonances

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{dos.png}
\caption{DOS at \( R = (0,0) \) as a function of \( \Delta r \) for two identical impurities with \( U_0 = 700 \text{ meV} \), corresponding to the unitary limit, in agreement with Refs. [3,4]. While the specific form of the DOS changes with \( U_0 \), its qualitative features remain unchanged. To study the effects of \( \alpha \) and \( \Delta r \) on the DOS separately, we first consider for definiteness two impurities located along the crystal \( \hat{x} \)-axis at \( r_1 = (0,0) \) and \( r_2 = (\Delta r, 0) \) with \( \alpha = 0 \). In Fig. 1, we present the DOS at \( R = (0,0) \), i.e., at one of the impurity sites, as a function of \( \Delta r \). For comparison, we note that for a single impurity with \( U_0 = 700 \text{ meV} \), the resonances are located \( \omega_{\text{res}} = \pm 1.5 \text{ meV} \). As \( \Delta r \) 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 \( |\omega_{\text{res}}| \) decreases, the frequency width decreases as well [3,4]. In the case of two impurities, we find that \( |\omega_{\text{res}}| \) 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 \( \omega_{\text{res}} = \pm 4.0 \text{ meV} \), but the width of the resonances.
\end{figure}
are considerably larger in the second case. Moreover, for some values of $\Delta r$, 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 $R = (0, 0)$ 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, 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%.

An additional important result of Fig. 1 is that the number of observable low-energy resonances changes with $\Delta r$. In particular, for $\Delta r \leq 6$, 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 $\Delta r$, as shown in Fig. 2. Here, we plot the DOS as a function of the single impurity $R = (0, 0)$ for two impurities located at $r_1 = (0, 0)$ and $r_2 = (\Delta r, 0)$. The uppermost curve corresponds to the midpoint between the two impurities, the dashed line represents the DOS at $r_2$. For $\Delta r = 2$ (Fig. 2a), there exist only two low-energy resonances at $\omega_{\text{res}} \pm 4$ meV. In contrast, for $\Delta r = 7$ (Fig. 2b), we find two broader resonances at $\omega_{\text{res}} = \pm 3$ meV, and two sharper resonances at $\omega_{\text{res}} = \pm 0.25$ meV. Note, that the resonances for $\Delta r = 2$ at $\omega_{\text{res}} \pm 4$ meV have a considerably larger amplitude than those for $\Delta r = 7$ at $\omega_{\text{res}} = \pm 3$ meV. This result again differs from the single impurity case, where the resonance with the smaller $|\omega_{\text{res}}|$ always possesses a larger amplitude in the DOS.

While sharp resonances can only be identified for $\omega_{\text{res}} \ll \Delta_0$, oscillations in the DOS exist for basically all energies $|\omega| \leq \Delta_0$. To study these oscillations in more detail, we present in Fig. 3 the DOS along $R = (R, 0)$ for various frequencies and the same impurity arrangement as in Fig. 2a; the locations of the impurities are indicated by arrows. The solid and dashed lines in Fig. 3a represent the DOS at $\omega_{\text{res}} = \pm 4$ meV, corresponding to peak (1) and (2) in Fig. 2a. The DOS at $|\omega_{\text{res}}| \leq \Delta_0$ and resonance energy $\omega_{\text{res}} = \pm 1.5$ meV. A comparison shows that the amplitude of the DOS oscillations induced by 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 particle-like 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 $r_n \approx 4-5$, while in the single-impurity case, the oscillations are already substantially reduced at $r_n \approx 2$. In Fig. 3b, we present the DOS along $R = (R, 0)$ for several frequencies with $|\omega_{\text{res}}| < |\omega| < \Delta_0$. While there exist no evidence for a resonance at higher energies, we still find considerable oscillations in the DOS. As $\omega_{\text{res}}$ decreases, the wave-vectors of these oscillations decreases, as can clearly be 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. 1.

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 devia-
variations in for the impurities are located along the lattice diagonal, i.e.,

$$\Delta r$$, we chose two different impurity arrangements which can be realized experimentally, and possess almost identical values for $$\Delta r$$. In the first case, the impurities are located along the lattice diagonal ($$\alpha = \pi/4$$) at $$r_1 = (0, 0)$$ and $$r_2 = (3, 3)$$ (dotted line, $$\Delta r \approx 4.2$$). In the second arrangement, the impurities are aligned along the crystal $$\hat{x}$$-axis ($$\alpha = 0$$) at $$r_1 = (0, 0)$$ and $$r_2 = (4, 0)$$ (dashed line, $$\Delta r = 4$$). We verified that the DOS for $$r_2 = (4, 0)$$, which would yield identical values of $$\Delta r$$, but is experimentally not realizable, differs only slightly from that for $$r_2 = (4, 0)$$. The DOS at $$R = (0, 0)$$ and $$R = (1, 0)$$ is 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 which 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 non-magnetic impurities in a $$d_{x^2-y^2}$$-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 novel tool to identify the symmetry of unconventional superconductors, such as Sr$_2$RuO$_4$, where the symmetry of the superconducting state is still a topic of controversy.

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1. A.V. Balatsky, M.I. Salkola, and A. Rosengren, Phys. Rev. B 51, 15547 (1995); M.I. Salkola, A.V. Balatsky, J.R. Schrieffer, Phys. Rev. B 55, 12648 (1997); M.I. Salkola, A.V. Balatsky, and D.J. Scalapino, Phys. Rev. Lett. 77, 1841 (1996).
2. M.E. Flatté, and J.M. Byers, Phys. Rev. Lett. 78, 3761 (1997); M.E. Flatté, Phys. Rev. B 61, 14920 (2000).
3. S. Haas and K. Maki, Phys. Rev. Lett. 85, 2172 (2000); H. Tsuchiura et al., Phys. Rev. Lett. 84, 3165 (2000); J.-X. Zhu and C.S. Ting, Phys. Rev. B 64, 060501(R) (2001).
4. A. Polkovnikov, S. Sachdev, and M. Vojta, Phys. Rev. Lett. 86, 296 (2001).
5. A. Yazdani et al., Phys. Rev. Lett. 83, 176 (1999); S.H. Fan et al., Nature (London) 403, 746 (2000).
6. E.W. Hudson et al., Nature (London) 411, 920 (2001).
7. D.J. Derro et al., Phys. Rev. Lett. 88, 097002 (2002).
8. H.C. Manoharan, C.P. Lutz, and D.M. Eigler, Nature (London) 403, 512 (2000).
9. G.A. Fiete et al., Phys. Rev. Lett. 86, 2392 (2001); A.A. Aliaga, Phys. Rev. B 64, 121102 (2001); K. Hallberg, A.A. Correa, and C.A. Balseiro, Phys. Rev. Lett. 88, 066802 (2002).
10. D.K. Morr and A.V. Balatsky, preprint, cond-mat/0106616.
11. Y. Maeno, T.M. Rice, and M. Sigrist, Physics Today 54, 42 (2001), and references therein.
12. D.K. Morr et al., in preparation.
13. H. Shiba, Prog. Theoret. Phys. 40, 435 (1968).
14. M.E. Flatté, and D.E. Reynolds, Phys. Rev. B 61, 14810 (2000).
15. D.K. Morr and N.A. Stavropoulos, preprint, cond-mat/0205328.
16. H. Ding et al., Phys. Rev. Lett. 76, 1533 (1996).
17. J. Mesot et al., Phys. Rev. Lett. 83, 840 (1999).
18. D.S. Marshall et al., Phys. Rev. Lett. 76, 4841 (1996); A. Ino et al., Phys. Rev. B 65, 094504 (2002).

FIG. 4: DOS at (a) $$R = (0, 0)$$ and (b) $$R = (1, 0)$$ for two impurities with $$U = 700$$ meV. One impurity is located at $$r_1 = (0, 0)$$, the other one either at $$r_2 = (3, 3)$$ (dotted line) or at $$r_2 = (4, 0)$$ (dashed line).