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Andreev states near short-ranged pairing potential impurities

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We study Andreev states near atomic scale modulations in the pairing potential in both s- and d-wave superconductors with short coherence lengths. For a moderate reduction of the local gap, the states exist only close to the gap edge. If one allows for local sign changes of the order parameter, however, resonances can occur at energies close to the Fermi level. The local density of states (LDOS) around such pairing potential defects strongly resembles the patterns observed by tunneling measurements around Zn impurities in $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO). We discuss how this phase impurity model of the Zn LDOS pattern can be distinguished from other proposals experimentally.

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Motivated by the experimental ability to determine the LDOS with high resolution in both energy and real space using scanning tunneling microscopy (STM), there has recently been a large interest in the perturbations caused by impurities in superconductors. This is because impurities disturb the underlying superconducting state and hence constitute a natural probe of the state in which they are embedded[1]. For magnetic adatoms on the surface of conventional s-wave superconductors such experiments were performed by Yazdani *et al*[2]. In the superconducting state of BSCCO, STM measurements have provided detailed information about the electronic structure near Ni and Zn impurities[3, 4, 5]. Near Zn it was found that each impurity generates a sharp conductance peak close to the Fermi level ($\omega_B \sim -1.5$meV). By fixing the bias voltage between the tip and the sample at ω_B, the spatial structure of this state can be mapped out: it is strongly localized near the Zn atom with maximum intensity on the impurity site and second largest intensity on the next-nearest neighbor sites.

Although there exists a large number of theoretical treatments dealing with the resonant states generated by nonmagnetic impurities in d-wave superconductors, no consensus has been reached on their relevance to experiments[1]. Within the most straightforward scenario where Zn is modelled as a delta-function potential scatterer, low-energy resonant states are generated in the unitary limit where the potential is large compared to all other energy scales of the problem[6]. For realistic bands with particle-hole asymmetry, a particular value of the impurity potential V must be chosen to tune the resonance energy ω_B to be close to the Fermi level. Thus, the potential scattering model can reproduce the energetics of the resonant state. However, as is well-known, it produces a low-energy spatial LDOS pattern with a severely suppressed amplitude on the impurity site, in contrast to experimental results on Zn[5]. Physically, this is clear since a large on-site potential V penalizes any substantial amplitude of the impurity-state wavefunction on the impurity site. In fact, within this model the largest intensity is found on the nearest neighbor site to the impurity. These properties of the delta-function potential scatterer are shown in Fig.1. The discrepancies between experiments and the potential scattering scenario have led to the suggestion of various filter functions motivated by the fact that the measurements are performed on the topmost BiO layer whereas the nonmagnetic impurity substitutes a Cu atom in the CuO_2 plane two layers below the top BiO layer[8, 9, 10]. The significance of the filter functions remains controversial. Other scenarios have focused on the formation of local moments near the Zn impurities[11, 12, 13]. For instance, if the main effect of nonmagnetic impurities in cuprate superconductors is to locally break spin singlet bonds, the sharp conductance peak has been interpreted as a Kondo resonance[12].

While most models assume that an impurity produces a screened electrostatic potential and possible magnetic exchange effects, little attention has been paid to the possibility that a defect can cause local distortions of the interactions which lead to BCS pairing. We proposed this idea recently in a phenomenological approach to understanding the correlations between dopant atoms and gap inhomogeneity in BSCCO[14]. In that paper, it was shown that by assuming that out of plane dopant atoms

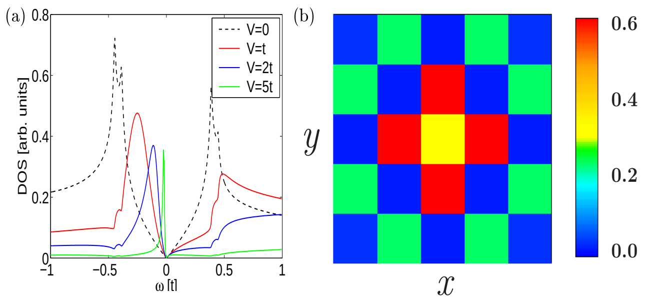

FIG. 1: (Color online) Left: LDOS in a d-wave superconductor at the impurity site for varying potential scattering strengths V (clean case: dashed curve). As V increases the resonant state sharpens and moves to lower energy. Right: Real-space LDOS pattern at the resonant energy ω_B with a delta-function impurity potential ($V = 5t$) at the center[7].

locally enhance the pair interaction, many of the peculiar experimental correlations could be understood[20]. Here, we continue this phenomenological approach, and calculate the Andreev states associated with atomic scale perturbations in the pairing potential relevant for superconductors with very short coherence lengths. This is contrary to the conventional study of Andreev states within the quasiclassical approach where physical quantities are assumed to vary slowly on the atomic scale. From the results for the d-wave case, we show that the low-energy conductance peaks observed near in-plane nonmagnetic impurities in BSCCO can be explained in terms of localized Andreev states. We further investigate the robustness of this picture and suggest some measurements that could be used to test this scenario.

The model is given by the usual BCS Hamiltonian

$$\mathcal{H}_0 = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} + \text{H.c.} \right), \quad (1)$$

where $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$ denotes the quasiparticle dispersion with nearest (next-nearest) neighbor hopping $t(t')$. For s-wave pairing, $\Delta_{\mathbf{k}} = \Delta_0$, whereas for d-wave pairing, $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)$. In terms of the Nambu spinor $\hat{\psi}^\dagger_{\mathbf{k}} = (\hat{c}^\dagger_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow})$, the corresponding Green's function $\mathcal{G}^0(\mathbf{k}, i\omega_n) = -\int d\tau d\mathbf{r} \langle T_\tau \hat{\psi}(0,0) \hat{\psi}^\dagger(\mathbf{r},\tau)\rangle \exp(i(\mathbf{k}\cdot\mathbf{r} - \omega_n \tau))$ in Matsubara representation is given by

$$\mathcal{G}^0(\mathbf{k}, i\omega_n) = \frac{i\omega_n \tau_0 + \xi_{\mathbf{k}} \tau_3 + \Delta_{\mathbf{k}} \tau_1}{(i\omega_n)^2 - E^2_{\mathbf{k}}}, \quad (2)$$

where $E^2_{\mathbf{k}} = \xi^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}$, and τ_i denote the Pauli matrices. In real-space, the perturbation due to delta-function potential impurities in the diagonal τ_3 channel and modulated pairing in the off-diagonal τ_1 channel is given by

$$\mathcal{H}'(\mathbf{r}, \mathbf{r}') = \hat{\psi}^\dagger_{\mathbf{r}} \left[V\delta(\mathbf{r})\delta(\mathbf{r}')\tau_3 - \delta\Delta(\mathbf{r},\mathbf{r}')\tau_1 \right] \hat{\psi}_{\mathbf{r}'}. \quad (3)$$

To obtain the resulting LDOS as a function of energy and lattice sites, one needs to determine the full Green's function $\mathcal{G}(\mathbf{r}, i\omega_n)$ given by the Dyson equation

$$\mathcal{G}(\mathbf{r},\mathbf{r}') = \mathcal{G}^0(\mathbf{r}-\mathbf{r}') + \sum \mathcal{G}(\mathbf{r},\mathbf{r}'') H'(\mathbf{r}'',\mathbf{r}''') \mathcal{G}^0(\mathbf{r}'''-\mathbf{r}'). \quad (4)$$

Thus, by calculating the matrix elements of

$$\mathcal{G}^0(\mathbf{r}, i\omega_n) = \sum_{\mathbf{k}} \frac{(i\omega_n \tau_0 + \xi_{\mathbf{k}} \tau_3 + \Delta_{\mathbf{k}} \tau_1)}{(i\omega_n)^2 - E^2_{\mathbf{k}}} \exp(i\mathbf{k}\cdot\mathbf{r}), \quad (5)$$

the remaining problem is that of a matrix inversion. The solution is presented in terms of the so-called T-matrix

$$\mathcal{G}(\mathbf{r},\mathbf{r}') = \mathcal{G}^0(\mathbf{r}-\mathbf{r}') + \sum \mathcal{G}^0(\mathbf{r}-\mathbf{r}'') T(\mathbf{r}'',\mathbf{r}''') \mathcal{G}^0(\mathbf{r}'''-\mathbf{r}'). \quad (6)$$

The poles of the T-matrix, or equivalently, the determinant of $(1 - H'G^0)$, determine the bound state energies.

For s-wave superconductors, it is well-known that nonmagnetic impurities cannot generate states inside the gap[16]. However, as shown by Yu and Shiba, point-like magnetic impurities ($\mathcal{H}'(\mathbf{r},\mathbf{r}') = \hat{\psi}^\dagger_{\mathbf{r}} \left[V_m \delta(\mathbf{r})\delta(\mathbf{r}')\tau_0 \right] \hat{\psi}_{\mathbf{r}'}$) of strength V_m produce bound states at $\omega_B = \pm\Delta_0 (1 - (V_m \pi N(0))^2)/(1 + (V_m \pi N(0))^2)$, where $N(0)$ is the density of states at the Fermi level in the normal state[17, 18]. Assuming, as a toy-model, a point-like τ_1 scatterer in an s-wave superconductor, a straightforward calculation shows that an attractive delta-function τ_1 scatterer generates Andreev bound states with energies given by $\omega_B = \pm\Delta_0 |(1 - (\pi N(0)\delta\Delta)^2)/(1 + (\pi N(0)\delta\Delta)^2)|$. Here, $\delta\Delta$ is treated as a free parameter and not necessarily just the self-consistent response of the order parameter to e.g. an electrostatic potential. A cursory examination of this expression for the bound state energies ω_B shows that as the local gap decreases from the bulk value Δ_0, the Andreev states are pushed further into the gap. While initially located near the gap edge, for increased scattering strength the bound states can in principle be tuned all the way to zero energy, but this requires $\delta\Delta$ of order the Fermi energy, outside the framework of conventional weak-coupling BCS theory.

What about d-wave superconductors? For a single nonmagnetic τ_3 delta-function impurity, the T-matrix is diagonal with $T_{11} = \delta(\mathbf{r})[V^{-1} - \sum_{\mathbf{k}} \frac{\omega+\xi_{\mathbf{k}}}{\omega^2 - E^2_{\mathbf{k}}}]^{-1} \delta(\mathbf{r}')$, $T_{22} = \delta(\mathbf{r})[-V^{-1} - \sum_{\mathbf{k}} \frac{\omega-\xi_{\mathbf{k}}}{\omega^2 - E^2_{\mathbf{k}}}]^{-1} \delta(\mathbf{r}')$. It is the poles of these matrix elements that largely determine the properties presented in Fig.1. We expect short-ranged τ_1 scatterers to be more relevant in the case of d-wave cuprate superconductors due to the short coherence length of these materials. In the d-wave case, a point-like τ_1 impurity is defined as a modulation of the pairing potential on the four links attached to the impurity site. Following Shnirman *et al.*[15], in the case of a particle-hole symmetric band, one can determine the subgap poles from the determinant $D(\omega)$ given by

$$D(\omega) = 1 - \alpha L(\omega) \left(2 - \alpha L(\omega) + \alpha\omega P(\omega) \right), \quad (7)$$

where α parameterizes the local gap suppression, $\delta\Delta = \alpha\Delta_0$. Here, $P(\omega)$ and $L(\omega)$ are given by

$$(P(\omega), L(\omega)) = -\sum_{\mathbf{k}} \frac{(\omega, \Delta^2_{\mathbf{k}})}{\omega^2 - \xi^2_{\mathbf{k}} - \Delta^2_{\mathbf{k}}}. \quad (8)$$

We can rewrite Eq. (7) in terms of: $\tilde{P}(\omega) = \tilde{\omega} K(1/(1-\tilde{\omega}^2)/(\sqrt{1-\tilde{\omega}^2})$, $\tilde{L}(\omega) = \tilde{\omega}^2/(\sqrt{1-\tilde{\omega}^2}) K(1/(1-\tilde{\omega}^2)) + (\sqrt{1-\tilde{\omega}^2}) E(1/(1-\tilde{\omega}^2))$, where $E(x)$ ($K(x)$) is the complete elliptic integral (of the first kind), and $\tilde{\omega} = \omega/\Delta_0$ and $\tilde{\alpha} = 4\pi N(0)\Delta_0 \alpha$. In Fig.2a we plot the real part of the determinant, Re$D(\omega)$, for different values of the strength of the off-diagonal impurity potential. The imaginary part, Im$D(\omega)$ (not shown), is a monotonically decreasing function as $\omega \to 0$ with Im$D(0) = 0$.

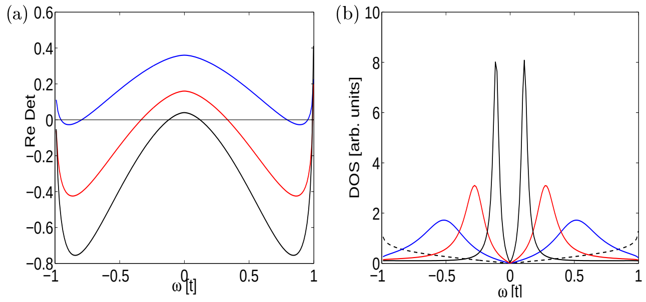

FIG. 2: (Color online) (a) Real part of the determinant, Re$D(\omega)$, with $\tilde{\alpha} = 0.4$ (top), $\tilde{\alpha} = 0.6$ (middle), and $\tilde{\alpha} = 0.8$ (bottom). (b) LDOS at the impurity site for the same values of $\tilde{\alpha}$ as in (a), the dashed curve displays the clean result.

Thus, the point-like τ_1 impurity in a d-wave superconductor also supports Andreev resonant states. The resulting LDOS at the impurity site is shown in Fig.2b: for increased strength of the gap suppression the Andreev resonance sharpens up and moves to lower energy. As opposed to the τ_3 point-like impurity, the resonance exists symmetrically around zero energy with strongly increased amplitude as $\omega_B \rightarrow 0$. In general, this symmetry is broken by including e.g. weak τ_3 potentials. One expects the same to be true for more realistic non-particle-hole symmetric band structures. In this case, however, it is advantageous to resort to numerics. Since we will be mostly interested in the case of optimally doped BSCCO, in the following we fix $t' = -0.3t$, $\Delta_0 = 0.4t$, and $\mu = -t$ corresponding to 17% hole doping.

In Fig.3 we show the LDOS for this band structure at the three sites nearest to the impurity. Clearly, in this case the particle-hole symmetry is broken, and the negative bias resonance dominates the LDOS at the impurity site. Fig.3(d) shows explicitly that the τ_1 scattering channel produces the *largest maximum on the impurity site and has a second maximum on the next-nearest neighbor site*. If we apply the filter function of Ref. [9], the LDOS pattern becomes similar to the one shown in Fig.1(b) in disagreement with experiments. When including the τ_3 scattering channel the asymmetry in Figs.3a,b,c becomes more pronounced. Depending on the specific band structure, we find that in general the main features of Fig.3 remain valid for $V \lesssim t$. Therefore, if the conventional argument is eventually proven correct that a closed unscreened d-shell on Zn necessarily implies a local potential of several eV, then the present model cannot be applied to explain the low-energy conductance peak seen near these impurities in BSCCO[5].

The important point of the results presented here is that point-like τ_1 scatterers generate well-defined Andreev states in both s- and d-wave superconductors. As a specific example (Fig.3), we found that in order to model the sharp zero bias conductance peak near Zn impurities in BSCCO, the local gap has reversed sign compared to

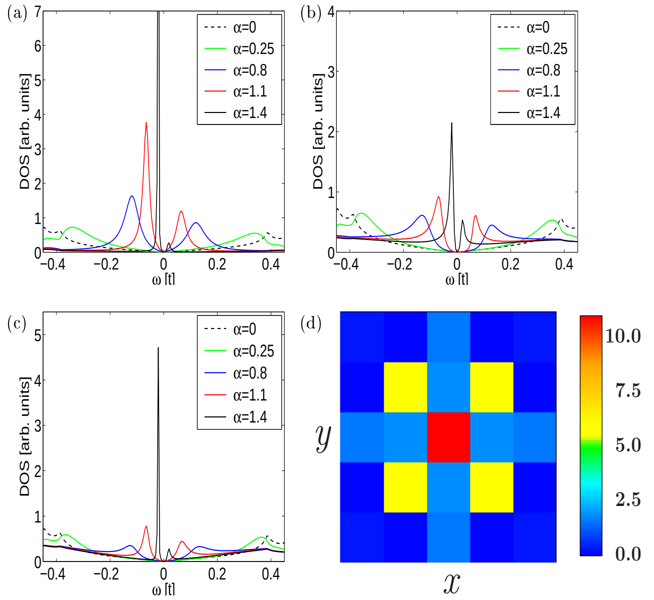

FIG. 3: (Color online) LDOS for various strengths of the τ_1 scatterer at the impurity site (a), on the nearest neighbor site (b), and the next-nearest neighbor site (c). In each figure, the dashed curve shows the bulk LDOS. (d) The real-space LDOS distribution at the resonance energy ω_B when $\alpha = 1.4$.

its value in the bulk[19]. Thus, it is intriguing to consider the idea that nonmagnetic planar impurities in cuprate superconductors act mainly as *phase impurities* changing locally the sign of Δ on the x and y links compared to the bulk. The particular value $\delta\Delta_B$ necessary to generate well-defined low-energy Andreev states near the impurity site depends on band structure, possible nonzero τ_3 scattering, and the spatial extent of the pairing modulation. Regarding the last, we find that for longer ranged phase impurities, the necessary strength $\delta\Delta_B$ is substantially reduced. For example, for a τ_1 impurity ranging over two lattice constants, $\alpha = 0.5$ generates LDOS similar to the solid black curves of Fig.3. Thus, $\delta\Delta_B$ of order Δ_0 is sufficient to generate well-defined low-energy states.

Though the approach here is phenomenological and the microscopic origin of these phase impurities is unknown, they clearly must be generated by the local perturbations resulting from a Zn ion replacing a Cu. In recent work, it was found that the main features of the LDOS spectra in the inhomogeneous nano-scale regions of BSCCO materials can be accounted for by local dopant induced modulations of the pairing interaction[14, 20]. In the present context, we find that self-consistent solutions of the Bogoliubov-de Gennes equations generate phase impurities if the pair interaction near the Zn impurity position is repulsive. Local pairing modulations can be generated, for instance, by locally modified magnetic exchanges and/or electron-phonon couplings. A similar approach has been used previously to explain the enhanced

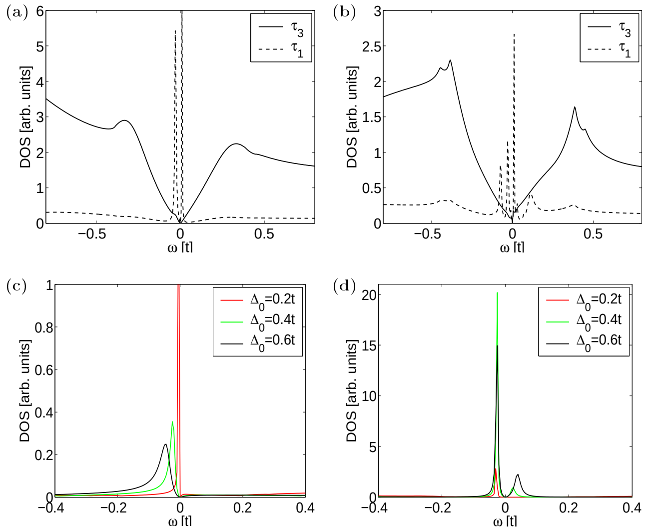

FIG. 4: (Color online) LDOS at $(0,0)$ (a) and $(2,0)$ (b) when two impurities are positioned at $(-1,1)$ and $(1,-1)$ for both the τ_3 (solid) and τ_1 (dashed) channel. In both cases, the τ_3 LDOS has been rescaled for clarity. (c-d) LDOS at the impurity site for a single τ_3 (c) and τ_1 (d) scatterer of fixed strength ($V = 5t$ for τ_3, and $\alpha = 1.4$ for τ_1) but varying Δ_0.

T_c in twinning-plane superconductors[21].

We end this section by suggesting alternative experimental tests of whether the τ_1 or τ_3 channel is dominating the LDOS near Zn in the BSCCO materials. In both scenarios the appearance of the resonance peak is tied to the superconducting transition temperature T_c. Recently, there has been an increased interest in the quantum interference caused by nearby impurity states[22, 23, 24]. Figs.4a,b show the resulting LDOS from two interfering τ_3 or τ_1 impurities. Here, the two impurities are fixed in close proximity at $(-1,1)$ and $(1,-1)$ and the LDOS is shown at $(0,0)$ (a) and $(2,0)$ (b). Evidently, there is a qualitative difference in the resulting interference pattern between the two scenarios: whereas the τ_3 resonances are absent, the well-defined Andreev resonances are split and enhanced by the interference. The latter point remains valid for other sites (except at the impurity site) in the vicinity of the two Andreev resonances. Another possible experimental test utilizes the ubiquitous gap inhomogeneities observed near the surface of BSCCO[25, 26, 27]. Specifically, as shown in Figs.4c,d the LDOS near Zn impurities in large and small gap regions is different in the two scenarios: whereas τ_3 scatterers change both ω_B and the resonance amplitude, the τ_1 case exhibits mainly amplitude modulations with the largest resonance amplitude for intermediate gap Δ_0.

In summary, we have studied the states near short-ranged off-diagonal impurities in both s- and d-wave superconductors. In both cases we find that the impurities generate low-energy Andreev states. This offers a new possibility for the origin of the low-energy conductance peak observed near Zn impurities in BSCCO .

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