Impurity resonances in the mixed state of high-\(T_c\) superconductors

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We study the quasiparticle resonance states near strong impurities in the mixed state of a \(d\)-wave superconductor. These states give rise to zero-bias peaks in the local density of states, observed in scanning tunneling microscopy experiments. The field dependence of the peaks is obtained by averaging with respect to the spatially non-uniform Doppler shifts in the energy of excitations. The hybridization of the magnetic field-induced nodal quasiparticles with the impurity resonances results in the suppression and broadening of the zero-bias peaks. The height of the peaks is found to scale as \((H_{c2}/H)^{1/2}\). The magnetic field response of the peaks is shown to be strongly dependent on the field orientation.

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One of the striking features of high-\(T_c\) superconductors (HTSC’s) is that even a single impurity has a notable effect on the superconducting state, creating a sharp resonance state in its vicinity, which becomes a true bound state of zero energy in the limit of strong impurity potential (the unitary limit) [1, 2, 3, 4, 5, 6]. These bound states manifest themselves as sharp peaks near zero bias in the energy dependence of the single-particle density of states (DoS), which have been observed in scanning tunneling microscopy (STM) experiments on BSCCO compound [7, 8, 9, 10].

The bound states near non-magnetic impurities are specific to unconventional superconductors with an anisotropic order parameter and the gap nodes at the Fermi surface [11]. The zero width of these states in the unitary limit follows from the absence of hybridization with the extended quasiparticle states: HTSC compounds are \(d\)-wave superconductors, and the DoS, \(N_0(\omega)\), of the extended states vanishes at small energy linearly in \(\omega\). However, this is no longer true if the superconductor is placed in an external magnetic field \(H\). The field-induced supercurrents act as pair breakers, filling the gap nodes and creating a finite density of bulk quasiparticles at low energies. These quasiparticles are responsible for a number of peculiar properties of the HTSC’s, such as a non-analytical in \(H\) behavior of the electronic specific heat and the thermal conductivity in the mixed state at low temperatures (the Volovik effect) [12]. One can expect that the hybridization with the field-induced bulk quasiparticles gives rise to a finite width of the impurity bound states. A simpler version of this problem, applicable, for instance, to the case of \(\mathbf{H} \parallel ab\) in the Meissner state, was studied in Ref. [13], where a uniform supercurrent \(q_\|\) was considered and it was shown that the bound states indeed acquire a non-zero width which depends non-analytically on \(q_\|\). In this paper, we study the effect of the magnetic field on the quasiparticle states near unitary impurities in the mixed state for \(\mathbf{H} \parallel c\). In the presence of vortices, the supercurrent is non-uniform, which qualitatively changes the magnetic field response of the impurity resonances. The unitary limit of scattering is of particular interest because the most profound effects related to the impurity resonances have been observed in the vicinity of Zn impurities in BSCCO, which have the \(s\)-wave phase shift \(\delta_0\) close to \(\pi/2\) [7].

Suppose we have a repulsive point-like impurity which is described by the potential \(U(\mathbf{r}) = u\delta(\mathbf{r})\) \((u > 0)\) in a two-dimensional \(d\)-wave superconductor. The external magnetic field \(\mathbf{H}\) is directed along the \(c\) axis. We assume that \(H_{c1} < H \ll H_{c2}\). In these conditions, the Abrikosov vortices are well separated and the amplitude of the superconducting order parameter is constant almost everywhere, except from the core regions, whose size is of the order of the coherence length, \(\xi_0 \sim 1\) nm. The average distance between vortices, \(a_v\), is estimated from the requirement that there is one flux quantum per vortex: \(a_v = \sqrt{\Phi_0/\pi H}\), where \(\Phi_0 = \hbar c/2e\). In typical experimental situations, \(\xi_0 \ll a_v < \lambda_L\), where \(\lambda_L\) is the London penetration depth, which allowed us to replace the internal induction \(B\) by the applied field \(H\).

The quantity measured in STM experiments is the local differential tunneling conductance, which is proportional to the local DoS, \(N(\mathbf{r}, \omega) = -(1/\pi) \text{Im} G^R_{11}(\mathbf{r}, \mathbf{r}; \omega)\), where \(G^R\) is the retarded Gor’kov-Nambu matrix Green function. In the presence of a single scalar impurity, one can express \(G^R\) in terms of the Green function, \(G^R_{0}(\mathbf{r}_1, \mathbf{r}_2; \omega)\), of a clean superconductor in the mixed state: \(G^R = G^R_0 + G^R_0T G^R_0\), where \(T(\omega) = \omega \tau_3 [1 - u g_0(\omega) \tau_3]^{-1}\) is the T-matrix, with \(g_0(\omega) = G^R_0(\mathbf{0}, \mathbf{0}; \omega)\). Then,

\[
N(\mathbf{r}, \omega) = N_0(\mathbf{r}, \omega) + N_{imp}(\mathbf{r}, \omega),
\]

where \(N_0\) is the local DoS for a \(d\)-wave superconductor in the mixed state in the absence of impurity, and

\[
N_{imp} = -\frac{1}{\pi} \text{Im} \left[ G^R_0(\mathbf{0}, \mathbf{0}; \omega) T(\omega) G^R_0(\mathbf{0}, \mathbf{0}; \omega) \right]_{11}
\]

is the impurity-induced contribution. The unitary limit corresponds to strong scattering: \(u \rightarrow \infty\) and \(T(\omega) \rightarrow -g_0^{-1}(\omega)\). In this limit, \(N(\mathbf{0}, \omega) = 0\) because the quasiparticles are prevented from occupying the impurity site
by a strong repulsive potential. Thus, in order to study the effect of magnetic field on the bound state near a unitary impurity, one should calculate the local DoS at one of its nearest neighbors, e.g. at $\mathbf{r} = \mathbf{a}$, where $N(\mathbf{r}, \omega)$ reaches its maximum. That the STM pictures show the maximum of the tunneling conductance directly above the impurity can be attributed to the blocking effect of Bi-O layers and does not invalidate the standard theoretical model of the impurity bound states. It should be mentioned that there are alternative explanations of this effect. For example, it was suggested that superconductivity is completely destroyed in the vicinities of this effect. For example, it was suggested that superconductivity is completely destroyed in the vicinities of this effect. Creating an effectively normal region with high DoS.

In this article, creating an effectively normal region with high DoS. Another possibility is the Kondo screening of the local magnetic moment induced around the Zn impurity, see Ref. [15], creating an effectively normal region with high DoS. It is still an open question, whether the peak in the STM conductance right above the impurity site is related to the details of the tunneling measurements or is an intrinsic property of the CuO layers. In this article, we adopt the former point of view.

We shall see that the energy dependence of $N_{imp}(\mathbf{a}, \omega)$ is determined mostly by that of the $T$-matrix. A closed analytical expression for $g_0(\omega) = G^R_0(0, 0; \omega)$ can be obtained only in the case of a uniform supercurrent, when a gauge transformation can be applied to make the order parameter real and independent of $\mathbf{r}$, so that the Fourier transform of $G^R_0(\mathbf{r}, 0; \omega)$ is given by

$$G^R_{0, \text{uniform}}(\mathbf{k}, \omega) = \frac{(\omega + v_F q_x) \tau_0 + \xi_k \tau_3 + \Delta_k \tau_1}{(\omega - v_F q_x)^2 - \xi_k^2 - \Delta_k^2}. \quad (3)$$

Here $\omega_+ = \omega + i0$, $\tau_i$ are the Pauli matrices, $\xi_k$ is the normal state spectrum, $v_F = \nabla_k \xi_k$ is the Fermi velocity, $q_x$ is the superfluid momentum, and $\Delta_k = 2\Delta_0 (\cos k_x d - \cos k_y d)$. The mean-field order parameter, corresponding to $d_{x^2-y^2}$ symmetry ($d$ is the lattice constant). We do not calculate the order parameter self-consistently and assume $\Delta_0$ to be constant. The numerical investigation of the self-consistency effects shows some suppression of the order parameter near the impurity site, which leads only to a renormalization of the effective impurity strength towards the unitary limit. It follows from Eq. (3) that the quasiparticle energy is Doppler-shifted in the presence of supercurrent: $E_k = \pm \sqrt{\xi_k^2 + \Delta_k^2} + v_F q_x$.

The relevant energies of the problem are small compared to the gap magnitude: according to Refs. [12], the energy scale associated with the Doppler shift in the mixed state is given by $E_H = v_F/a_0 \ll \Delta_0$. The Zeeman splitting is neglected because $\mu_B H \ll E_H$ at all experimentally relevant fields along the $c$ axis (the field at which the Zeeman splitting becomes comparable to $E_H$ is of the order of $H_{c2}^2/H_{c2}$, where $H_{c2}$ is the paramagnetic limiting field). Assuming an electron-hole symmetric band, the momentum integrals can be easily calculated, giving the following result at real frequencies: $g_0(\omega) = \pi N_F F(\omega)\tau_0$, where $z = \omega/\Delta_0$ and

$$F(z) = \sum_{n=1}^4 \left[ \frac{1}{2\pi} (z - z_n) \ln |z - z_n| - \frac{i}{4} |z - z_n| \right]. \quad (4)$$

Here $N_F$ is the DoS in the normal state at the Fermi level, $n$ labels the gap nodes, $z_n = v_n q_x/\Delta_0$ are the dimensionless Doppler shifts, and $v_n$ are the Fermi velocities at the nodes (we label the nodes in such a way that $z_1 = -z_3$, and $z_2 = -z_4$). Expression (4) is valid at $|z| \ll 1, |z_n| \ll 1$. Finally, $T(z) = u c_\tau [c - F(\omega)\tau_3]^{-1}$, where $c = 1/(\pi u N_F) = \cot \delta_0 > 0$ for a repulsive impurity.

The spectrum of the bound states is determined by the poles of the $T$-matrix, i.e. by the equation $F(z) = \pm c$. In zero field, $F(z) \rightarrow F_0(z) = (2/\pi) \ln |z - i|$. At $c \ll 1$, the equation $F_0(z) = \pm c$ has the solution $z_0 = \mp \pi c/|z - i|$, with logarithmic accuracy, describing a narrow impurity-induced resonance. In the unitary limit $c = 0$, the resonance is coupled from the continuum of bulk excitations and becomes a true bound state of zero width, which manifests itself as a sharp peak in the tunneling DoS. In the presence of a non-zero supercurrent, the DoS of the bulk excitations does not vanish at $\omega = 0$, which leads to a stronger hybridization of the bound state and the continuum of propagating states. As a result, the bound state is replaced by a sharp resonance whose width is proportional to $v_F q_x/|\ln(v_F q_x/\Delta_0)| \ll \Delta_0$.

In the mixed state, the supercurrent and the order parameter amplitude are non-uniform, and Eq. (3) is no longer valid. Further progress can be achieved by using the so-called Doppler-shift approximation [12, 13]. The basic assumption of this approach that the low-energy properties of a superconductor with the gap nodes are determined by the extended quasiparticle states and the contribution from the vortex cores can be neglected. The effect of the magnetic field can be described quasiclassically by introducing a non-uniform Doppler shift of the excitation energy: $E_k \rightarrow E_k(\mathbf{r}) = E_k + v_F q_x(\mathbf{r})$. In particular, the Green function at coinciding arguments becomes $G^R_0(\mathbf{r}, \mathbf{r}; \omega) = \pi N_F F(\omega)\tau_0$, where $F$ is defined by Eq. (4), in which the Doppler shifts $z_n$ now depend on the coordinate: $z_n \rightarrow z_n(\mathbf{r}) = v_n q_x(\mathbf{r})/\Delta_0$. It is expected that the Doppler-shift approximation works well at low fields $H \ll H_{c2}$ (for a discussion of its applicability and limitations, see, e.g., Ref. [20]).

The Doppler-shift approximation should be used with caution in the calculation of the local DoS because the impurity-induced contribution rapidly oscillates as a function of $\mathbf{r}$ with the period of the order of $k_F^{-1}$. We assume that the impurity is unitary, so that

$$N(\mathbf{r}, \omega) = N_0(\mathbf{r}, \omega) + \frac{1}{\pi^2 N_F} \text{Im} \left\{ F^{-1} \left( \frac{\omega}{\Delta_0} \right) \times \left[ G^R_0(\mathbf{r}, 0; \omega) G^R_0(0, \mathbf{r}; \omega) \right] \right\}. \quad (5)$$
Due to the smallness of the energy scale \(E_H\), only the limit \((\omega, v_F q_a) \leq E_H \ll \Delta_0\) is relevant. In this limit, one can neglect \(N_0(\mathbf{r}, \omega)\) compared to \(N_{\text{imp}}(\mathbf{r}, \omega)\), which is peaked at small \(\omega\) because of the singularity of \(F^{-1}(\omega/\Delta_0)\). In addition, the product of two Green functions in the second term on the right-hand side of Eq. 6 depends weakly on \(\omega\) and \(q_s\) and can therefore be replaced by its value at \(\omega = q_s = 0:\)

\[
[G^R_0(\mathbf{r}, 0; 0)G^R_0(0, \mathbf{r}; 0)]_{11} = (\pi N_F)^2 \gamma(\mathbf{r}).
\]  

(6)

Here \(\gamma = |I_1|^2 + |I_2|^2\) is a real number, which depends on the order parameter and the shape of the Fermi surface,

\[
I_1(\mathbf{r}) = \frac{1}{\pi N_F} \int \frac{d^2 k}{(2\pi)^2} \frac{\xi_{k}}{\xi_{k}^2 + \Delta_{k}^2},
\]

\[
I_2(\mathbf{r}) = \frac{1}{\pi N_F} \int \frac{d^2 k}{(2\pi)^2} \frac{\xi_{k}}{\xi_{k}^2 + \Delta_{k}^2},
\]

where the \(k\)-integration goes over the first Brillouin zone \(-\pi/d \leq k_x, k_y \leq \pi/d\). Thus, in the unitary limit and at \(\omega \ll \Delta_0\),

\[
\frac{N_{\text{imp}}(\mathbf{a}, \omega)}{N_F} = \gamma(\mathbf{a}) \text{Im} F^{-1}\left(\frac{\omega}{\Delta_0}\right).
\]

(7)

For a dispersion \(\xi_{k} = -2t(\cos k_x d + \cos k_y d) - 4t_1 \cos k_x d \cos k_y d - \mu\), and \(\mathbf{r} = \mathbf{a} = \hat{x} d\), we have \(\gamma(\mathbf{a}) = 0.63\) (we used the parameters representative of BSCCO near the optimum doping: \(t_1/t = -0.3\), \(\mu/t = -1\), \(\Delta_0/t = 0.04\), \(\Delta_0 = 10\) meV).

When calculating the energy dependence of the impurity resonance contribution to the local DoS, \(N_{\text{imp}}(\omega) = N_{\text{imp}}(\mathbf{a}, \omega)\), one can use the values of the Doppler shifts at the impurity site, \(z_n = z_n(\mathbf{0})\), since the variation of the supercurrent at the atomic length scale is negligibly small. As a final step, one should average over all impurity positions (or, equivalently, over the vortex positions relative to the impurity site):

\[
\frac{N_{\text{imp}}(\omega)}{N_F} = \gamma \langle \text{Im} F^{-1}\left(\frac{\omega}{\Delta_0}\right) \rangle_{\mathcal{P}}.
\]

(8)

Here \(\langle \text{Im} F^{-1} \rangle_{\mathcal{P}} = \int dz_1 dz_2 \mathcal{P}(z_1, z_2) \text{Im} F^{-1}\), where \(F\) is defined in Eq. 4, and \(\mathcal{P}\) is the distribution function of the Doppler shifts:

\[
\mathcal{P}(z_1, z_2) = \frac{1}{\mathcal{A}} \int d^2 r \delta\left(z_1 - \frac{\mathbf{v}_1 q_s(\mathbf{r})}{\Delta_0}\right) \times \delta\left(z_2 - \frac{\mathbf{v}_2 q_s(\mathbf{r})}{\Delta_0}\right),
\]

(9)

where \(\mathcal{A}\) is the system area.

According to Ref. 10, Zn impurities in BSCCO act as pinning centers for the vortices, so that a sizeable fraction (\(\sim 50\%)\) of the vortices reside at the impurity sites, creating a disordered vortex solid. Because of a strong variation of the order parameter in the vortex core, the Doppler-shift approach is clearly inapplicable for the bound states near such impurities. On the other hand, in the experimental conditions of Ref. 11, the majority of Zn atoms are found in the space between the vortex cores and exhibit zero-bias peaks in the tunneling DoS. The field dependence of these peaks can be analyzed using the Doppler-shift approximation. The overlap of the impurity resonances and the core states is neglected.

The probability distribution, Eq. 9, of the Doppler shifts at the inequivalent gap nodes depends on the vortex configuration. In the case of a disordered vortex solid, which is relevant to the experiment, the probability density is peaked around the zero Doppler shift. In Ref. 20, different models for the supercurrent distribution were discussed giving rise to different \(\mathcal{P}(z_1, z_2)\). One possible choice, which agrees with the results of numerical simulations and is believed to capture the physics reasonably well, is given by

\[
\mathcal{P}(z_1, z_2) = \frac{1}{\pi} \frac{z_H^2}{(z_1^2 + z_2^2 + z_H^2)^2},
\]

(10)

where \(z_H = E_H/\Delta_0 \simeq \sqrt{H/H_c2}\). We use this distribution in Eq. 8 to calculate the average DoS.

At zero field, \(z_H = 0\), and \(\mathcal{P}(z_1, z_2) = \delta(z_1)\delta(z_2)\). In this case, the local DoS has a divergent peak near zero bias: \(N_{\text{imp}}(\omega) / N_F = \gamma \text{Im} F^{-1}_0(\omega)\). It is not a \(\delta\)-function peak because \(F^{-1}_0(z)\) does not have a simple pole structure. At finite \(H\), the height of the peak at \(\omega = 0\)
becomes finite and can be calculated exactly:

\[ \frac{N_{\text{imp}}(0)}{N_F} = 2\gamma \left\langle \frac{1}{|z_1| + |z_2|} \right\rangle_{\mathcal{P}} \]
\[ = \frac{2\sqrt{2}\ln(\sqrt{2} + 1)\gamma}{z_H} \sqrt{\frac{H_{c2}}{H}}. \quad (11) \]

For the band dispersion described above, \( N_{\text{imp}}(0)/N_F \approx 1.57 \sqrt{H_{c2}/H} \). This should be contrasted to the uniform supercurrent model considered in Ref. [13], according to which \( N_{\text{imp}}(0)/N_F \propto H^{-1} \).

It can also be shown that the result \( N_{\text{imp}}(0)/N_F \propto \sqrt{H_{c2}/H} \) is actually independent of the choice of \( \mathcal{P}(z_1, z_2) \). Indeed, \( \mathcal{P}(z_1, z_2) \) is even in both \( z_1 \) and \( z_2 \) and also symmetric with respect to the interchange \( z_1 \leftrightarrow z_2 \).

If the only energy scale of the Doppler shift distribution is \( E_H \), then \( \mathcal{P} \) can always be written in the form

\[ \mathcal{P}(z_1, z_2) = \frac{1}{z_H} f \left( \frac{z_1}{z_H}, \frac{z_2}{z_H} \right). \quad (12) \]

where \( f(x, y) \) is a dimensionless function such that \( f(x, y) = f(y, x) \), \( f(\pm x, \pm y) = f(x, y) \), and \( \int_0^\infty dx \int_0^\infty dy f(x, y) = 1 \) in order to satisfy the normalization condition for \( \mathcal{P} \). Then,

\[ \frac{N_{\text{imp}}(0)}{N_F} = \frac{2\gamma}{z_H^2} \int \frac{dz_1}{|z_1|} \int \frac{dz_2}{|z_2|} f \left( \frac{z_1}{z_H}, \frac{z_2}{z_H} \right) \]
\[ = A \frac{\Delta_0}{E_H}. \quad (13) \]

where \( A = 2\gamma \int dx dy f(x, y)/(|x| + |y|) \).

At arbitrary bias, the impurity contribution to the local DoS given by Eq. (13) can be calculated numerically. In Fig. 1 we plot \( N_{\text{imp}}(\omega)/N_F \) for several values of \( z_H \). The most prominent feature of these graphs is that the peaks are indeed quickly suppressed as \( H \) grows, in accordance with the result (11). To see that this suppression is accompanied by broadening and to facilitate comparison of the results at different \( z_H \), we plot in Fig. 2 the local DoS normalized to its maximum value, \( N_{\text{imp}}(\omega)/N_{\text{imp}}(0) \). The broadening of the peaks can be attributed to the hybridization of the impurity bound states with the field-induced nodal quasiparticles, whose density of states at zero energy increases with field as \( \sqrt{H/H_{c2}} \) [12]. One should keep in mind that since the expressions (4) and (8) are applicable only at \( z, z_H \ll 1 \), they give a quantitatively correct picture only in the vicinity of the zero-bias peaks at fields far from \( H_{c2} \).

In conclusion, we have studied the influence of magnetic field on the impurity bound states in \( d \)-wave superconductors. The magnetic field effects are treated semi-classically, using the Doppler-shift approach. The main result is that the bound states are destroyed by magnetic field, which manifests itself as the suppression and broadening of the zero-bias peaks in the tunneling DoS. The height of the peaks scales as \( H^{-1/2} \) for any non-uniform supercurrent distribution, depending on a single energy scale \( E_H \). This result is sensitive to the orientation of the field: if \( H \) is parallel to the \( ab \) planes, then the uniform supercurrent model of Ref. [13] should be more appropriate, which predicts that the height of the peaks is proportional to \( H^{-1} \). As mentioned above, the impurity resonance model is not the only possible explanation of the zero-bias anomalies in the tunneling conductance of HTSC’s. It would be interesting to look at the magnetic-field response in the other models, which might help to resolve the controversy about the origin of the zero-bias peaks.

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