Effect of magnetic field on impurity bound states in high-$T_c$ superconductors

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We consider the influence of a magnetic field $H$ on the quasiparticle bound states near scalar impurities in $d$-wave superconductors. A “Doppler shift” in the excitation energies induced by the supercurrent leads to several important effects. At large but finite impurity strength, there are corrections to the energy and width of the impurity-induced resonance, proportional to $H^2$. On the other hand, in the limit of very strong impurity potential (unitary limit), the bound state is destroyed and acquires a finite width proportional to $H(\ln H)^{-1}$. There are also considerable changes in the asymptotic behaviour of the bound state wave functions.

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High-temperature superconductors (HTSC) belong to a class of unconventional superconductors with $d$-wave symmetry [1]. A non-trivial orbital structure of the order parameter, in particular the presence of the gap nodes, leads to the effects of disorder in HTSC being much richer than in conventional materials. For instance, in contrast to the $s$-wave case, the Anderson theorem does not work and non-magnetic impurities exhibit a strong pair-breaking effect. Also, a finite concentration of disorder produces a non-zero density of quasiparticle states at zero energy, which results in a considerable modification of the thermodynamic and transport properties at low temperatures [8].

One of the striking features of $d$-wave superconductors is that even a single scalar impurity has a notable effect on the superconducting state, creating a quasiparticle impurity bound state (IBS) in its vicinity whose energy and width tend to zero in the limit of strong impurity potential [3]. Various aspects of the theory of IBS have been elaborated by many authors, both analytically [3–5] and numerically [8]. From the practical point of view, the high sensitivity of IBS to the symmetry of the order parameter and the impurity strength makes these states a powerful tool for probing the properties of HTSC. This has been done recently in beautiful scanning tunneling microscopy (STM) experiments on BSCCO compounds [10–14], in which many of the theoretically predicted features of IBS were observed, such as (i) sharp peaks in the energy dependence of the single-particle density of states (DoS), (ii) a cross-shape anisotropy of the quasiparticle wave functions in $a$-$b$ plane, and (iii) a slow power-law decay of the wave functions away from the impurity. (Some apparent discrepancies between the theory and the experiment, such as the position of the maximum local DoS directly above the impurity site as seen in STM pictures, can be attributed to the blocking effect of Bi-O layers [10] and thus do not invalidate the standard theoretical picture of IBS.)

All previous studies have neglected the influence of an external magnetic field on IBS. It is known, however, that in the presence of the gap nodes, the supercurrent induced by a magnetic field acts as an effective pair breaker and gives rise to a finite density of bulk quasiparticles at low energies. This should affect the properties of IBS because of the hybridization of localized and delocalized states. The purpose of the present article is to study the combined effect of magnetic field and strong impurity scattering in $d$-wave superconductors. We neglect the Zeeman splitting and concentrate on the physical properties relevant to the $c$-axis STM experiments which probe the local DoS at various distances from an impurity site. The influence of the magnetic field on the disorder-averaged density of states in $d$-wave superconductors with randomly distributed unitary impurities was studied in Ref. [1].

Let us consider a repulsive point-like impurity with potential $U(r) = u \delta(r) \ (u > 0)$ in a two-dimensional $d$-wave superconductor. The external magnetic field can be directed either in the $a$-$b$ plane or along the $c$ axis. In both cases, we assume that the supercurrent $\mathbf{p_s}$ is locally uniform, and use the gauge in which the order parameter is real [12]. The model Hamiltonian can be written in the following form:

$$\mathcal{H} = \sum_{kk'} C_{kk'}^\dagger \mathcal{H}_{kk'} C_{kk'},$$

where $C_k = (c_{k\uparrow}, c_{-k\downarrow})^T$ are Nambu operators, and

$$\mathcal{H}_{kk'} = \left( \frac{H^\perp}{\Delta_k} - H^\perp \right).$$

is the Bogoliubov-de Gennes (BdG) operator. The normal part of $\mathcal{H}_{kk'}$ depends on the supercurrent via the gauge transformation: $H^\perp = \xi_{kk'} \mathbf{p_s} + U_{k-k'} \simeq \xi_k \pm v_F \mathbf{p_s} + U_{k-k'}$, where $\xi_k = k^2/(2m) - \mu$ is the normal state spectrum (we assume a spherical Fermi surface, which does not restrict the generality of our results, but considerably simplifies the calculations), $v_F = \nabla_k \xi_k$ is the Fermi velocity, and $U_k$ is the Fourier transform of the impurity potential. The mean-field order parameter, corresponding to $d_{x^2-y^2}$ symmetry, has the form $\Delta_k = \Delta_0 (\hat{\mathbf{t}}_x^2 - \hat{\mathbf{t}}_y^2) = \Delta_0 \cos 2\varphi$, where $\varphi$ is the azimuthal
angle in $a$-$b$ plane. Note that we do not calculate the order parameter self-consistently and assume $\Delta_0$ to be constant. The numerical investigation of the self-consistent BdG equations shows that there is some suppression of the order parameter magnitude near an impurity site [13], which can affect the low-energy behaviour of DoS in a system with a finite number of impurities [14]. Here we study the single-impurity limit, which corresponds to a dilute disorder concentration. In this case, it has been demonstrated in Ref. [15] that the order parameter variation leads only to renormalization of the effective impurity strength towards the unitary limit.

The quantity measured in STM experiments is the local differential conductance $dI/dV$, which is proportional to the local density of states:

$$N(r, \omega) = -\frac{1}{\pi} \text{Im} \, G^R_{11}(r, r; \omega),$$

where $G^R$ is the retarded Gor’kov-Nambu matrix Green’s function. In the presence of a single scalar impurity, one can express $G^R$ in terms of the Green’s function of a clean superconductor. Thus,

$$G^R(r_1, r_2; \omega) = G^R_0(r_1 - r_2, \omega) + G^R_0(\mathbf{r}_1, \omega) T(\omega) G^R_0(-\mathbf{r}_2, \omega),$$

where the $T$-matrix is given by $T(\omega) = \omega \tau_3 \left[1 - u g(\omega) \tau_3\right]^{-1}$, and $g(\omega) = G^R_0(0, \omega) = \int d\mathbf{k}/(2\pi)^2 \, G^R_0(k, \omega)$. The Green’s function $G^R_0$ describes a homogeneous system without an impurity, but in the presence of a uniform supercurrent. The effect of the supercurrent in a translationally invariant system amounts to a “Doppler shift” in the quasiparticle energy. In the momentum representation, we have

$$G^R_0(k, \omega) = \frac{i\omega + v_F p_s \tau_0 + \xi_k \tau_3 + \Delta_k \tau_1}{i\omega - v_F p_s \Delta_0 \tau_2 + \xi_k \tau_3 - \Delta_k \tau_1},$$

where $\omega = \omega + i0$, and $\tau_i$ are the Pauli matrices.

The energies of the impurity-induced IBS correspond to the poles of the $T$-matrix and satisfy the equation $\det T(\omega) = 0$, whose solutions can be complex. We are interested in the limit of small supercurrent and strong impurity scattering, so that the relevant energies are expected to be small compared to the gap magnitude. This case is of particular interest because the most profound effects related to IBS have been observed in the vicinity of Zn impurities in BSCCO, which have the s-wave phase shift $\delta_0 \approx 0.48\pi$ and thus are very close to the unitary limit [1]. The momentum integrals can be easily calculated, giving the following result at $\text{Im} \, \omega = 0$:

$$\text{Im} \, g(\omega, p_s) = g_0(\omega, p_s) \tau_0 + g_1(\omega, p_s) \tau_1,$$

where, in leading order in $(v_F p_s/\Delta_0)^2$,

$$g_0 = -\frac{\pi N_F}{4\Delta_0} \sum_{i=1}^{4} |\omega - v_i p_s|,$$

$$g_1 = -\frac{\pi N_F}{8\Delta_0} \left[\mathbf{z} \times p_s\right] \cdot \sum_{i=1}^{4} (-1)^i v_i |\omega - v_i p_s|.$$  

In these expressions, $N_F$ is the DoS in the normal state at the Fermi level [12], $i$ labels the gap nodes, and $v_i$ are the Fermi velocities at the nodes. We see that, at small supercurrents, it is possible to neglect the off-diagonal terms in (9) (retaining these terms would give the corrections of the order of $(v_F p_s/\Delta_0)^4$ to the results below). From the Kramers-Kronig relations, we obtain

$$g(\omega) = \frac{\pi N_F}{2\Delta_0} \sum_{i=1}^{4} \frac{(\omega - v_i p_s) \ln \Delta_0}{|\omega - v_i p_s|} \tau_0. \quad (8)$$

The next step in the derivation of the $T$-matrix is to continue $g(\omega)$, whose real and imaginary parts at the real axis are given by Eqs. (6) and (10), to the whole complex plane of $\omega$. Introducing the notation $z = \omega/\Delta_0$, we have $g(\omega) = \pi N_F F(z) \tau_0$, where

$$F(z) = \frac{1}{2\pi} \sum_{i=1}^{4} \left(z - z_i\right) \ln(z - z_i) - iz \quad (9)$$

with $z_i = v_i p_s/\Delta_0 \sum_i z_i = 0$. Four logarithmic branch cuts go down from $z = z_i$ parallel to the negative imaginary axis. Finally,

$$T(z) = \begin{pmatrix} uc & 0 \\ c - F(z) & -uc \end{pmatrix}$$

where $c = (\pi u N_F)^{-1} \approx \cot \delta_0 > 0$ for a repulsive impurity. This expression for the $T$-matrix is valid at $|z|, |z_i| \ll 1$.

The IBS spectrum is determined by the equation

$$F(z) = \pm c. \quad (11)$$

In the absence of a supercurrent, $F(z) \to F_0(z) = (2/\pi) z \ln z - iz$, and Eq. (11) can be easily solved at $c \ll 1$, giving the IBS energy of the form $\omega_0 = z_0 \Delta_0$, where $\text{Re} \, z_0 = \mp \pi c/2 \ln |c|$, $\text{Im} \, z_0 = -\pi^2 c/4 \ln^2 c$ with logarithmic accuracy [3]. The presence of a non-zero imaginary part indicates that the impurity-induced bound state is in fact a narrow resonance.

At $p_s \neq 0$, the effect of supercurrent on IBS strongly depends on the relation between the Doppler shift $v_F p_s$ and the “bare” energy $\omega_0$. If $p_s$ is parallel to one of the crystallographic axes, e.g. (100), then $z_{1.4} = -z_{2.3} = z_s = v_F p_s/\sqrt{2} \Delta_0$, and Eq. (11) takes the form

$$F(z) = -iz + \frac{1}{\pi} (z + z_s) \ln(z + z_s) + \frac{1}{\pi} (z - z_s) \ln(z - z_s). \quad (12)$$
For $z_s \ll |z_0|$, the solution of Eq. (11) can be found perturbatively in $z_s$. Using the expansion $F(z) = F_0(z) + z_s^2/\pi z$, we find

$$\begin{align*}
\text{Re } z &= \text{Re } z_0 + \frac{1}{\pi} \frac{z_s^2}{2}, \\
\text{Im } z &= \text{Im } z_0 - \frac{1}{2c \ln^2 c} z_s^2. \quad (13)
\end{align*}$$

These expressions are valid as long as $|\delta z(z_s)/z_0| \ll 1$. Thus, in the presence of a small magnetic field, the corrections to the IBS energy and width are proportional to $H^2 (z_s^2 = 0.5|H/H_c(0)|^2$ for $\mathbf{H} \perp z$).

More interesting is the opposite limit of “large” supercurrents, which is relevant when the impurity scattering is close to the unitary limit. In zero field, the bare IBS current, which is relevant when the impurity scattering width. The dominant energy scale in this case is provided by the Doppler shift $v_F p_s$, which makes it possible to treat the right-hand side of Eq. (11) as a small perturbation. It can be checked that the equation $F(z) = 0$ has only one solution in the complex plane:

$$z_s = -\frac{i}{2|\ln z_0|} \frac{\pi z_s}{z} \quad (14)$$

At $c \neq 0$, we look for a solution in the form $z = z_s + \delta z(c)$ and obtain

$$\begin{align*}
\text{Re } z &= \frac{\pi c}{2|\ln z_0|}, \\
\text{Im } z &= -\frac{1}{2|\ln z_0|} + O(c^2). \quad (15)
\end{align*}$$

These expressions are valid as long as $|\text{Re } z/z_s| \ll 1$, i.e. at $z_s \gg c$. From Eqs. (13) we see that the zero-energy IBS in the unitary limit is destroyed by magnetic field, getting replaced by a resonance whose width is proportional to $H^2$. The physical reason for this is clear from Eqs. (3) and (6): at non-zero supercurrent, the DoS of the bulk excitations does not vanish at $\omega = 0$, which leads to a stronger hybridization of the IBS and the continuum of propagating states. We would like to stress that the result (13) is manifestly non-perturbative in magnetic field.

The calculations for other directions of supercurrent can be done in a similar fashion. Solution of Eq. (11) leads to the expressions analogous to (13) and (14), albeit with different numerical coefficients. Therefore, the qualitative effect of magnetic field on the IBS energy does not depend on the direction of $\mathbf{p}_s$.

In order to visualize our results and facilitate the comparison with STM experiments, we have computed the local DoS at the impurity site:

$$N(0, \omega) = -N_F \frac{c F(z)}{c - F(z)}, \quad (16)$$

where $F$ is given by Eq. (3). The dependence of $N(0, \omega)$ on energy and supercurrent is plotted in Fig. 1. We see that the asymmetric peak in the local DoS, which corresponds to a hole-like resonance at $c > 0$, gets shifted and broadened in the presence of supercurrent.

It follows from (14) that $N(0, \omega) = 0$ at $c = 0$. For this reason, the STM measurements directly at the impurity site are not useful in the unitary limit. To study the effect of supercurrent on IBS in this case, one should calculate the local DoS away from the point $r = 0$, e.g. at one of the nearest neighbors of the impurity site, where the local DoS is known to reach its maximum value at $p_s = 0$. According to Eqs. (3), (4) and (10), the local DoS at site $r$ in the unitary limit can be represented in the form

$$N(r, \omega) = N_0(\omega) + \frac{1}{\pi^2 N_F} \text{Im } \frac{F(z)}{F(z)} \left[ G_0^R(r, \omega) G_0^R(-r, \omega) \right]_{11}, \quad (17)$$

where $N_0(\omega) = -(1/\pi) g_0(\omega)$ is the DoS for a clean d-wave superconductor in the presence of supercurrent, and $G_0^R(r, \omega)$ is the Fourier transform of Eq. (3). At $r = a$ and $(\omega, v_F p_s)/\Delta_0 \to 0$, one can neglect the first term on the right hand side of Eq. (17) compared to the second one, which is singular in this limit. The singularity comes from $F^{-1}(z)$, while the product of two Green’s functions is not singular and can be replaced by its value at $\omega = p_s = 0$, which is real. Therefore, $N(a, \omega)/N_F \sim \text{Im } F^{-1}(z)$. We have calculated the energy dependence of $\delta N(a, \omega) = N(a, \omega) - N_0(\omega)$ for $p_s \parallel a$ and plotted the results in Fig. 2. As the supercurrent increases, so does the width of the zero-energy peak, whereas its magnitude decreases. Experimentally, a notable suppression of the c-axis zero-bias conductance peaks (ZBCP) has been reported in Ref. [17] for YBCO/Ag and TBCCO/Au planar junctions. It is tempting to attribute this observation to the effect of magnetic field on the IBS induced by strong defects at the surface of those materials.

Another peculiar property of IBS, which was predicted in Ref. [13] and observed in recent STM experiments [14], is a sharp four-fold anisotropy of the IBS wave functions at zero bias, with a characteristic $1/r^2$-tails at large distances from the impurity. This not only reflects the microscopic symmetry of superconducting state, but also has important consequences for the quasiparticle transport in HTSC. It was argued in Ref. [13] that, in the presence of many impurities, the overlap of the extended IBS wave functions along the gap node directions can result in the formation of an impurity band, where all states are delocalized and can thus participate in quasiparticle transport. This should be contrasted to the propagating excitations which are localized in the presence of short-range disorder potential [14].

Here we address the following question: What is the effect of magnetic field on the asymptotics of the IBS
wave functions in the unitary limit? We study the decay of \( \delta N(r, \omega) = N(r, \omega) - N_0(\omega) \) along the nodal direction (110) at \( \omega = 0 \). The coordinate dependence of \( G_0^{\|}(r, \omega) \) in Eq. (1) is described by rather cumbersome expressions (the details of calculations will be given in a separate publication), which take on a particularly simple form in the limit of large distances from the impurity \( r \gg p_s^{-1} \gg \xi_0 = v_F/\Delta_0 \). In contrast to our results for the IBS energies, the asymptotic behaviour of the wave functions strongly depends on the direction of the supercurrent. If \( p_s \) is perpendicular to the nodal direction (110), then, in leading order in \( 1/r \),

\[
\delta N(r, 0) = \frac{\gamma(p_s) N_F \xi_0^2}{4\pi^2} \frac{\sin^2 k_F r}{r^2},
\]

for \( k_F \xi_0 \gg p_s r \gg 1 \), and

\[
\delta N(r, 0) = -\frac{\gamma(p_s) p_s 1}{8\pi^2 \Delta_0} \frac{1}{r},
\]

for \( p_s r \gg k_F \xi_0 \gg 1 \) (we introduced the notation \( \gamma(p_s) = \text{Im} F^{-1}(z = 0) \)). If \( p_s \) is parallel to (110), then

\[
\delta N(r, 0) = -\frac{N_F p_s \xi_0^2}{8\pi} \text{Im} \left[ F^{-1}(0) e^{2ik_F r} \right].
\]

Eq. (18) is essentially the zero-field result, whereas Eqs. (19) and (20) show that magnetic field leads to a slower power-law decay of the envelope IBS wave functions along the nodal directions, or even the disappearance of the Fermi oscillations at very large distances from the impurity. These changes reflect the contributions from the nodal quasiparticles excited by supercurrent. In particular, the non-oscillatory tail in Eq. (19) comes from the (110) and (110) nodal states for which \( k_F = 0 \).

In conclusion, we have studied the influence of magnetic field on the impurity bound states in \( d \)-wave superconductors. We have found several effects, which can be directly measured in STM experiments, such as a non-linear shift of the electron-hole asymmetric peak in the local DoS at \( c \neq 0 \), and also strong suppression and broadening of the zero-bias peak in the unitary limit. The changes in the wave function asymptotics can lead to a stronger long-range overlap between the bound states at different impurities, which might considerably affect the quasiparticle transport in HTSC.

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FIG. 1. Evolution of the DoS at the impurity site as a function of energy at increasing magnetic field ($p_s \parallel a$, $c = 0.1$).

FIG. 2. Suppression and broadening of the impurity-induced DoS peak at a nearest neighbor site in the unitary limit at increasing magnetic field for $p_s \parallel a$ (a sharp peak at zero field is not shown).