Zeeman effects on the impurity-induced resonances in $d$-wave superconductors

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Recent scanning tunneling microscopy (STM) measurements in BSCCO high-$T_c$ superconductors have recorded clear images of quasiparticle resonant states around intrinsic defects and individual Au and Zn impurity atoms. A common result of these different measurements is that, in average, the resonances are observed just below the Fermi energy, indicating a resonant energy $\omega_0$ much smaller than the superconducting energy gap $\Delta$ ($|\omega_0| \sim \Delta/30$). For the case of Zn-impurity doping, the spatial dependence of the resonant states exhibits a large signal at the impurity site with local maxima on the second neighbour Cu sites (i.e., along the node-gap directions) followed by somewhat weaker peaks along the directions of the gap maxima.

Low-lying quasiparticle resonant states have been predicted to occur in $d_{x^2-y^2}$-wave superconductors doped with spinless impurities close to the unitary limit. According to such model, the resonance at $\omega_0 \approx 1.5$ meV for Zn-substituted samples implies a scattering parameter $c = 1/\pi N_F V_{\text{imp}}$ of about 0.1, where $V_{\text{imp}}$ is the s-wave impurity potential and $N_F$ is the normal-state density of states for each spin species at the Fermi level. Similar values of $c$ are estimated for Au impurities and generic intrinsic defects. Furthermore, the observed power-law decay $G(r) \sim 1/r^{1.97}$ of the angle-averaged differential conductance $G(r)$ at large distances $r$ from the impurity site is in very good accord with $G(r) \sim 1/r^2$, predicted in Ref.

Despite of the agreements between theory and experiments, the spatial dependence of the resonant states reported in Ref.

The images recorded by the STM measurements appear therefore rotated by $\pi/4$ with respect to those resulting from a spinless quasi-unitary impurity potential. Recently, it has been proposed that a blocking effect of the BiO and SrO layers between the tunneling tip and the Cu$_2$O$_2$ layer would actually give rise to the same spatial dependence recorded in experiments. On the other hand, according to a recent theoretical analysis, the observed spatial dependence would rather arise from a local antiferromagnetic spin re-arrangement induced by a nominal zero-spin weak impurity. From this perspective, the Zn-atom behaves effectively as a magnetic impurity with non-local coupling to the charge carriers leading to the X-shaped geometry of the resonant state. Such a picture would be consistent also with the presence of unpaired $S = 1/2$ moments in the vicinity of Zn atoms as observed by NMR experiments.

From the above discussion and the contrasting claims reported in recent literature, it appears that the problem of deciding whether nominal spinless impurities behaves as non-magnetic or effectively magnetic scattering centers in high-$T_c$ cuprates is still an open issue. However, models based on purely non-magnetic impurity potentials predict resonant states quite sensitive to impurity strength and charge carrier doping, while the picture proposed in Ref.

The aim of this paper is two-fold. First, it is shown how the resonant states induced by a single spinless impurity in a $d_{x^2-y^2}$-wave superconductor evolve under the effect of an applied Zeeman magnetic field. Second, it is demonstrated that the spin-orbit coupling to the impurity potential becomes especially important when the impurity is close to the unitary limit and can have important effects on the resonant states and their response to a Zeeman field. According to whether the spin-orbit scattering is irrelevant or not, the Zeeman response of the resonant state behaves in two distinct ways. For zero or very small spin-orbit interaction, the resonances become Zeeman splitted and the spatial dependence can change from electron-like to hole-like for already quite small values of the imposed magnetic field. On the contrary, when the spin-orbit coupling to the quasi-unitary impurity becomes relevant, new low-lying sharp resonances arise which do not show Zeeman splitting. In this latter case, the spatial dependence at fixed energy can be
made to change from electron-like to a novel, spin-orbit induced, symmetry for a suitable value of the Zeeman field.

The differential conductance recorded in a STM experiment is proportional to the local density of states (LDOS) \( N(r, \omega) = -\frac{1}{\pi} \text{Im} \{ G_R^{\text{imp}}(r, r, \omega) \} \), where \( G_R^{\text{imp}}(r, r, \omega) \) is the retarded 4 \( \times \) 4 matrix Green’s function defined in the particle-hole-spin space and \( r \), \( \omega \) is the vector position with respect to the impurity located at the origin. The (11) and (22) components refer to the two pseudospin states of the quasiparticles. For the single impurity case, \( G_R^{\text{imp}}(r, r, \omega) \) is obtained by the Fourier transform of \( G(k, k^\prime; \omega) = \delta_{k, k^\prime} G_0(k, \omega) + G_0(k, \omega) T(k, k^\prime; \omega) G_0(k^\prime, \omega) \), where \( G_0(k, \omega) \) is the Green’s function for the pure superconductor and \( T(k, k^\prime; \omega) \) is the \( T \)-matrix associated to the impurity scattering: \( T(k, k^\prime; \omega) = V(k, k^\prime) + \sum_{k^\prime^\prime} V(k, k^\prime^\prime) G_0(k^\prime^\prime, \omega) T(k^\prime^\prime, k^\prime; \omega) \), where \( V(k, k^\prime) \) is the impurity potential in momentum space. In the following, an external magnetic field \( H \) is assumed to be directed parallel to the conducting \( x-y \) plane, for example \( H \parallel \hat{x} \), and the spins are quantized along the direction of \( H \). Under the assumption of strong two-dimensionality, the coupling of the planar magnetic field to the quasiparticle spins becomes predominant over the coupling to the quasiparticle orbital motion. In the limiting case for which the orbital coupling can be neglected, the Green’s function \( G_0(k, \omega) \) is simply given by \( G_0^{-1}(k, \omega) = \omega - c(k) \rho_3 - \Delta(k) \rho_2 + h \rho_3 \sigma_3 \), where \( c(k) \) is the quasiparticle dispersion, \( \Delta(k) \equiv \Delta(\phi) = \Delta \cos(2\phi) \) is the gap function, and \( h = \mu_B H \) is the Zeeman energy \( (\mu_B \equiv \text{Bohr magneton}) \). The Pauli matrices \( \rho_i \) and \( \sigma_j \) \((i, j = 1, 2, 3) \) act on the particle-hole and spin subspaces, respectively. For sufficiently low values of \( h/\Delta \), the Fulde-Ferrel-Larkin-Ovchinnikov state can be ignored, and the effect of \( H \) is merely to split the pseudospin degeneracy of the quasiparticle excitations.

The impurity atom is assumed to have a simple \( \delta \)-function potential: \( V_{\text{imp}}(r) = V_{\text{imp}} \delta(r) \). According to the Elliott-Yafet theory, the spin-orbit coupling to \( V_{\text{imp}} \) can be modelled as \( V_{\text{so}}(r) = \delta g V_{\text{imp}} (\mathbf{k} \times \mathbf{k}^\prime) \times \mathbf{p} \cdot \mathbf{\sigma} \), where \( \mathbf{p} = -i \nabla \) and \( \mathbf{\sigma} \) are respectively the momentum and spin operators, \( k_F \) is the Fermi momentum and \( \delta g \) is of the order of the shift of the \( g \)-factor. Here, \( \delta g \) is treated as a free parameter, however not exceeding \( \delta g \approx 0.1 - 0.2 \), which is the expected order of magnitude for CuO\(_2\) systems. Since the charge carriers are confined to move on the \( x-y \) plane, only the \( \sigma_x \) component of \( V_{\text{so}}(r) \) is nonzero. Hence, in the particle-hole spin subspace, the total impurity potential \( V(k, k^\prime) \) reduces to \( V(k, k^\prime) = V_{\text{imp}} \rho_3 + i \delta g V_{\text{imp}} (\mathbf{k} \times \mathbf{k}^\prime) \tau_1 \).

The \( \mathbf{k} \times \mathbf{k}^\prime \) dependence of the spin-orbit contribution permits to decouple the \( T \)-matrix into two components: \( T(k, k^\prime; \omega) = T_{\text{imp}}(\omega) + T_{\text{so}}(k, k^\prime; \omega) \), where \( T_{\text{imp}}(\omega) \) is treated as a free parameter, however not exceeding \( \delta g \approx 0.1 - 0.2 \), which is the expected order of magnitude for CuO\(_2\) systems. Since the charge carriers are confined to move on the \( x-y \) plane, only the \( \sigma_x \) component of \( V_{\text{so}}(r) \) is nonzero. Hence, in the particle-hole spin subspace, the total impurity potential \( V(k, k^\prime) \) reduces to \( V(k, k^\prime) = V_{\text{imp}} \rho_3 + i \delta g V_{\text{imp}} (\mathbf{k} \times \mathbf{k}^\prime) \tau_1 \).

The \( \mathbf{k} \times \mathbf{k}^\prime \) dependence of the spin-orbit contribution permits to decouple the \( T \)-matrix into two components:

\[
T_{\text{so}}(k, k^\prime; \omega) = i \delta g V_{\text{imp}} (\mathbf{k} \times \mathbf{k}^\prime) \tau_1
\]

**FIG. 1.** LDOS without spin-orbit interaction as a function of \( \omega/\Delta \) for \( c = 0.08 \) and \( h = 0 \) (solid lines), \( h/\Delta = 0.02 \) (dotted lines), and \( h/\Delta = 0.04 \) (dashed lines). (a): LDOS at the impurity site \( r = (0, 0) \). (b): LDOS along the direction of gap maxima \( r = (4/\sqrt{2}, 0) \).

\[
+i \delta g V_{\text{imp}} \sum_{k''} [\mathbf{k} \times \mathbf{k}''] \tau_1 G_0(k'', \omega) T_{\text{so}}(k'', k''); \omega
\]

\[
+ i \delta g V_{\text{imp}} \sum_{k''} [\mathbf{k} \times \mathbf{k}''] \tau_1 G_0(k'', \omega) T_{\text{so}}(k'', k''); \omega
\]

is the \( T \)-matrix for the spin-orbit coupling to the impurity. The resulting LDOS is therefore the sum of three contributions:

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

From now on, the LDOS contributions are given in units of the normal-state DOS summed over the two spin directions, \( 2N_F \), and particle-hole symmetry is assumed. Moreover, \( N_0(\omega) = [\text{Im} g_0(\omega) + \text{Im} g_0(\omega_-)]/2 \), where \( g_0(\omega) = \int \frac{d\omega}{\pi} \omega/|\Delta(\phi)/\omega|^2 - \omega^2/\Delta(\phi)^2 + \omega \mp h \), is the LDOS for the pure superconductor, while \( \delta N_{\text{imp}}(r, \omega) = \delta N_{\text{imp}}(r, \omega) + \delta N_{\text{imp}}(r, \omega) \) is the LDOS contribution induced by the interaction with the impurity (spin-orbit) potential. The impurity part of the LDOS is just the superposition of the zero-field LDOS reported in Ref. 10 shifted by \( \pm h \):

\[
\delta N_{\text{imp}}(r, \omega) = -\frac{1}{2} \text{Im} \left[ \frac{g_0(\omega, \omega_\pm)}{g_0(\omega_\pm) + c} \right] + \frac{f_0(\omega, \omega_\pm)}{g_0(\omega_\pm) - c}
\]

where

\[
\left[ \begin{array}{c}
g_0(\omega_\pm)
g_0(\omega_\pm)
\end{array} \right] = \int \frac{d\phi}{2\pi} e^{-ik_F \cdot r} \left[ \begin{array}{c}
\omega_\pm
\omega_\pm
\end{array} \right].
\]

A crucial effect of the Zeeman magnetic field is that the poles arising from the denominators of Eq. 2 are splitted by \( h \). In fact, for small values of \( c \) and \( h \), the energy
The value of the scattering parameter, $h$, has been chosen in order to reproduce a zero-field maximum signal on the impurity site, $r = 0$ (Fig.1a), for $\omega/\Delta = -0.03$, i.e. the resonant energy reported in Ref. [1]. For nonzero values of $h$, the resonance becomes Zeeman splitted in good agreement with $\omega_0(h) \simeq \omega_0 \pm h$. This is also true for the LDOS signals away from $r = 0$, as it is shown in Fig.1b where the LDOS is plotted for $r = (4/k_F, 0)$ (i.e., along the direction of the gap maxima).

The spatial dependence of the LDOS as a function of $h$ for $\omega/\Delta = -0.03$ is shown in Fig.2. The pattern shown in Fig.2a, $h = 0$ (Fig.2b) closely resembles the spatial dependence obtained by Haas and Mak[3] and it is characteristic of an electron-like bound state. However, already for $h/\Delta = 0.02$ (Fig.2b), which for $\Delta = 44$ meV corresponds to a magnetic field of about 15 T, the resonance acquires a predominant hole-character, signalled by the contemporary suppression of the central peak at $r = 0$ and the signals along the gap-node directions. This pattern is equal to that reported in Fig.2 of Ref.[3] but here it has been obtained without reversing the sign of $\omega$. As can be also inferred from Fig.1, higher values of $h$ modify the intensity of the signal, but its spatial dependence remains equal to that of Fig.2b. It is important to stress that Fig.2 refers to the spatial dependence on the CuO$_2$ layer and no blocking effect has been considered.

Let us consider now under which conditions the results of Figs 1 and 2 are modified by the presence of spin-orbit coupling to the impurity. The spin-orbit $T$-matrix contribution, Eq.(1), is obtained by setting $T_{so}(k, k'; \omega) = i\delta V_{imp}[k \times t(k', \omega)]\tau_1$, where $t(k, \omega) = k + i\delta V_{imp}\sum_k k'\tau_1 G_0(k', \omega)[k' \times t(k, \omega)]\tau_1$. The equation for $t(k, \omega)$ is easily solved in terms of its components, $t_x$ and $t_y$, and after some algebra the resulting spin-orbit part of the LDOS reduces to:

$$\delta N^\pm_{so}(r, \omega) = -\frac{1}{2} \text{Im}\{A^\pm(\omega)[g_\tau(r, \omega^\pm)^2 + g_\tau(r, \omega^\pm)^2] + f_\tau(r, \omega^\pm)^2 + f_\tau(r, \omega^\mp)^2\} - \text{Im}\{B^\pm(\omega)[g_\tau(r, \omega^\pm)f_\tau(r, \omega^\pm) + g_\tau(r, \omega^\pm)f_\tau(r, \omega^\pm)]\},$$

where

$$A^\pm(\omega) = \frac{c^2_{so}g(\omega^\pm)\pm[f(\omega^\pm)^2 - g(\omega^\pm)^2]}{D(\omega)},$$

$$B^\pm(\omega) = \frac{c^2_{so}f(\omega^\pm)\mp[f(\omega^\pm)^2 - g(\omega^\pm)^2]}{D(\omega)} \times \{\epsilon^{c^2_{so} - [f(\omega_-) + g(\omega_+)]}) + [f(\omega_+) + g(\omega_-)]\}\$$

where $c_{so} = 1/(\pi\hbar gV_{imp}) = c/\delta g$ and:

$$\left[\frac{g(\omega^\pm)}{f(\omega^\pm)}\right] = \int \frac{d\phi}{2\pi} \frac{\sin(\phi)^2}{\Delta(\phi)^2 - \omega^\pm_0} \frac{\omega^\pm_0}{\Delta(\phi)},$$

$$\left[\frac{g_\tau(r, \omega^\pm)}{f_\tau(r, \omega^\pm)}\right] = \int \frac{d\phi}{2\pi} \frac{\cos(\phi)e^{ik\cdot r}}{\Delta(\phi)^2 - \omega^\pm_0} \frac{\omega^\pm_0}{\Delta(\phi)}.$$
FIG. 3. Effect of the spin-orbit contribution to the LDOS at $r = (2/k_F, 2/k_F)$ for $c = 0.08$ and different values of the spin-orbit parameter $\delta g$ for $h = 0$ (a) and $h/\Delta = 0.1$ (b). Solid lines: $\delta g = 0.01$; dotted lines: $\delta g = 0.05$; dashed lines: $\delta g = 0.1$; long dashed lines: $\delta g = 0.15$; dot-dashed lines: $\delta g = 0.2$. The arrows indicate the positions of the coherence peaks for $\delta g = 0.01$.

too much into details, the main feature of the spin-orbit poles is that, at $h = 0$, $D(\omega)$ vanishes at $\omega = 0$ when $c_{so} = 1/\pi$. Away from this limit the poles acquire a finite imaginary part and move rapidly towards high energies. Note however that $\delta N_{so}(r, 0) = 0$, the resonance becomes sharper as $c_{so} \rightarrow 1/\pi$ without reducing to a $\delta$-function at $\omega = 0$ for $c_{so} = 1/\pi$. Finally, due to the spin-mixing processes of the spin-orbit interaction, the effect of $h$ is not merely a Zeeman split of the zero-field poles.

These features are demonstrated in Fig. 3, where the total LDOS including the spin-orbit contribution is plotted as a function of $\omega$ for $r = (2/k_F, 2/k_F)$, $c = 0.08$ and different values of $\delta g$. For $h = 0$ (Fig. 3a) and $\delta g = 0.01$ the presence of the coherence peaks at $\omega = \pm \Delta$ indicate that the LDOS is very close to that of a $d$-wave superconductor without impurities. However, as $\delta g$ is enhanced, the coherence peaks are depleted and a symmetric broad resonance develops and moves towards low energies with contemporary reduction of its peak-width. The symmetry with respect to $\omega = 0$ merely reflects the particle-hole symmetry conservation of the spin-orbit interaction. At $\delta g = 0.2$, the coherence peaks at $\omega = \pm \Delta$ are completely suppressed and a sharp resonance is built at $\omega = \pm \omega_{so}$ with $\omega_{so} \ll \Delta$. The origin of such low-lying resonances stem from the poles of Eq. (7). Note in fact that for $\delta g = 0.2$ the value of the spin-orbit scattering parameter, $c_{so} = c/\delta g = 0.4$, nearly fulfills the condition $c_{so} = 1/\pi$ for which, as discussed above, the spin-orbit $T$-matrix has a pole at $\omega_{so} = 0$ with vanishing imaginary part. The effect of the magnetic field is shown in Fig. 3b, where the LDOS is plotted for $h/\Delta = 0.1$ and for the same set of $\delta g$ values of Fig. 3a. As expected, for $\delta g = 0.01$ the coherence peaks at the gap edge are split by $\pm h$. However, for higher values of $\delta g$, the low-lying spin-orbit resonances do not show Zeeman splitting because of the presence of important spin-flip processes.

Although the low-lying spin-orbit resonances are not Zeeman splitted, they nevertheless show some dependence on $h$. This is shown in Fig. 4, where $\omega_{so}$ is plotted as a function of $h$ for $\delta g = 0.15$ and $\delta g = 0.2$. Note however that the $h$-dependence of $\omega_{so}$ is rather weak, at least for low values of $h$.

The spatial dependence of the total LDOS with $\delta g = 0.2$ is plotted in Fig. 5 for the same parameters of Fig. 2 ($c = 0.08$ and $\omega/\Delta = -0.03$). For $h = 0$ (Fig. 5a) the poles of the spin-orbit $T$-matrix are at energies higher than $\omega = -0.03$ and the spatial dependence of the LDOS resembles closely that of Fig. 2, where $\delta g = 0$. Note however that the weight of the central peak is somewhat extended along the diagonals leading to an X-shaped geometry. For $h/\Delta = 0.02$ (Fig. 5b), the spatial dependence is radically different from that shown in Fig. 5a. Now, a signal arises along the diagonals in the vicinity of $r = 0$ with a contemporary shift of the peaks in the $(\pm 1, 0)$ and $(0, \pm 1)$ directions at higher distances from the impurity site. This particular geometry of the LDOS is characteristic of the spin-orbit coupling to the impurity and, as inferred from Fig. 5a, it can be obtained also at $h = 0$ when $\omega$ is close to the spin-orbit $T$-matrix poles.

In summary, two possible scenarios can be drawn about the Zeeman field effects on the LDOS of a $d_{x^2-y^2}$-wave superconductor around a quasi-unitary impurity atom. First, if the spin-orbit coupling is absent or weak ($c_{so} \gg 1/\pi$), the imposed magnetic field splits the quasiparticle resonance peaks by $\pm h$ and, at fixed energy $\omega$, the spatial
conducting condensate is efficient against spin-flip transitions induced by the magnetic field.

Note added - As shown in a recent publication [H. Tsuchiura, Y. Tanaka, M. Ogata, and S. Kashiwaya, Phys. Rev. Lett. 84, 3165 (2000)] a Zeeman splitting of the quasiparticle resonances can be induced also by classical magnetic impurities.

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