

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

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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. Moreover, it is demonstrated that the spin-orbit coupling to the impurity potential can have important and characteristic effects on the resonant states and their response to the Zeeman field, especially when the impurity is close to the unitary limit. For zero or very small spin-orbit interaction, the resonant states become Zeeman split by the magnetic field while when the spin-orbit coupling is important, new low-lying resonances arise which do not show any Zeeman splitting.

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Recent scanning tunneling microscopy (STM) measurements in  $\text{Bi}_2\text{Sr}_2\text{CaCuO}_{8+\delta}$  high- $T_c$  superconductors have recorded clear images of quasiparticle resonant states around intrinsic defects<sup>1</sup> and individual Au- (Ref. 2) and Zn- (Ref. 3) impurity atoms. A common result of these different measurements is that, on 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-neighbor Cu sites (i.e., along the node-gap directions) followed by somewhat weaker peaks along the directions of the gap maxima.<sup>3</sup>

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.<sup>4</sup> According to such a 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,<sup>3</sup> where  $V_{\text{imp}}$  is the  $s$ -wave impurity potential and  $N_F$  is the normal-state density of states (DOS) for each spin species at the Fermi level. Similar values of  $c$  are estimated for Au impurities and generic intrinsic defects.<sup>1,2</sup> Furthermore, the observed power-law decay  $\bar{G}(r) \sim 1/r^{1.97}$  of the angle-averaged differential conductance  $\bar{G}(r)$  at large distances  $r$  from the impurity site<sup>1</sup> is in very good accord with  $\bar{G}(r) \sim 1/r^2$ , predicted in Ref. 4.

Despite the agreements between theory and experiments, the spatial dependence of the resonant states reported in Ref. 3 is quite at odds with that expected by strong spinless impurities. These, in fact, would generate, in addition to the peak at the impurity site, a fourfold symmetric signal with maxima along the directions where the gap is fully opened.<sup>4,5</sup>

The images recorded by the STM measurements appear therefore rotated by  $\pi/4$  with respect to those resulting from a spinless quasiunitary impurity potential. Recently, it has been proposed that a blocking effect of the BiO and SrO layers between the tunneling tip and the  $\text{CuO}_2$  layer would actually give rise to the same spatial dependence recorded in experiments.<sup>6</sup> On the other hand, according to a recent theoretical analysis,<sup>7</sup> the observed spatial dependence would rather arise from a local antiferromagnetic spin rearrangement induced by a nominal zero-spin weak impurity. From this perspective, the Zn atom behaves effectively as a mag-

netic impurity with nonlocal 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.<sup>8</sup>

From the above discussion and the contrasting claims reported in recent literature, it appears that the problem of deciding whether nominal spinless impurities behave 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,<sup>4,9</sup> while the picture proposed in Ref. 7 has been claimed to yield results much more robust. This qualitative difference could therefore be used as a tool for discriminating between the two pictures by, for example, studying the response to some external applied perturbation.

The aim of this paper is twofold. 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<sup>10</sup> 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 split and the spatial dependence can change from electronlike to holelike for already quite small values of the imposed magnetic field. On the contrary, when the spin-orbit coupling to the quasiunitary 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 electronlike 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)  $N(\mathbf{r}, \omega) = -(1/\pi) \text{Im}[G_{11}^R(\mathbf{r}, \mathbf{r}; \omega) + G_{22}^R(\mathbf{r}, \mathbf{r}; \omega)]$ , where  $G^R(\mathbf{r}, \mathbf{r}; \omega)$  is the retarded  $4 \times 4$  matrix Green's function defined in the particle-hole-spin space and  $\mathbf{r}$  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,  $G^R(\mathbf{r}, \mathbf{r}; \omega)$  is obtained by the Fourier transform of  $G(\mathbf{k}, \mathbf{k}'; \omega) = \delta_{\mathbf{k}, \mathbf{k}'} G_0(\mathbf{k}, \omega) + G_0(\mathbf{k}, \omega) T(\mathbf{k}, \mathbf{k}'; \omega) G_0(\mathbf{k}', \omega)$ , where  $G_0(\mathbf{k}, \omega)$  is the Green's function for the pure  $d_{x^2-y^2}$ -wave superconductor and  $T(\mathbf{k}, \mathbf{k}'; \omega)$  is the  $T$  matrix associated to the impurity scattering:  $T(\mathbf{k}, \mathbf{k}'; \omega) = V(\mathbf{k}, \mathbf{k}') + \sum_{\mathbf{k}''} V(\mathbf{k}, \mathbf{k}'') G_0(\mathbf{k}'', \omega) T(\mathbf{k}'', \mathbf{k}'; \omega)$ , where  $V(\mathbf{k}, \mathbf{k}')$  is the impurity potential in momentum space. In the following, an external magnetic field  $\mathbf{H}$  is assumed to be directed parallel to the conducting  $x$ - $y$  plane, for example,  $\mathbf{H} \parallel \hat{\mathbf{x}}$ , and the spins are quantized along the direction of  $\mathbf{H}$ . 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.<sup>11</sup> In the limiting case for which the orbital coupling can be neglected,<sup>12</sup> the Green's function  $G_0(\mathbf{k}, \omega)$  is simply given by  $G_0^{-1}(\mathbf{k}, \omega) = \omega - \epsilon(\mathbf{k})\rho_3 - \Delta(\mathbf{k})\rho_2\tau_2 + h\rho_3\tau_3$ , where  $\epsilon(\mathbf{k})$  is the quasiparticle dispersion,  $\Delta(\mathbf{k}) \equiv \Delta(\phi) = \Delta \cos(2\phi)$  is the gap function, and  $h = \mu_B H$  is the Zeeman energy ( $\mu_B \equiv$  Bohr magneton). The Pauli matrices  $\rho_i$  and  $\tau_j$  ( $i, j = 1, 2, 3$ ) 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.<sup>13-15</sup>

The impurity atom is assumed to have a simple  $\delta$ -function potential:  $V_{\text{imp}}(\mathbf{r}) = V_{\text{imp}}\delta(\mathbf{r})$ . According to the Elliott-Yafet theory,<sup>16</sup> the spin-orbit coupling to  $V_{\text{imp}}$  can be modeled as  $V_{\text{so}}(\mathbf{r}) = (\delta g/k_F^2)[\nabla V_{\text{imp}}(\mathbf{r}) \times \mathbf{p}] \cdot \boldsymbol{\sigma}$ , where  $\mathbf{p} = -i\nabla$  and  $\boldsymbol{\sigma}$  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.<sup>11,16</sup> 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  $\text{CuO}_2$  systems.<sup>17</sup> Since the charge carriers are confined to move on the  $x$ - $y$  plane, only the  $\sigma_z$  component of  $V_{\text{so}}(\mathbf{r})$  is nonzero. Hence, in the particle-hole spin subspace, the total impurity potential  $V(\mathbf{k}, \mathbf{k}')$  reduces to  $V(\mathbf{k}, \mathbf{k}') = V_{\text{imp}}\rho_3 + i\delta g V_{\text{imp}}[\hat{\mathbf{k}} \times \hat{\mathbf{k}}']_z \tau_1$ .

The  $\mathbf{k} \times \mathbf{k}'$  dependence of the spin-orbit contribution permits to decouple the  $T$  matrix into two components:  $T(\mathbf{k}, \mathbf{k}'; \omega) = T_{\text{imp}}(\omega) + T_{\text{so}}(\mathbf{k}, \mathbf{k}'; \omega)$ , where  $T_{\text{imp}}(\omega) = V_{\text{imp}}\rho_3 + \sum_{\mathbf{k}} V_{\text{imp}}\rho_3 G_0(\mathbf{k}, \omega) T_{\text{imp}}(\omega)$  is the usual  $T$  matrix for the scalar potential and

$$T_{\text{so}}(\mathbf{k}, \mathbf{k}'; \omega) = i\delta g V_{\text{imp}}[\hat{\mathbf{k}} \times \hat{\mathbf{k}}']_z \tau_1 + i\delta g V_{\text{imp}} \sum_{\mathbf{k}''} [\hat{\mathbf{k}} \times \hat{\mathbf{k}}'']_z \tau_1 G_0(\mathbf{k}'', \omega) T_{\text{so}}(\mathbf{k}'', \mathbf{k}'; \omega) \quad (1)$$

is the  $T$  matrix for the spin-orbit coupling to the impurity.<sup>10</sup> The resulting LDOS is therefore the sum of three contributions:  $N(\mathbf{r}, \omega) = N_0(\omega) + \delta N_{\text{imp}}(\mathbf{r}, \omega) + \delta N_{\text{so}}(\mathbf{r}, \omega)$ . 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. Hence,  $N_0(\omega) = [\text{Im}g_0(\omega_+) + \text{Im}g_0(\omega_-)]/2$ , where  $g_0(\omega_{\pm}) = \int (d\phi/2\pi) \omega / [\Delta(\phi)^2 - \omega_{\pm}^2]^{1/2}$  and  $\omega_{\pm} = \omega \mp h$  is the LDOS for the pure superconductor, while  $\delta N_{\text{imp},(\text{so})}(\mathbf{r}, \omega)$

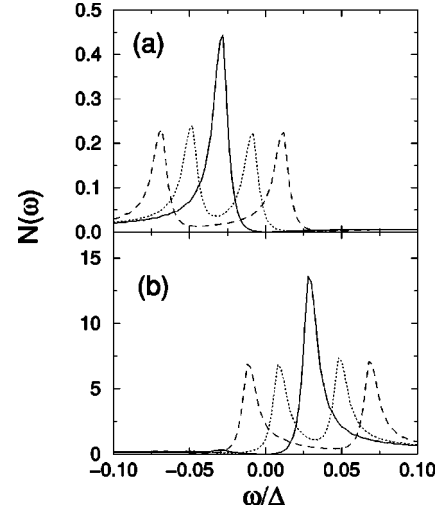


FIG. 1. LDOS without spin-orbit interaction as a function of  $\omega/\Delta$  for  $c=0.08$  and  $h=0$  (solid lines),  $h/\Delta=0.02$  (dotted lines), and  $h/\Delta=0.04$  (dashed lines). (a) LDOS at the impurity site  $\mathbf{r}=(0,0)$ . (b) LDOS along the direction of gap maxima  $\mathbf{r}=(4/k_F,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

$= \delta N_{\text{imp},(\text{so})}^+(\mathbf{r}, \omega) + \delta N_{\text{imp},(\text{so})}^-(\mathbf{r}, \omega)$  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. 4 shifted by  $\pm h$ :

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

where

$$\begin{bmatrix} g_0(\mathbf{r}, \omega_{\pm}) \\ f_0(\mathbf{r}, \omega_{\pm}) \end{bmatrix} = \int \frac{d\phi}{2\pi} \frac{e^{i\mathbf{k}_F \cdot \mathbf{r}}}{[\Delta(\phi)^2 - \omega_{\pm}^2]^{1/2}} \begin{bmatrix} \omega_{\pm} \\ \Delta(\phi) \end{bmatrix}. \quad (3)$$

A crucial effect of the Zeeman magnetic field is that the poles arising from the denominators of Eq. (2) are split by  $h$ . In fact, for small values of  $c$  and  $h$ , the energy resonance  $\omega_0(h)$  is simply  $\omega_0(h) \approx \omega_0 \pm h$ , where  $\omega_0 \approx \Delta(c\pi/2)/\ln(8/\pi c)$  is the resonance energy for  $h=0$ .<sup>4</sup> Hence, for quasiunitary scattering ( $\omega_0 \ll \Delta$ ), already quite small values of  $h$  compared to  $\Delta$  are sufficient to deeply modify the impurity-induced resonance.

This is clearly seen in Fig. 1 where the  $\omega$  dependence of  $N_0(\omega) + \delta N_{\text{imp}}(\mathbf{r}, \omega)$  is plotted for  $h/\Delta = 0, 0.02, 0.04$ . The value of the scattering parameter,  $c=0.08$ , has been chosen in order to reproduce a zero-field maximum signal on the impurity site,  $\mathbf{r}=\mathbf{0}$  [Fig. 1(a)], for  $\omega/\Delta = -0.03$ , i.e., the resonant energy reported in Ref. 3. For nonzero values of  $h$ , the resonance becomes Zeeman split in good agreement with  $\omega_0(h) \approx \omega_0 \pm h$ . This is also true for the LDOS signals away from  $\mathbf{r}=\mathbf{0}$ , as it is shown in Fig. 1(b) where the LDOS is plotted for  $\mathbf{r}=(4/k_F, 0)$  (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. 2(a) ( $h=0$ ) closely resembles the spatial dependence obtained by Haas and Maki,<sup>5</sup> and it is characteristic of an

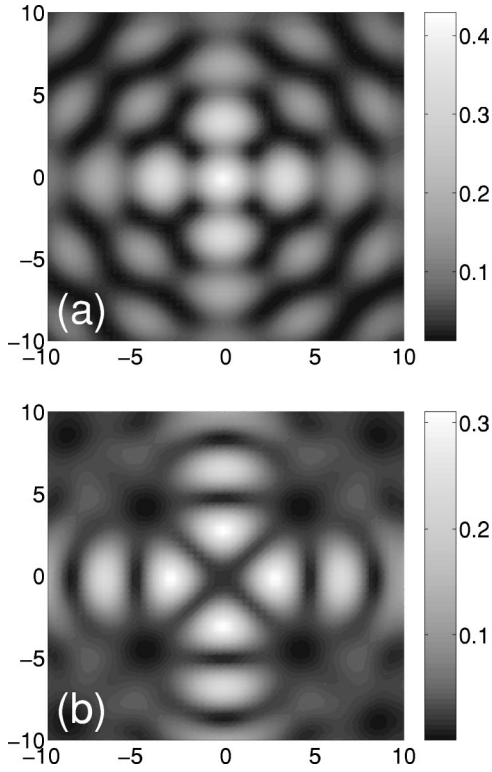


FIG. 2. Spatial dependence of the LDOS without spin-orbit interaction for  $c=0.08$  and  $\omega/\Delta = -0.03$ . (a)  $h=0$ . (b)  $h/\Delta=0.02$ .

electronlike bound state. However, already for  $h/\Delta=0.02$  [Fig. 2(b)], which for  $\Delta=44$  meV Ref. (3) corresponds to a magnetic field of about 15 T, the resonance acquires a predominant hole character, signaled by the contemporary suppression of the central peak at  $\mathbf{r}=\mathbf{0}$  and the signals along the gap-node directions. This pattern is equal to that reported in Fig. 2 of Ref. 5, 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. 2(b). It is important to stress that Fig. 2 refers to the spatial dependence on the  $\text{CuO}_2$  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  $T_{\text{so}}(\mathbf{k}, \mathbf{k}'; \omega) = i\delta g V_{\text{imp}}[\hat{\mathbf{k}} \times \mathbf{t}(\hat{\mathbf{k}}', \omega)]_z \tau_1$ , where  $\mathbf{t}(\hat{\mathbf{k}}, \omega) = \hat{\mathbf{k}} + i\delta g V_{\text{imp}} \sum_{\mathbf{k}'} \hat{\mathbf{k}}' \tau_1 G_0(\mathbf{k}', \omega)[\hat{\mathbf{k}}' \times \mathbf{t}(\hat{\mathbf{k}}, \omega)]_z$ .<sup>10</sup> The equation for  $\mathbf{t}(\hat{\mathbf{k}}, \omega)$  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

$$\begin{aligned} \delta N_{\text{so}}^{\pm}(\mathbf{r}, \omega) = & -\frac{1}{2} \text{Im} \{ A^{\pm}(\omega) [g_c(\mathbf{r}, \omega_{\pm})^2 + g_s(\mathbf{r}, \omega_{\pm})^2 \\ & + f_c(\mathbf{r}, \omega_{\pm})^2 + f_s(\mathbf{r}, \omega_{\pm})^2] \} \\ & - \text{Im} \{ B^{\pm}(\omega) [g_s(\mathbf{r}, \omega_{\pm}) f_s(\mathbf{r}, \omega_{\pm}) \\ & - g_c(\mathbf{r}, \omega_{\pm}) f_c(\mathbf{r}, \omega_{\pm})] \}, \end{aligned} \quad (4)$$

where

$$A^{\pm}(\omega) = \frac{c_{\text{so}}^2 g(\omega_{\mp}) + [f(\omega_{\mp})^2 - g(\omega_{\mp})^2] g(\omega_{\pm})}{D(\omega)}, \quad (5)$$

$$B^{\pm}(\omega) = \frac{c_{\text{so}}^2 f(\omega_{\mp}) - [f(\omega_{\mp})^2 - g(\omega_{\mp})^2] f(\omega_{\pm})}{D(\omega)}, \quad (6)$$

$$\begin{aligned} D(\omega) = & \{ c_{\text{so}}^2 - [f(\omega_-) + g(\omega_-)][f(\omega_+) + g(\omega_+)] \} \\ & \times \{ c_{\text{so}}^2 - [f(\omega_-) - g(\omega_-)][f(\omega_+) - g(\omega_+)] \} \end{aligned} \quad (7)$$

where  $c_{\text{so}} = 1/(\pi N_F \delta g V_{\text{imp}}) = c/\delta g$  and

$$\begin{bmatrix} g(\omega_{\pm}) \\ f(\omega_{\pm}) \end{bmatrix} = \int \frac{d\phi}{2\pi} \frac{\sin(\phi)^2}{[\Delta(\phi)^2 - \omega_{\pm}^2]^{1/2}} \begin{bmatrix} \omega_{\pm} \\ \Delta(\phi) \end{bmatrix}, \quad (8)$$

$$\begin{bmatrix} g_c(\mathbf{r}, \omega_{\pm}) \\ f_c(\mathbf{r}, \omega_{\pm}) \end{bmatrix} = \int \frac{d\phi}{2\pi} \frac{\cos(\phi) e^{i\mathbf{k}_F \cdot \mathbf{r}}}{[\Delta(\phi)^2 - \omega_{\pm}^2]^{1/2}} \begin{bmatrix} \omega_{\pm} \\ \Delta(\phi) \end{bmatrix}. \quad (9)$$

The expressions for  $g_s(\mathbf{r}, \omega_{\pm})$  and  $f_s(\mathbf{r}, \omega_{\pm})$  are obtained by replacing  $\cos(\phi)$  with  $\sin(\phi)$  in the right-hand side of Eq. (9).

There are two important general features characteristic of the spin-orbit LDOS. First, as can be inferred from Eqs. (4)–(9), the spin-orbit LDOS vanishes at the impurity site:  $\delta N_{\text{so}}^{\pm}(\mathbf{0}, \omega) = 0$ . Moreover, at  $h=0$ ,  $\delta N_{\text{so}}(\mathbf{r}, 0) = 0$  for every  $\mathbf{r}$ . This is due to the  $\mathbf{k} \times \mathbf{k}'$  factor appearing in Eq. (1) which makes the spin-orbit coupling particle-hole symmetry conserving. The second important feature is that the spin-orbit interaction can induce additional resonances driven by the zeros of Eq. (7). Without entering too much into detail, the main feature of the spin-orbit poles is that, at  $h=0$ ,  $D(\omega)$  vanishes at  $\omega=0$  when  $c_{\text{so}} = 1/\pi$ .<sup>18</sup> Away from this limit the poles acquire a finite imaginary part and move rapidly towards high energies. Note however that since  $\delta N_{\text{so}}(\mathbf{r}, 0) = 0$ , the resonance becomes sharper as  $c_{\text{so}} \rightarrow 1/\pi$  without reducing to a  $\delta$  function at  $\omega=0$  for  $c_{\text{so}} = 1/\pi$ . 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  $\mathbf{r} = (2/k_F, 2/k_F)$ ,  $c=0.08$ , and different values of  $\delta g$ . For  $h=0$  [Fig. 3(a)] 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 a 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  $\omega = \pm \omega_{\text{so}}$  with  $\omega_{\text{so}} \ll \Delta$ . The origin of such low-lying resonances stems from the poles of Eq. (7). Note in fact that for  $\delta g=0.2$  the value of the spin-orbit scattering parameter,  $c_{\text{so}} = c/\delta g = 0.4$ , nearly fulfills the condition  $c_{\text{so}} = 1/\pi$  for which, as discussed above, the spin-orbit  $T$  matrix has a pole

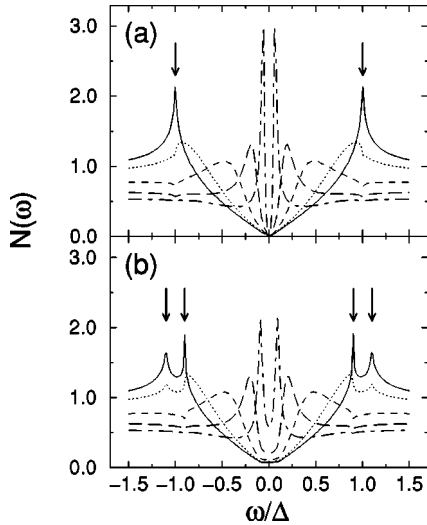


FIG. 3. Effect of the spin-orbit contribution to the LDOS at  $\mathbf{r} = (2/k_F, 2/k_F)$  for  $c=0.08$  and different values of the spin-orbit parameter  $\delta g$  for  $h=0$  (a) and  $h/\Delta=0.1$  (b). Solid lines:  $\delta g=0.01$ , dotted lines:  $\delta g=0.05$ , dashed lines:  $\delta g=0.1$ , long-dashed lines:  $\delta g=0.15$ , and dot-dashed lines:  $\delta g=0.2$ . The arrows indicate the positions of the coherence peaks for  $\delta g=0.01$ .

at  $\omega_{so}=0$  with a vanishing imaginary part. The effect of the magnetic field is shown in Fig. 3(b), where the LDOS is plotted for  $h/\Delta=0.1$  and for the same set of  $\delta g$  values of Fig. 3(a). 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 split, 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. 5(a)] 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(a) 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  $h/\Delta=0.02$

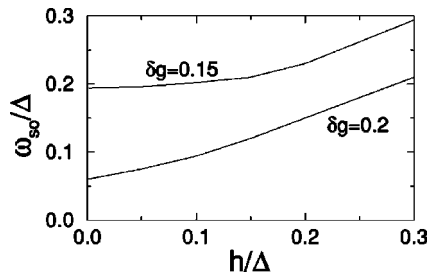


FIG. 4. Spin-orbit resonant energies  $\omega_{so}$  for  $c=0.08$  as a function of the external field.

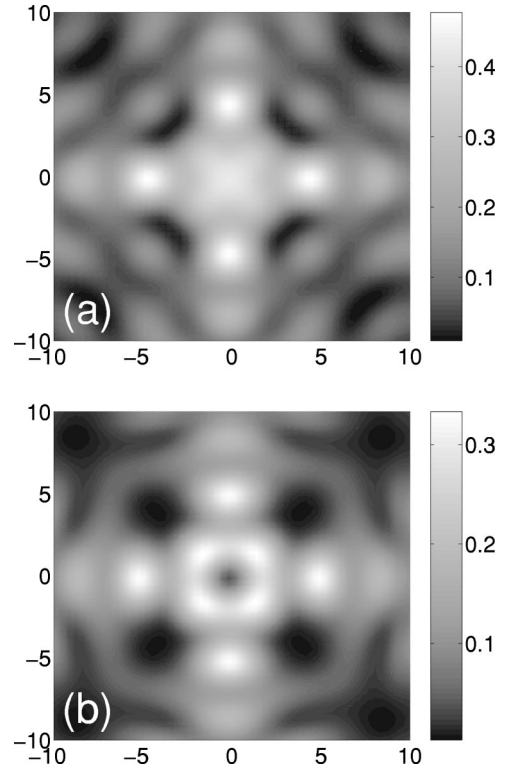


FIG. 5. Spatial dependence of the LDOS with spin-orbit interaction for  $c=0.08, \delta g=0.2$ , and  $\omega/\Delta=-0.03$ . (a)  $h=0$ . (b)  $h/\Delta=0.02$ .

[Fig. 5(b)] the spatial dependence is radically different from that shown in Fig. 2(b). Now, a signal arises along the diagonals in the vicinity of  $\mathbf{r}=\mathbf{0}$  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. 3, 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 quasiunitary 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 dependence can be modified from electronlike to holelike. Second, if the spin-orbit scattering is sufficiently strong ( $c_{so} \approx 1/\pi$ ), the LDOS acquires a novel off-site and particle-hole symmetric resonance at low energies which does not show Zeeman splitting at  $h \neq 0$ . Which of these two possibilities is actually realized would produce important information on the nature of the resonant states in high- $T_c$  superconductors.

A last remark regards the possibility of having very high (small) values of  $\delta g(c)$  in such a way that  $c_{so} \ll 1$ . In fact, when  $c_{so} \rightarrow 0$ , Eqs. (5) and (6) reduce to  $A^\pm(\omega) = g(\omega_\pm)/[f(\omega_\pm)^2 - g(\omega_\pm)^2]$  and  $B^\pm(\omega) = -f(\omega_\pm)/[f(\omega_\pm)^2 - g(\omega_\pm)^2]$ , respectively. In this case,  $\delta N_{so}^\pm(\omega)$  does no longer contain spin-mixed terms and the two spin channels are perfectly decoupled. As explained in Ref. 19, this situation is due to the fact that, as long as the charge carriers are confined to move in the  $x$ - $y$  plane, the spin-orbit impurity

operator commutes with  $\sigma_z$ . For very strong spin-orbit interaction, it is found that also in the presence of an external magnetic field perpendicular to the  $z$  direction the (singlet) Cooper pairs are formed by electrons with opposite spins in the  $z$  direction and the spin rigidity of the superconducting

condensate is efficient against spin-flip transitions induced by the magnetic field.

*Note added in proof.* As shown in a recent publication,<sup>20</sup> a Zeeman splitting of the quasiparticle resonances can be induced also by classical magnetic impurities.

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