Impurity-induced bound states in superconductors with spin-orbit coupling

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(Dated: October 20, 2014)

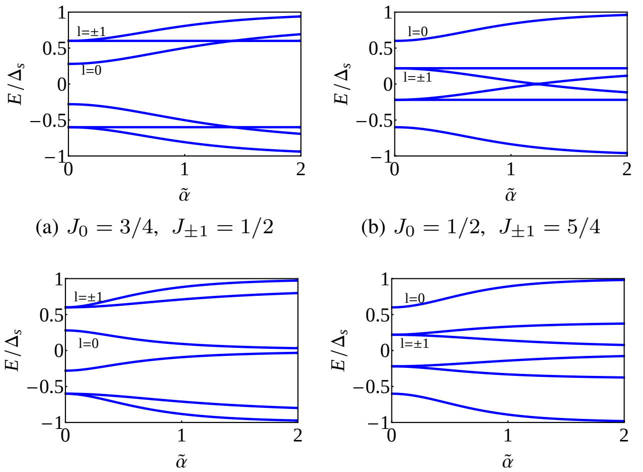
We study the effect of strong spin-orbit coupling on bound states induced by impurities in superconductors. The presence of spin-orbit coupling breaks the $\mathbb{SU}(2)$-spin symmetry and causes the superconducting order parameter to have generically both singlet (s-wave) and triplet (p-wave) components. As a result, impurity-induced bound states corresponding to different angular momentum channels hybridize and display a number of qualitatively different features from that of the well-known Yu-Shiba-Rusinov states in conventional s-wave superconductors. In particular, we find that in the presence of spin-orbit coupling the spectrum of the impurity-induced bound states depends on the orientation of the magnetic moment of the impurity. Our predictions can be used to distinguish the symmetry of the order parameter and have implications for the Majorana proposals based on chains of magnetic atoms placed on the surface of superconductors with strong spin-orbit coupling [1].

PACS numbers: 73.20.Hb, 74.78.-w, 75.70.Tj,

The presence of impurities is almost always unavoidable in condensed matter systems. Often impurities are regarded as a nuisance that spoils the properties of a clean system and complicates the understanding of its properties. However, impurities are in many instances essential to obtain desirable physical effects and can be used as unique atomic-scale probes of the ground state of the host system [2–10]. The study of the effect of impurities in superconductors has been a very active field of research [10]. In an s-wave superconductor magnetic impurities cause the formation of bound states, the Yu-Shiba-Rusinov (YSR) states [11–13]. There has been a significant interest in the properties of YSR states due to theoretical proposals suggesting that a chain of magnetic impurities placed on the surface of a superconductor (SC) would be a very robust, self-tuning, system that should exhibit non-abelian, Majorana, states [14–18]. In these proposals the bound states induced by the chain of magnetic impurities form an impurity band with non-trivial topological character. More recently it has been pointed out that the presence of Rashba spin-orbit coupling (SOC) should facilitate the realization of a topological impurity band of YSR states. [1, 19–21]. On the surface, due to the lack of inversion symmetry, some amount of Rashba SOC will be present. Therefore, for the systems considered to realize a topological band of YSR states the presence of Rashba SOC is both unavoidable and beneficial. This assessment has very recently been confirmed by the experimental results presented in Ref. 1, that show evidence of the presence of Majorana modes at the end of a chain of Fe atoms placed on the surface of a SC with strong SOC, Pb. The recent developments in the search of systems that can resiliently host Majorana fermions [22–43] strongly motivates the study of the effect of SOC on YSR states. However, so far the effects of SOC on YSR states have been almost completely neglected.

In this work we present the general theory of the impurity-induced bound states in the presence of Rashba SOC. We show that SOC, which breaks $\mathbb{SU}(2)$-spin symmetry and results in the mixture of s-wave and p-wave pairing correlations [44] profoundly modifies the spectrum of the YSR states [45] Our theory takes into account the fact that the impurity potential normally has both a scalar and a magnetic component. We consider the realistic, and general, case in which both the scalar and the magnetic part of the impurity potential has angular momentum components (l) higher than $l = 0$. This is also motivated by the fact that partial waves beyond s-wave have been shown to often be essential to explain experimental data [46–48]. We find that the presence of SOC, by mixing YSR states with different l, profoundly changes the spectrum of the impurity-induced bound states. Moreover, we show that in the presence of SOC the scalar part of the disorder potential can qualitatively modify the nature of the spectrum of the YSR states. When the p-wave component of the order parameter becomes larger than the s-wave one, the scalar potential alone may induce bound states well within the gap [49–51]. These results are directly relevant to recent scanning-tunneling-spectroscopy (STS) measurements of the states induced in thin films of Pb by the presence of magnetic adatoms [47]. One important consequence of the presence of SOC and higher angular momentum components of the impurity potential, is that the spectrum of the YSR states becomes dependent on the orientation of the magnetic moment of the impurity. This result allows us to make novel predictions on the properties of the YSR states that can be tested experimentally. In addition, it opens up the possibility to use the orientation of the magnetic impurity, that can be modified via external magnetic fields, to tune the spectrum of the YSR states. This additional degree of tunability could be extremely helpful to realize, and verify, the conditions necessary to obtain a topological band of YSR states hosting Majorana zero-energy modes.

Model. We consider a superconductor described by the mean-field Hamiltonian $\mathcal{H}_{\rm SC} = \sum_{\mathbf{p}} \psi^\dagger_{\mathbf{p}} H_{\rm SC}(\mathbf{p})\psi_{\mathbf{p}}$ where $\psi_{\mathbf{p}}$ is the Nambu spinor $(c_{\mathbf{p}\uparrow}, c_{\mathbf{p}\downarrow}, c^\dagger_{-\mathbf{p}\downarrow}, -c^\dagger_{-\mathbf{p}\uparrow})^T$, with $c^\dagger_{\mathbf{p}\sigma}$ ($c_{\mathbf{p}\sigma}$) the creation (annihilation) operator for an electron with



(a) $J_0 = 3/4,\ J_{\pm1} = 1/2$ (b) $J_0 = 1/2,\ J_{\pm1} = 5/4$

(c) $J_0 = 3/4,\ J_{\pm1} = 1/2$ (d) $J_0 = 1/2,\ J_{\pm1} = 5/4$

FIG. 1. Bound state spectrum for a purely magnetic impurity in a s-wave SC as a function of Rashba SOC. Lines correspond to the different angular momentum channels defined at $\alpha = 0$. $U_0 = U_{\pm1} = 0$, $\mathbf{S} = \hat{z}$(top) and $\hat{x}$(bottom) were used.

momentum $\mathbf{p} = (p_x, p_y)$ and spin σ, and

$$H_{\rm SC}(\mathbf{p}) = \tau_z \otimes (\xi_{\mathbf{p}} + \alpha \mathbf{l}_{\mathbf{p}} \cdot \boldsymbol{\sigma}) + \tau_x \otimes (\Delta_s + \frac{\Delta_t}{p_F} \mathbf{l}_{\mathbf{p}} \cdot \boldsymbol{\sigma}). \quad (1)$$

$\mathcal{H}_{\rm SC}$ describes effectively two-dimensional superconducting thin films, and surfaces of 3D superconductors with strong Rashba SOC. In (1) $\hbar = 1$, τ_j, σ_i are the Pauli matrices in Nambu and spin space respectively, $\xi_{\mathbf{p}} = p^2/2m - \mu$, with m the effective mass of the fermionic quasiparticles and μ the chemical potential, $p_F = \sqrt{2m\mu}$ is the Fermi momentum, $\mathbf{l}_{\mathbf{p}} = (p_y, -p_x)$[52], α is the strength of the Rashba SOC, and Δ_s, Δ_t are the singlet, triplet, pairing order parameters respectively, that, without loss of generality, we take to be real.

In the presence of an impurity the term $H_{\rm imp} = \hat{U}(|\mathbf{r} - \mathbf{R}|)\tau_z \otimes \sigma_0 + \hat{J}(|\mathbf{r} - \mathbf{R}|)\tau_0 \otimes \mathbf{S} \cdot \boldsymbol{\sigma}$ must be added to $H_{\rm SC}$. $\mathbf{R}$ is the position of the impurity, and $\hat{U}$ and $\hat{J}$ are the charge and magnetic potential respectively. Without loss of generality, we set $\mathbf{R} = 0$. Using the density of states (per spin) $\nu_F = m/\pi$, and the Fermi velocity $v_F = p_F/m$, we can define the dimensionless potentials $U \equiv \hat{U}\pi\nu_F$, $J \equiv \hat{J}\pi\nu_F|\mathbf{S}|$, and the dimensionless Rashba SOC $\tilde{\alpha} \equiv \alpha/v_F$ which are used in the remainder of the paper.

To find the spectrum $\{E\}$ of the impurity-induced states we have to solve the Schrödinger equation $(H_{\rm SC} + H_{\rm imp})\psi(\mathbf{r}) = E\psi(\mathbf{r})$. Let $G = [E - H_{\rm SC}]^{-1}$, then the Schrödinger equation can be rewritten as $[1 - G(E, \mathbf{r})H_{\rm imp}]\psi(\mathbf{r}) = 0$ [18]. In particular, the spectrum of the impurity bound states is obtained by finding the values of E such that $\det[1 - G(E, \mathbf{r})H_{\rm imp}] = 0$. In momentum space the Schrödinger equation takes the form:

$$\psi(\mathbf{p}) - G(E, \mathbf{p}) \int_{\mathbf{p}'} H_{\rm imp}(|\mathbf{p} - \mathbf{p}'|)\psi(\mathbf{p}') = 0. \quad (2)$$

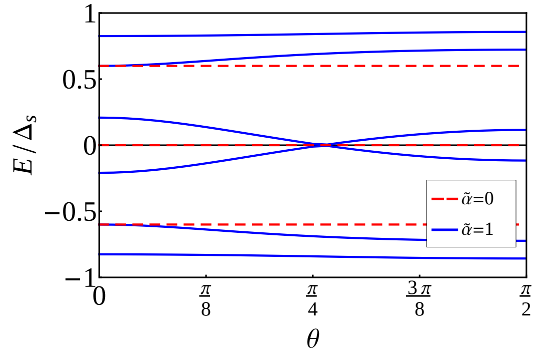


FIG. 2. Bound state spectrum for a magnetic impurity pointing in an arbitrary direction in an s-wave SC. Here $J_0 = 1$, $J_1 = 1/2$ and $U_0 = U_1 = 0$.

G can be written as the sum $(G(E, \mathbf{p}) = [G^+(E, \mathbf{p}) + G^-(E, \mathbf{p})]/2)$ of the two spin helical bands [44]

$$G^{\pm}(E, \mathbf{p}) = \begin{pmatrix} E + \xi_{\pm} & \Delta_{\pm} \\ \Delta_{\pm} & E - \xi_{\pm} \end{pmatrix} \otimes \frac{\sigma_0 \pm \sin\theta\sigma_x \mp \cos\theta\sigma_y}{E^2 - \xi_{\pm}^2 - \Delta_{\pm}^2}.$$

Here $p = |\mathbf{p}|$, $\xi_{\pm} = p^2/2m \pm \alpha p - \mu$ and $\Delta_{\pm} = \Delta_s \pm \Delta_t p/p_F$. To make further progress we rewrite all the functions, $f(\mathbf{p})$, of momentum that enter Eq. (2) in terms of their angular momentum components f_l: $f(\mathbf{p}) = \sum_l f_l(p) e^{il\theta}$. Assuming that close to the Fermi momentum $H_{\rm imp}(\mathbf{p})$ depends only very weakly on p, Eq. (2) can be rewritten in the form:

$$\sum_l \psi_l(p) e^{il\theta} - 2\pi \sum_{n,l'} G_n(E, p) e^{i(n+l')\theta} H_{\rm imp}^{l'} \times \int \frac{dp'}{(2\pi)^2} p' \psi_{l'}(p') = 0 \quad (3)$$

where

$$H_{\rm imp}^l = \begin{pmatrix} U_l \sigma_0 + J_l \frac{\mathbf{S}\cdot\boldsymbol{\sigma}}{|\mathbf{S}|} & 0 \\ 0 & -U_{-l}\sigma_0 + J_{-l}\frac{\mathbf{S}\cdot\boldsymbol{\sigma}}{|\mathbf{S}|} \end{pmatrix}. \quad (4)$$

Since $H_{\rm imp}$ is Hermitian and even with respect to $\theta - \theta'$, we require $U_l(= U_{-l})$ and $J_l(= J_{-l})$ to be real. Let $\overline{\psi_l} = \int \frac{dp}{(2\pi)^2}\, p\, \psi_l(p)$ and $\overline{G_n(E)} = \int \frac{dp}{(2\pi)^2} 2\pi p\, G_n(E, p)$. Integrating Eq. (3) over momenta we find:

$$\overline{\psi_l} - \sum_n \overline{G_n(E)} H_{\rm imp}^{l-n} \overline{\psi_{l-n}} = 0. \quad (5)$$

In our case $\overline{G_n} = 0$ for $|n| \geq 2$ so that Eq.(5) becomes:

$$\overline{\psi_l} - \overline{G_0(E)} H_{\rm imp}^l \overline{\psi_l} + \overline{G_1(E)} H_{\rm imp}^{l-1} \overline{\psi_{l-1}} + \overline{G_{-1}(E)} H_{\rm imp}^{l+1} \overline{\psi_{l+1}} = 0. \quad (6)$$

with $\overline{G_n(E)} = (\overline{G_n^+(E)} + \overline{G_n^-(E)})/2$. Assuming that most of the contributions come from the region close to the Fermi surface, we find

$$\overline{G_0^\lambda(E)} = -\frac{\pi\nu_\lambda}{\sqrt{\tilde{\Delta}_\lambda^2 - E^2}}\left(E\tau_0 + \tilde{\Delta}_\lambda\tau_x\right)\otimes\sigma_0, \tag{7}$$

$$\overline{G_{\pm1}^\lambda(E)} = \frac{\pi\lambda\nu_\lambda}{\sqrt{\tilde{\Delta}_\lambda^2 - E^2}}\frac{(E\tau_0 + \tilde{\Delta}_\lambda\tau_x)\otimes(\sigma_y \pm i\sigma_x)}{2} \tag{8}$$

where $\lambda = \pm$, $\nu_\pm = \nu_F(1 \mp \tilde{\alpha}/\sqrt{1+\tilde{\alpha}^2})$, $\tilde{\Delta}_\pm = \Delta_s \pm \Delta_t$. Henceforth, we assume that the impurity potential has only large $l = 0, 1$ components and neglect higher angular momentum channels. There are two different phases of non-centro-symmetric SC [53–55]: s-wave ($|\Delta_s| \gg |\Delta_t|$) and p-wave ($|\Delta_s| \ll |\Delta_t|$) pairing dominating regimes. As we show below, impurity-bound-state spectra are qualitatively different in the two regimes.

s-wave dominating regime. For a SC for which s-wave singlet pairing is dominant, $\Delta_s \gg \Delta_t$, each non-zero angular momentum component of the magnetic impurity potential, J_n, creates a bound state [13]. In the presence of Rashba SOC, for the case when the magnetic moment of the impurity is perpendicular to the 2D surface, $\mathbf{S} = \hat{z}$, we find that the energy levels of the impurity-induced bound states are given by the following expressions:

$$\frac{|E_{l=0,1}|}{\Delta_s} = \frac{\gamma^2 - J_0^2J_1^2 \pm \gamma^{\frac{3}{2}}\sqrt{(J_0^2-J_1^2)^2 + (\gamma-1)(J_0-J_1)^4}}{\gamma^2(1+(J_0-J_1)^2) + 2\gamma J_0J_1 + J_0^2J_1^2} \tag{9}$$

$$\frac{|E_{l=-1}|}{\Delta_s} = \frac{1-J_1^2}{1+J_1^2} \tag{10}$$

where $\gamma = 1 + \tilde{\alpha}^2$. For zero Rashba SOC $H_{\rm imp}^1$ and $H_{\rm imp}^{-1}$ have the same structure and therefore the $l = \pm1$ levels are degenerate. However, as soon as we turn on the SOC, the levels corresponding to different ls mix. This mixing is a new qualitative feature of superconductors with SOC. We find that the effect of the SOC is qualitatively different depending on the orientation of $\mathbf{S}$. For $\mathbf{S}$ perpendicular to the surface the SOC causes mixing of the $l = 0$ and $l = 1$ states. This hybridization causes a splitting of the $l = 1, -1$ states: as $\tilde{\alpha}$ grows the energy of both hybridized particle-like (hole-like) states increases (decreases) whereas the energy of the $l = -1$ state remains unchanged, as shown in Fig. 1 (a), (b). For the case in which $\mathbf{S}$ is in the plane of the 2D SC all the three states, $l = 0, -1, 1$, hybridize, as shown in Fig. 1 (c), (d). The $l = 1, -1$ states split and their energy grows (decreases) with $\tilde{\alpha}$ if they are particle-like (hole-like). The energy of the hybridized $l \approx 0$ states on the other hand in this case follows an opposite trend and decreases (increases) with $\tilde{\alpha}$ for the particle-like (hole-like). This behavior can be qualitatively understood by considering the perturbative regime $\tilde{\alpha} \ll \min\{1, |J_0 - J_1|\}$, for which we can obtain analytic expressions for the energies of the YSR states to lowest order in $\tilde{\alpha}$ for an arbitrary direction of $\mathbf{S} = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)$ [56]:

$$\frac{|E_{l=0}|}{\Delta_s} \approx \frac{1-J_0^2}{1+J_0^2} + \frac{4\tilde{\alpha}^2J_0^2J_1(J_0\cos^2\theta - J_1)}{(1+J_0^2)^2(J_0^2 - J_1^2)} \tag{11}$$

$$\frac{|E_{l=\pm1}|}{\Delta_s} \approx \frac{1-J_1^2}{1+J_1^2} + \frac{2\tilde{\alpha}^2J_0J_1^2(J_0 - J_1\cos^2\theta \pm F(\theta))}{(1+J_1^2)^2(J_0^2 - J_1^2)}$$

where $F = \sqrt{(J_0 - J_1)^2\cos^2\theta + J_1^2\sin^4\theta}$. The expressions above are valid as long as the hybridized states are not degenerate. To describe this situation we solved Eq. (6) numerically. Fig. 2 shows an example of the evolution of the spectrum of the YSR states with θ. We see that, for a given set of values of $J_0, J_1, \tilde{\alpha}$, there can be a value of θ for which the energy levels of the different YSR states cross. In this situation, by varying the orientation of $\mathbf{S}$, the fermion parity of the impurity-bound ground state can be modified. This feature is useful to tune between topological and non-topological regimes in the YSR-based Majorana proposals [18].

We now investigate the effect of the interplay between the scalar and the magnetic potential. Without SOC, the effect of $U_n \neq 0$ is to merely shift the energy of the $l = n$ level [10]. However, the presence of the SOC causes the scalar potential to qualitatively affect the spectrum of the YSR states created by the magnetic potential ($J_0, J_1 \neq 0$). In the perturbative regime $\alpha \ll 1$, for $\mathbf{S} \parallel \hat{z}$, we find that when $U_0 \neq 0$ the energies of the $l = 0, 1$ states are given by the following analytical expressions:

$$\frac{|E_{l=0}|}{\Delta_s} \approx \frac{1-J_0^2+U_0^2}{\sqrt{(1-J_0^2+U_0^2)^2+4J_0^2}} + \frac{4\tilde{\alpha}^2J_0^2J_1((1-J_0J_1)(1+J_0^2+U_0^2)+2J_0J_1U_0^2)}{((1-J_0J_1)(J_0+J_1)+J_1U_0^2)((1-J_0^2+U_0^2)^2+4J_0^2)^{\frac{3}{2}}} \tag{12}$$

$$\frac{|E_{l=1}|}{\Delta_s} \approx \frac{1-J_1^2}{1+J_1^2} + \frac{4\tilde{\alpha}^2J_1^2(J_0(1-J_0J_1)+J_1U_0^2)}{(1+J_1^2)^2((1-J_0J_1)(J_0+J_1)+J_1U_0^2)} \tag{13}$$

whereas the energy of the $l = -1$ states remains unchanged (see Eq. (10)). From these expressions we can see that the SOC correction to the energy of the $l = 1$ level depends in a non-trivial way on U_0. Analogously, we found that the energy of the $l = 0$ level qualitatively depends on U_1. To go beyond the perturbative regime we solved Eq. (6) with $U_0 \neq 0$ numerically. Fig. 3 shows the evolution of the YSR-states spectrum as a function of J_1 when both U_0 and $\tilde{\alpha}$ are not zero. This figure clearly shows the qualitative effect that U_0 has on the YSR-spectrum in the presence of SOC: for $\mathbf{S} \parallel \hat{z}$ the interplay of SOC and scalar potential creates avoided crossings between the particle-like $l = 0$ and the hole-like $l = 1$ levels. For in-plane direction $\mathbf{S}$ there is an additional avoided crossing between particle-like and hole-like $l = 1$ levels.

p-wave dominating regime. Superconductors with dominantly p-wave pairing, $\Delta_t > \Delta_s$, have properties which are more similar to unconventional superconductors. Triplet superconductivity can be due to effective electron-electron interactions (such as the ones originating from spin fluctuations) that favor a Cooper instability in the p-wave channel, or SOC itself, in which case Δ_t depends on the strength of the SOC.

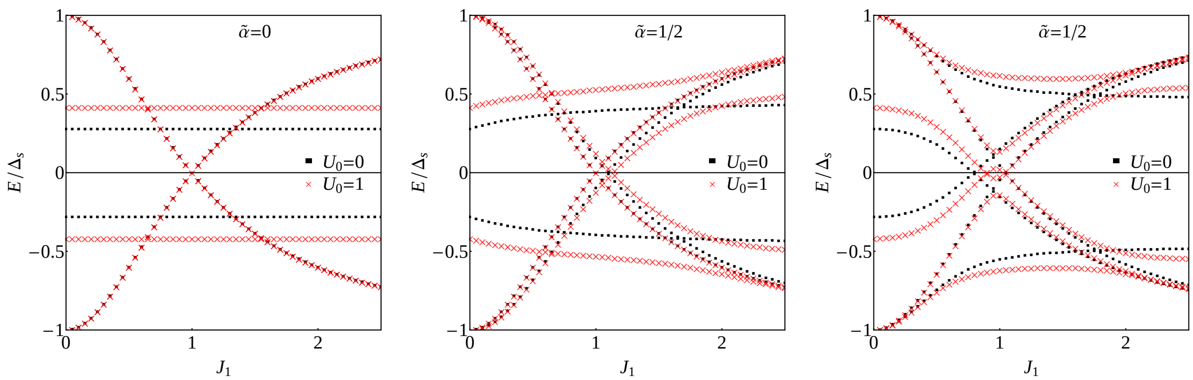
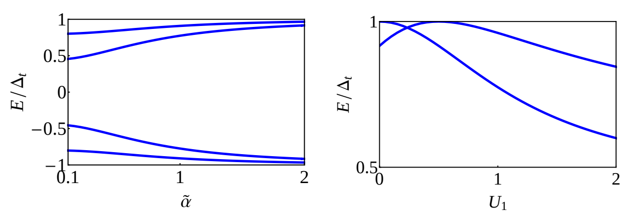


FIG. 3. Bound state spectrum for a magnetic impurity with or without scalar potential in a s-wave SC as a function of J_1. $J_0 = 3/4$, $U_1 = 0$, $\mathbf{S} = \hat{z}$ (left, middle panel) and $\mathbf{S} = \hat{x}$ (right panel) were used.

Because we are exclusively interested on the effect of the parity of the order parameter on the YSR states in the presence of SOC, we assume Δ_t to be fixed and do not obtain it self-consistently.



(a) $U_0 = 1/2, \; U_{\pm1} = 2$ (b) $\tilde{\alpha} = 1/2, \; U_0 = 1/2$

FIG. 4. Bound state spectrum for a purely scalar impurity in a p-wave SC as a function of Rashba SOC. Each of the levels is doubly degenerate here due to time reversal symmetry.

One can show that even in the presence of time-reversal symmetry, scattering off non-magnetic impurities alone leads to the formation of subgap bound states in the p-wave dominated regime [49–51]. The presence of SOC modifies the spectrum. In the limit of no magnetic potential, for $\tilde{\alpha} \ll 1$, we find the following analytical expressions for the energy levels of the bound states:

$$\frac{|E_{l=0}|}{\Delta_t} \approx \frac{U_0U_1 + 1}{\sqrt{(U_0^2+1)\,(U_1^2+1)}} + \frac{\tilde{\alpha}^2(U_0-U_1)^2((U_0+U_1)^2+1-U_0^2U_1^2)}{2(1+U_0U_1)((1+U_0^2)(1+U_1^2))^{3/2}} \tag{14}$$

$$\frac{|E_{l=1}|}{\Delta_t} \approx \frac{1+\tilde{\alpha}^2U_1^2/2}{\sqrt{1+U_1^2}} \tag{15}$$

Fig. 4 (a) shows the evolution of these levels with $\tilde{\alpha}$. In Fig. 4 (b) we show the effect of U_1 for fixed values of $\tilde{\alpha}$ and U_0. We see that there can be a value of U_1 for which the energy levels cross. Notice that the YSR levels given by Eqs (14), (15) are doubly degenerate due to time reversal symmetry. The presence of a magnetic potential ($J_n \neq 0$) leads to splitting of these Kramers doublets. Next, we find that the YSR spectrum of triplet SC depends strongly on the direction of $\mathbf{S}$ as shown in Fig. 5 even for small Rasbha SOC. From this figure we can see that, as we found for s-wave dominated SCs, also in p-wave dominated SCs the fermion parity of the impurity ground state can be changed by varying the direction of $\mathbf{S}$.

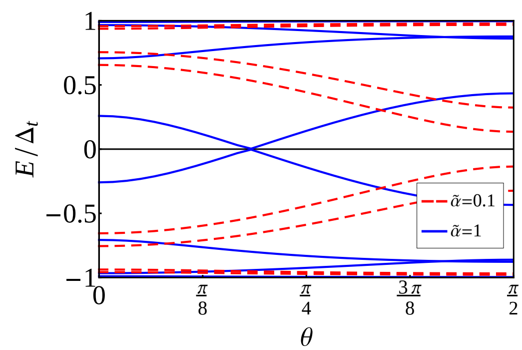


FIG. 5. Bound state spectrum for a magnetic impurity pointing arbitrary direction in a p-wave SC. Here $J_0 = 2$, $J_1 = 1$, $U_0 = U_1 = 0$.

Conclusions. We have studied the effect of spin-orbit coupling on the impurity-induced resonances in the local density of states of a 2D superconductor. Our treatment is general in that (i) it takes into account both the scalar and the magnetic part of the impurity potential; (ii) it includes higher ($|l| \geq 1$) angular momentum components of the impurity potential. We show that SOC mixes YSR states with different angular momentum and therefore strongly modifies their spectrum.

Our results have important implications for the scanning tunneling microscopy (STM) experiments trying to reveal the nature of the superconducting pairing in non-centrosymmetric superconductors. Since Pb has large SO coupling [1], our results shed some light on the measurements presented in Ref. [47]. We also find that in the presence of SOC the spectrum of the YSR states is sensitive to the direction of the magnetic moment $\mathbf{S}$ of the impurity. Our results for the dependence of the YSR on the direction of $\mathbf{S}$ constitute a novel prediction which can be tested experimentally using STM.

Our findings are also directly relevant to the ongoing efforts to use magnetic atom chains placed on the surface of a superconductor with strong SOC, such as Pb, to realize topological superconducting phases with Majorana end states [1]. Given that strong SOC leads to the dependence of the YSR spectrum on the direction of the atom magnetization, one might be able to control the fermion parity of the ground states (i.e. drive the topological phase transition) by changing the direction of the magnetization. Furthermore, we argue that higher angular momentum impurity resonances might be important for the interpretation of the experiment [1] since edges of the chain can induce in-gap states in $|l| > 0$ channels. The latter might give false positive signals in tunneling conductance measurements aimed to detect Majorana modes [1].

R.L. acknowledges the hospitality of the Aspen Center for Physics supported by NSF grant #1066293, where part of this work was done. Y.K. is supported by Samsung Scholarship. JZ and ER acknowledge support from ONR, Grant No. ONR-N00014-13-1-0321.

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