In-gap states of magnetic impurity in proximitized quantum spin Hall insulator

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We study the in-gap states of a single magnetic impurity embedded in a honeycomb monolayer proximitized to a s-wave bulk superconductor, analyzing a role played by the intrinsic spin-orbit coupling (SOC) introduced by Kane and Mele [Phys. Rev. Lett. 95, 226801 (2005)]. This interaction induces the quantum spin Hall insulating (QSHI) phase with a gap around the Fermi energy. In this gap, spin-polarized states reside, which, via the superconducting proximity effect, evolve into the Shiba-like bound states. We explore their spatial profiles and analyze the quantum phase transition (QPT), where the Shiba-like quasiparticles cross each other leading to abrupt reversal of the local currents circulating around the magnetic impurity. The mutual interplay of the Kane-Mele spin orbit interaction with the proximity induced electron pairing could be important for designing the edge modes of more complex nanostructures, such as magnetic nanowires or islands, in topological superconducting phase.

I. INTRODUCTION

Electrons native to materials such as graphene reveal a number of unique properties. Apart from their Dirac-like behavior, stemming from the honeycomb lattice, the intrinsic SOC could induce the QSHI state\textsuperscript{2} with perfect spin currents circulating along its boundaries. Realization of such effect has been experimentally observed in graphene layer randomly decorated with dilute Bi\textsubscript{2}Te\textsubscript{3} nanoparticles\textsuperscript{2} and in honeycomb type tungsten ditelluride monolayer at temperatures up to 100 K\textsuperscript{3}.

Further intriguing phenomena arise when honeycomb monolayer is proximitized to a superconducting bulk material\textsuperscript{4–9}. For instance, graphene deposited on aluminum films acquires superconductivity with the effective coherence length $\xi \approx 400$ nm\textsuperscript{9}, whereas grown on rhenium it shows high transparency of the interface, with the induced pairing gap $\Delta = 330 \pm 10$ $\mu$eV\textsuperscript{6}. Upon introducing impurities into graphene, various in-gap states can emerge, manifesting whether it is in the topologically trivial or non-trivial phase\textsuperscript{10}. In what follows we study the subgap states of a single impurity existing in the proximitized periodic honeycomb lattice, that have received a great deal of interest both in experimental\textsuperscript{11–15} and theoretical studies\textsuperscript{16–18}. In particular, more complex nanostructures embedded into such proximitized QSHI material could develop the Majorana-type quasiparticles\textsuperscript{19}.

The spin-orbit gap naturally depends on the material choice, in e.g. graphene it is often argued to be rather small, although Sichau \textit{et al.}\textsuperscript{20} have recently estimated its magnitude in to be 40 $\mu$eV by means of the resistively-detected electron spin resonance. Under such circumstances the superconducting gap would be comparable to the SOC and this could strongly affect the subgap bound states. In this paper we study the intrinsic SOC and consider its influence on observable phenomena associated with the Yu-Shiba-Rusinov (YSR) states of a single magnetic impurity embedded in a proximitized honeycomb monolayer. We inspect the topography of such states, analyze the QPT between different ground states, and study the currents induced around the impurity site.

The paper is organized as follows. In Sec. II we introduce the microscopic model and method for studying the bound states of magnetic impurity existing in honeycomb sheet. Sec. III discusses influence of the insulating and superconducting phases on the in-gap quasiparticles and presents their detailed properties. Finally, in Sec. IV, we summarize the results.

II. MODEL AND METHOD

We describe the magnetic impurity embedded in a honeycomb sheet (Fig. 1) by the tight-binding Hamiltonian

$$\hat{H} = \hat{H}_{imp} + \hat{H}_{K-M} + \hat{H}_{Rashba} + \hat{H}_{prox}. \quad (1)$$

In what follows, this impurity is treated classically

$$\hat{H}_{imp} = J \left( c_{i\sigma}^\dagger c_{j\sigma'} - c_{i\sigma'}^\dagger c_{j\sigma} \right), \quad (2)$$

where we denote the impurity site as $i_0$, and we apply the Kane-Mele scenario\textsuperscript{1} for description of the itinerant electrons

$$\hat{H}_{K-M} = t \sum_{\langle ij \rangle \sigma \sigma'} c_{i\sigma}^\dagger c_{j\sigma'} - \mu \sum_{i \sigma} c_{i\sigma}^\dagger c_{i\sigma} + i\lambda_{SO} \sum_{\langle \langle ij \rangle \rangle \sigma \sigma'} \nu c_{i\sigma}^\dagger c_{i\sigma'} s_{z \sigma} c_{j\sigma'}, \quad (3)$$

with the nearest-neighbor hopping $t$, the chemical potential $\mu$ (which we assume to be zero unless otherwise...
stated), and the imaginary, spin-dependent, next-nearest neighbor hopping amplitude $\lambda_{SO}$. The latter term is responsible for inducing the helical edge states. The sign $\nu_{ij} = \pm 1$ depends on the direction of electron hopping between the next-nearest-neighbor sites (+1 for clockwise and −1 for anticlockwise). The hopping terms involve the summation over (next-)nearest neighbors. Since substrate violates the mirror inversion $z \rightarrow -z$ symmetry, we also consider the Rashba spin-orbit interaction

\[ \hat{H}_{\text{Rashba}} = i\lambda_R \sum_{\langle ij \rangle \sigma \sigma'} c_{\sigma}^\dagger (\mathbf{s}^{\sigma \sigma'} \times \mathbf{d}_{ij})_z c_{\sigma'}. \]  

(4)

Here $\mathbf{s}^{\sigma \sigma'}$ is the vector of the Pauli matrices, referring to spin $\frac{1}{2}$, and the vector $\mathbf{d}_{ij}$ connects site $i$ with its nearest neighbor site $j$.

Finally, we assume that the honeycomb layer is proximitized to $s$-wave superconductor

\[ \hat{H}_{\text{prox}} = \sum_i \left( \Delta c_i^\dagger c_i^\dagger + \text{h.c.} \right) \]  

(5)

which induces the on-site pairing $\Delta$. For computing the observables of interest, we perform the Bogoliubov-Valatin transformation

\[ c_{\sigma} = \sum_n (u_{n\sigma}^i \gamma_n - \sigma v_{n\sigma}^i \gamma_n^\dagger), \]  

(6)

where $'$ denotes summation over the positive eigenvalues, and numerically solve the equations

\[ \sum_j \hat{H}_{ij} \hat{\Phi}_j = E_n \hat{\Phi}_i, \]  

(7)

in the auxiliary (Nambu spinor) representation $\Phi_i = (u_{1\sigma}^i, u_{2\sigma}^i, v_{1\sigma}^i, v_{2\sigma}^i)^T$. The matrix elements read

\[ \hat{H}_{ij} = \begin{pmatrix} i \delta_{ij} + t_{ij} & \lambda_{R}^\dagger & 0 & \Delta \\ -i \delta_{ii} & 0 & 0 & 0 \\ 0 & \Delta^* & - ( (\lambda_{R}^\dagger)^* (\lambda_{R}^\dagger)^* - (i \delta_{ii})^* ) \\ 0 & 0 & (\lambda_{R}^\dagger)^* & - (i \delta_{ii})^* \end{pmatrix}, \]  

(8)

where $t_{ij} = t_j \delta_{ij} - (\mu + \sigma \mu J \delta_{ii}) \delta_{ij} + \sigma i \lambda_{SO} \nu_j \delta_{ij}$ and $\lambda_{R}^{\sigma \sigma'} = i \lambda_R \sum_{\sigma' \langle \delta \rangle} (\mathbf{s}^{\sigma \sigma'} \times \mathbf{d}_{ij})_z (\lambda_{R}^{\sigma \sigma'})^*$.

Results discussed in this paper are obtained from numerical diagonalization of the Hamiltonian matrix on $40 \times 40$ lattice with the periodic boundary conditions in both directions. We do not consider any intrinsic pairing mechanism, assuming that it originates solely from the proximity effect (5). Self-consistent treatment of electron pairing is in general important (21, 22), however, in the present case it would not imply any significant changes of the local order parameter (23).

III. SUBGAP QUASIPARTICLES

For understanding the unique character of subgap quasiparticles of the proximitized honeycomb sheet it is useful to start from the QSHI state and next switch on the pairing $\Delta$.

A. Impurity bound states in QSHI phase

Let us consider the magnetic impurity in a finite-size honeycomb lattice, neglecting the superconducting substrate ($\Delta = 0$). Fig. 2 shows how the intrinsic spin-orbit interaction affects the low-energy quasiparticles. We notice that insulating energy gap of the QSHI phase grows linearly upon increasing the Kane-Mele coupling and, around $\lambda_{SO} = 0.2t$, it saturates to $\sim 1t$. Concomitantly there appear two in-gap states (purple-dotted lines in Fig. 2), which are fully spin-polarized. Similar bound states have been previously found for a single impurity whose magnetic moment is parallel to the graphene plane (24). When impurity is close enough to a perimeter of the sample they have been shown to hybridize with the topological edge states, inducing antiresonances in the transmission matrix. It has been also emphasized, that the bound states around point impurity in a two-dimensional insulator could distinguish between the topological and trivial phases of the host material (25).

Bottom panel in Fig. 2 displays the topography of the occupied ($E < E_F$) bound state for two different values of $\lambda_{SO}$. From careful examination of the spectral weight on the lattice sites adjacent to the impurity, we can notice an oscillatory decay of the wavefunction of the bound state. Practically its spatial extent does not exceed 10 atomic distances, and it quickly vanishes for higher magnitudes.
FIG. 3. Top panel: emergence of the YSR from the in-gap states of the QSHI phase driven by the proximity induced pairing $\Delta$ for $J = 6t$, $\lambda_{SO} = 0.1t$, $\mu = 0$. Bottom panel: same but for $\mu = 3\sqrt{3}\lambda_{SO}$.

of the SOC. This loss of spatial extent is accompanied by the simultaneous reduction of the spectral weight of the bound state. Closely related effects have been previously pointed out for the magnetic $^{26-30}$, non-magnetic $^{10,31,32}$ and both types of the scattering potential as well $^{33-35}$.

B. YSR quasiparticles

Upon coupling the honeycomb lattice to superconducting substrate, the energy gap around the Fermi energy results from a combined effect of the proximity induced pairing ($\Delta \neq 0$) and the insulating phase. In general, these phenomena are known to be competitive as indeed manifested by suppression of the bulk order parameter $\langle c_i \bar{c}_i \rangle$ (Sec. III C). From a perspective of the local physics (at impurity site), however, relationship between the QSHI and superconducting phases is much more intriguing. By gradually increasing the pairing potential $\Delta$, what can be achieved e.g. by reducing the external magnetic field or varying the temperature, we observe development of the YSR quasiparticles $^{36}$ directly from in-gap quasiparticles of the insulating phase (Fig. 3).

Let us focus in more detail on the YSR quasiparticles. In the present case they do not obey the original formula $E_{YSR} = \pm \Delta (1 - \pi \rho_n(E_F)J)/(1 + \pi \rho_n(E_F)J)$ derived for conventional superconductors because of the vanishing normal density of states in graphene $\rho_n(E_F) = 0$.$^{43,44}$ Fig. 4 displays the quasiparticle energies obtained numerically for our model as a function of the magnetic potential $J$ for several values of Kane-Mele coupling $\lambda_{SO}$. The dense (light-blue) dots refer to a continuum, whereas the single dotted lines represent the in-gap bound states. Amongst these in-gap branches we can recognize the Shiba-like quasiparticles by their strong variation with respect to $J$. In particular, at some critical value $J_C$ they eventually cross each other, signaling a qualitative changeover of the ground state $^{45}$. This QPT manifests itself by: sign-reversal of the local order parameter ($0 - \pi$ transition), abrupt onset of the spin polarization (Sec. III C), and by qualitative changes (both, in magnitude and vorticity) of the locally circulating currents (Sec. III E).

Our analysis indicates, that Kane-Mele coupling $\lambda_{SO}$ affects the QPT, by (i) shifting the critical coupling $J_C$ to higher values (Figs 4 and 6) and (ii) leading to substantial changes both in topography and spatial extent of the YSR-like states (Sec. III D). Thus the spin-orbit interaction weakens the efficiency of magnetic coupling $J$ between the impurity and conduction electrons. Furthermore, the YSR states no longer merge with a continuum even in the extremely strong coupling limit $J \rightarrow \infty$, in stark contrast to behavior of magnetic impurities in triangular lattice of the 2-dimensional superconductor$^{16}$ where the Kane-Mele interaction is absent.
The upper panel of Fig. 5 displays the bulk polarization, $\lambda$ ally evolves into the gap of QSHI which saturates around that energy gap of superconducting states (Fig. 2 but in presence of finite $\Delta$ and responding to the same set of model parameters as in Bottom panel of Fig. 5 presents the eigenenergies, corresponding to the on-site pairing and the spin-orbit interaction. It be instructive for understanding mutual relationship between the on-site pairing and the spin-orbit interaction. Even though variation of $J$ impurity potential of the YSR states) versus the Kane-Mele coupling $\lambda_{SO}$.

Let us now focus on the QPT, driven by the intrinsic SOC. Even though variation of $\lambda_{SO}$ would be rather not feasible experimentally, we deem that its effect can be instructive for understanding mutual relationship between the on-site pairing and the spin-orbit interaction. Bottom panel in Fig. 5 presents the eigenenergies, corresponding to the on-site pairing and the spin-orbit interaction. It be instructive for understanding mutual relationship between the on-site pairing and the spin-orbit interaction. Even though variation of $J$ impurity potential of the YSR states) versus the Kane-Mele coupling $\lambda_{SO}$.

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C. QPT

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The shift of $J_C$ with increasing $\lambda_{SO}$ is displayed as a phase diagram in Fig. 6. The black continuous line denotes the critical coupling $J_C$ at different values of $\lambda_{SO}$. Initially the shift of QPT is not meaningful, but starting from $\lambda_{SO} = 0.03t$ we observe onset of a linear variation. This increase also points out the fact that the spin-orbit interaction decreases the effective coupling of the impurity spin with the conduction electrons.

D. Topography of YSR quasiparticles

Let us now inspect the real-space shape (topography) of the YSR states. Fig. 7 presents spatial maps of the density of states at the energy of electron-like (occupied) bound state, both in absence and in presence of the intrinsic spin-orbit interaction. One can see that without the Kane-Mele interaction, the topography of YSR state has its usual character with exponential variation of the wavefunction $\sim \exp(-r/\xi)$. We remark, that spectral weight is differently distributed in each sublattice. Close to the impurity site $r_0 = (0,0)$ most of the spectral weight of the YSR quasiparticles appears in the B sublattice sites, whereas further away the A sublattice (in which the impurity resides) gains more and more spectral weight. Also the rotational symmetry of the topographic shape reveals a bipartite character. Close to the impurity site the shape has a $C_3$ rotational symmetry, reflecting the fact that every site has three nearest-neighbors (cf. bottom panels in Fig. 2), whereas at larger distances, the spectral weight distributed in the A sublattice resembles a hexagon with $C_6$ rotational symmetry. Precise evaluation of the bound states wavefunctions in this case would be a challenging task for future experimental measurements. Topography of the bound states changes dramatically, when the intrinsic SOC is taken into account. Bottom panel in Fig. 7 illustrates a strong tendency towards localization of the YSR states in vicinity of the magnetic impurity. Their spectral weight is spread over a few adjacent sites and we no longer observe any preference for dominance of only one sublattice. These prop-
The density of states \( \rho_{\lambda} \) convention \( \hbar \) YSR quasiparticle obtained for \( \Delta = 0 \).

FIG. 7. Spatial distribution of the occupied (negative value) impurity be seen by currents induced around the magnetic the Heisenberg equation \( i \partial_{t} \langle \sigma \rangle \) is normalized with respect to the occupation number. This effect is pronounced only for \( J > J_{C} \), as more sites around the impurity align their magnetic moments. The situation changes with increasing SOC which weakens the effective impurity coupling. For small \( J \) the magnetic moment is hardly screened by the closest neighboring sites and becomes more efficient when the coupling exceeds the critical value \( J_{C} \). Forcing the neighboring sites to align their magnetization with the impurity. This in turn reverses a direction of the current.

IV. CONCLUSIONS

We have theoretically investigated the spectral, magnetic and topographic features of the in-gap quasiparticles induced at magnetic impurity existing in a honeycomb sheet. We have addressed interplay between the intrinsic (Kane-Mele) spin-orbit interaction, responsible...
for energy gap of the QSHI phase, and the proximity-induced superconducting phase. Our results indicate, that the YSR quasiparticles (which are prone to superconductivity) could be developed directly from the bound states of insulating phase. This surprising behavior has no analogy to any previously reported phenomena and it can be verified empirically.

Further detailed analysis has shown, that by varying either the magnetic coupling $J$\textsuperscript{13} or the Kane-Mele interaction coupling $\lambda_{SO}$ the bound states eventually cross each other at the Fermi energy. This QPT of the ground state is manifested by sign-reversal of the local order parameter and in the present case would lead to reversal of vorticity and abrupt change of the total absolute magnitude of local currents. We have shown that the Kane-Mele coupling substantially pushes the QPT towards higher values of $J$ and strongly reduces the spatial extent of the YSR states, modifying their topographic patterns. We have also revealed the characteristic distributions of the bound states’ spectral weights in each sublattice of the proximitized honeycomb sheet.

Such phenomena might stimulate further considerations of topological insulating/superconducting phases in more complex structures, using e.g. magnetic nanowires\textsuperscript{19} or two-dimensional islands\textsuperscript{34} on honeycomb lattices, where the Majorana-type bound states could be realized.

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\begin{figure}
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\includegraphics[width=\textwidth]{figure8.png}
\caption{Spatial profiles of the currents around the magnetic impurity obtained for $J = 5t$ (a) and $J = 8.5t$ (b). Bottom panel (c) plots a magnitude of the integrated currents versus the coupling $J$. Other parameters: $\Delta = 0.2t$, $\lambda_{SO} = 0.1t$, $\lambda_{R} = 0.05t$.}
\end{figure}
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