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Impurity-induced states in superconducting heterostructures

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Heterostructures allow the realization of electronic states that are difficult to obtain in isolated uniform systems. Exemplary is the case of quasi-one-dimensional heterostructures formed by a superconductor and a semiconductor with spin-orbit coupling in which Majorana zero-energy modes can be realized. We study the effect of a single impurity on the energy spectrum of superconducting heterostructures. We find that the coupling between the superconductor and the semiconductor can strongly affect the impurity-induced states and may induce additional subgap bound states that are not present in isolated uniform superconductors. For the case of quasi-one-dimensional superconductor/semiconductor heterostructures we obtain the conditions for which the low-energy impurity-induced bound states appear.

Composite heterostructures provide an opportunity to realize states with novel and desirable properties that are different from the individual components. In the last decade, this principle has been implemented successfully to obtain *composite electronic systems* with novel and unique electronic properties. For example, heterostructures comprising a conventional s-wave superconductor (SC) and a semiconductor (SM) with strong spin-orbit coupling (SOC) may realize topological superconducting states supporting Majorana zero modes (MZMs)[1–9], of which preliminary signatures have been observed [10–24].

The presence of impurities is unavoidable in any condensed matter system. However, in heterostructures their effect can be particularly non-trivial due to the interplay between scattering processes involving different materials. Their effect in general varies significantly depending on the component of the heterostructure in which they are located. This fact makes the understanding of impurity effects in superconducting heterostructures non trivial and outside the scope of most previous works focusing on impurity effects in single-component homogeneous superconducting systems (for a recent review see Ref. [25]).

In this work we study the states induced by scalar impurities in heterostructures involving a SC and a SM with Rashba SOC. Previous studies mostly focused on the case of impurities located in the SM or at the SM/SC interface [26–43]. Here we consider in detail also the case when impurities are located in the SC. We focus on the case of an isolated impurity problem, and obtain analytical results that help to understand some recent numerical simulations [44]. We show that in general the self-energy describing the effect of an isolated impurity consists of two terms that may have opposite signs. We find that the complete or partial cancellation of these two terms is responsible for the presence of low-energy impurity-induced states that are not present in homogeneous SC systems [25]. We find that this cancellation may lead to impurity-induced subgap states even in the limit of vanishing magnetic field. This finding does not contra-

dict Anderson’s result [45] given that in our system the superconducting order parameter is not uniform. For the specific case of one-dimensional (1D) heterostructures we study how the spectrum of the impurity-induced states changes as a function of an external magnetic field. As shown in Refs. [46–49], a magnetic field may induce a quantum phase transition from a conventional (trivial) superconducting phase to a topological superconducting phase characterized by the presence of MZMs. We identify the regions in parameter space where very low-energy impurity-induced states might affect the observation and manipulation of MZMs.

The Hamiltonian H for the heterostructure can be written as $H = H_N + H_{SC} + H_T$, where H_N is the Hamiltonian for the normal, i.e. non-superconducting, component (either a SM or a metal), H_{SC} is the Hamiltonian for the SC and H_T is the term describing tunneling processes between the SC and the normal component. Specifically, H_N and H_{SC} are defined as (henceforth $\hbar = 1$)

$$H_N = \frac{1}{2} \sum_{\mathbf{k}} \psi_{N,\mathbf{k}}^\dagger [\epsilon_{N,\mathbf{k}} \sigma_0 \tau_z + \alpha \mathbf{l}_{\mathbf{k}} \cdot \boldsymbol{\sigma} \tau_z + V_x \sigma_x \tau_z] \psi_{N,\mathbf{k}}, \quad (1)$$

$$H_{SC} = \frac{1}{2} \sum_{\mathbf{k}} \psi_{SC,\mathbf{k}}^\dagger [\epsilon_{SC,\mathbf{k}} \tau_z \sigma_0 - \Delta_0 \tau_y \sigma_y] \psi_{SC,\mathbf{k}}. \quad (2)$$

where $\psi_{\mathbf{k},i}^\dagger = (c_{i,\mathbf{k}\uparrow}^\dagger, c_{i,\mathbf{k}\downarrow}^\dagger, c_{i,-\mathbf{k}\uparrow}, c_{i,-\mathbf{k}\downarrow})$ is the spinor with $i=N$ or $i=SC$, $c_{i,\mathbf{k}\sigma}^\dagger$ ($c_{i,\mathbf{k}\sigma}$) is the creation (annihilation) operator for an electron with momentum \mathbf{k} and spin σ in the i -th part of the heterostructure, $\epsilon_{i,\mathbf{k}} = (\mathbf{k}^2/2m_i - \mu_i)$ with m_i , μ_i the electron’s effective mass and chemical potential, respectively, in the i -th component, σ_j (τ_j) are the Pauli matrices in spin (Nambu) space, α is the strength of the Rashba SOC with $\mathbf{l}_{\mathbf{k}} = (0, k_z, -k_y)$, Δ_0 is the amplitude of the superconducting gap, and V_x is the Zeeman splitting due to the external magnetic field along the x -direction. The tunneling Hamiltonian can be written as

$$H_T = \frac{1}{2} \sum_{\mathbf{k}} \psi_{SC,\mathbf{k}}^\dagger \hat{h}_T(\mathbf{q}) \psi_{N,\mathbf{k}+\mathbf{q}} + h.c. \quad (3)$$

where $\hat{h}_T(\mathbf{q})$ is the tunneling matrix. In our case, assuming that the tunneling processes conserve the spin and the momentum parallel to the SC-N interface (\mathbf{k}_{\parallel}) we have $\hat{h}_T(\mathbf{q}) = t\sigma_0\tau_z\delta(\mathbf{q}_{\parallel})$ with t being the tunneling amplitude. To quantify the effect of the tunneling term it is helpful to introduce the parameter $\Gamma_t \equiv t^2\rho_{F,SC}$, where $\rho_{F,SC}$ is the density of states (DOS) of the SC at the Fermi energy, $E_{F,SC}$.

In the presence of impurities, the Hamiltonian for the system is modified by an additional term, H_{imp} , describing the scattering of electrons off the impurities. For a single isolated impurity located in the i -th ($i = \text{N, SC}$) component of the heterostructure

$$H_{\text{imp}} = \sum_{\mathbf{r}} \delta(\mathbf{r}) \psi_{i,\mathbf{r}}^\dagger \hat{h}_{\text{imp}} \psi_{i,\mathbf{r}} = \sum_{\mathbf{k}, \mathbf{k}'} \psi_{i,\mathbf{k}}^\dagger \hat{h}_{\text{imp}} \psi_{i,\mathbf{k}'}. \quad (4)$$

Here $\psi_{i,\mathbf{r}}^\dagger$ ($\psi_{i\mathbf{r}}$) is the creation (annihilation) operator for an electron at position \mathbf{r} in the i -th component of the heterostructure, and \hat{h}_{imp} is the matrix describing the structure of the impurity in spinor space. For a scalar impurity, using the convention specified above for spinors, we have $\hat{h}_{\text{imp}} = u_{\text{imp}}\sigma_0\tau_z$ where u_{imp} is the strength of the impurity potential.

The spectrum of the impurity-induced states can be obtained by locating the poles of the T matrix ([50] Sec. I). Using the diagrammatic approach, one can express the T -matrix in terms of the Green's function for the isolated components of the heterostructure $G_i^{(0)}(\mathbf{k}, \omega) = (\omega + i\eta - H_i)^{-1}$ with $i = \text{N, SC}$ and $\eta \rightarrow 0$. If the impurity is located in the i -th component of the heterostructure, the matrix T_i is given by

$$T_i(\omega) = \left[\mathbb{1} - \hat{h}_{\text{imp}} \Sigma_{i,\text{imp}}(\omega) \right]^{-1} \hat{h}_{\text{imp}}, \quad (5)$$

where $\Sigma_{i,\text{imp}}(\omega) = \int d\mathbf{k} G_i(\mathbf{k}, \omega)$ and $G_i(\mathbf{k}, \omega)$ is the Green's function of the i -th component of the heterostructure *dressed* by the self-energy $\Sigma_{i,t}(\mathbf{k}_{\parallel}, \omega)$ due to the tunneling term:

$$G_i(\mathbf{k}, \omega) = \left[(G_i^{(0)}(\mathbf{k}, \omega))^{-1} - \Sigma_{i,t}(\mathbf{k}, \omega) \right]^{-1} \quad (6)$$

$$\Sigma_{i,t}(\mathbf{k}, \omega) = \int d\mathbf{q} \hat{h}_T(\mathbf{q}) G_i^{(0)}(\mathbf{k} + \mathbf{q}, \omega) \hat{h}_T(-\mathbf{q}). \quad (7)$$

Here $G_i^{(0)}$ is the Green's function of the heterostructure's component coupled via the tunneling term to the i -th component. Using Eq.(3), we obtain

$$\Sigma_{i,t}(\mathbf{k}_{\parallel}, \omega) = t^2 \int d\mathbf{q}_{\perp} \sigma_0 \tau_z G_i^{(0)}(\mathbf{k}_{\parallel}, \mathbf{q}_{\perp}, \omega) \sigma_0 \tau_z. \quad (8)$$

To understand how the presence of the tunneling term affects the spectrum of the impurity-induced states it is useful to express T_i in the following equivalent form:

$$T_i = \left[\mathbb{1} - \hat{h}_{\text{imp}} \left(\Sigma_{i,\text{imp}}^{(0)}(\omega) + \Sigma_{i,\text{imp}}^{(1)}(\omega) \right) \right]^{-1} \hat{h}_{\text{imp}} \quad (9)$$

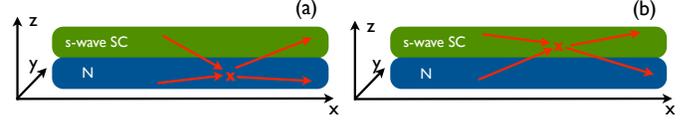


FIG. 1. (Color online) Sketch of 1D N/SC heterostructure with an isolated impurity, shown by the red “X”, in the semiconductor (N), in (a), and in the SC in (b). Red arrows represent impurity-induced scattering processes.

where

$$\Sigma_{i,\text{imp}}^{(0)}(\omega) = \int d\mathbf{k} G_i^{(0)}(\mathbf{k}, \omega), \quad (10)$$

$$\Sigma_{i,\text{imp}}^{(1)}(\omega) = \int d\mathbf{k} G_i^{(0)}(\mathbf{k}, \omega) \Sigma_{i,t}(\mathbf{k}, \omega) G_i(\mathbf{k}, \omega). \quad (11)$$

As follows from above, there are two contributions that determine the pole structure of T_i : $\Sigma_{i,\text{imp}}^{(0)}$ the term that appears if the component i were isolated, and $\Sigma_{i,\text{imp}}^{(1)}(\omega)$ the term due to tunneling processes between the i -th and \bar{i} -th component of the heterostructure. If tunneling is not a weak perturbation, the interplay between these two terms may lead to unusual properties for the spectrum of the impurity-induced states in the heterostructure.

For the case when the impurity is located in the normal component (in the remainder we assume it to be a semiconductor) the effect of the tunneling term is to induce a SC gap in it (Δ_{ind}) and it is straightforward from Eq. (5) to obtain $T_N(\omega) = [\tau_z \sigma_0 - u_{\text{imp}} \hat{\Sigma}_{N,\text{imp}}(\omega)]^{-1} u_{\text{imp}}$. When no SOC is present ($\alpha = 0$), $T_N(\omega)$ does not have poles ω^* below the induced gap (i.e. $|\omega^*| \geq \Delta_{\text{ind}}$). In the presence of SOC the induced superconductivity in the SM will be a mix of spin-singlet and spin-triplet pairing components even though in the SC only s-wave pairing is present [51–53]. To further investigate this case we consider the quasi-1D system shown in Fig. 1 in which $L_x \rightarrow \infty$ and L_y, L_z are small enough so that the spectrum is comprised of 1D subbands, $\epsilon_{k_x}^{(n)}$, with energy separation larger than Δ_0 . For concreteness, in the remainder we limit ourselves to the case in which only one spinful subband is occupied. When V_x is larger than a critical value, V_x^c , the system is expected to be in a topological phase [48, 49]. For parameter values relevant for current experiments ([50] Sec.II) for $V_x < V_x^c$ the impurity-induced states have energies, ω^* , very close to the induced-gap edge. When the chemical potential is much larger than the SC bulk gap ([50] Sec.III), in the trivial regime, $|\omega^*|$ can be smaller than Δ_{ind} , albeit it does not approaches zero. The spectrum of the impurity-induced states is completely different in the topological regime. In this regime the induced superconducting pairing is p-wave and we find that the energy of the bound states: (i) depends very strongly on u_{imp} , (ii) it is strongly asymmetric with respect to $u_{\text{imp}} = 0$, (iii) it can go to zero for finite (negative) values of u_{imp} [37]. This

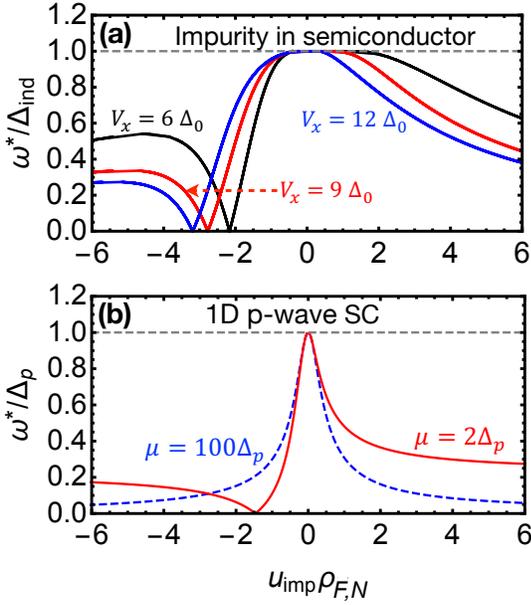


FIG. 2. (Color online) (a) Spectrum of impurity-induced bound states for 1D N/SC heterostructure as a function of $u_{\text{imp}}\rho_{F,N}$ for the case (a) of Fig.1 and $V_x > V_x^c$. Here $k_{F,N}^2/(2m_N) = 1.5\Delta_0$, $\alpha_{SO}k_{F,N} = 4.2\Delta_0$, $\Gamma_t = 5\Delta_0$, $V_x^c \approx 5.2\Delta_0$. (b) Spectrum of impurity-induced bound states for a 1D p-wave SC as a function $u_{\text{imp}}\rho_{F,N}$ for different values of μ .

can be seen in Fig. 2 (a) where the dependence of ω^* on $u_{\text{imp}}\rho_{F,N}$ ($\rho_{F,N}$ being the DOS of the semiconductor (N) at its Fermi energy $E_{F,N}$) for different values of the Zeeman splitting $V_x > V_x^c$.

The results shown in Fig. 2 (a) can be qualitatively understood considering a scalar impurity, Eq. (4), in a 1D p-wave superconductor for which: $H_{\text{pSC}} = \sum_{k_x, \sigma, \sigma'} [c_{k_x, \sigma}^\dagger (k_x^2/2m - \mu) \sigma_0 c_{k_x, \sigma'} + i\Delta_p(k_x/k_F) c_{k_x, \sigma}^\dagger \mathbf{d}_{k_x} \cdot \boldsymbol{\sigma} \sigma_y c_{-k_x, \sigma'}^\dagger + \text{h.c.}]$, where $\Delta_p(k_x/k_F) = -\Delta_p(-k_x/k_F)$ is the amplitude of the superconducting p-wave pairing and \mathbf{d}_{k_x} is the unit vector characterizing the polarization of the triplet state [54]. In this case $T(\omega) = u_{\text{imp}}[\tau_z - u_{\text{imp}} \int dk_x G_{\text{p-SC}}(\omega, k_x)]^{-1}$, where $G_{\text{p-SC}}(\omega, k_x) = (\omega + i\eta - H_{\text{p-SC}})^{-1}$. Due to the 1D nature of the carriers, one finds that, at low energies, the density of states is strongly dependent on their energy ϵ : $\rho(\epsilon) \approx 1/\sqrt{\epsilon}$. This fact makes the energy of the impurity bound state strongly dependent on u_{imp} when μ_N is close to the bottom of the band. This is shown in Fig. 2 (b) where we can see that the energy of the bound state depends strongly on u_{imp} when μ is small (solid line) and fairly weakly for large μ (dashed line) [55]. We should emphasize that this asymmetry effect is very relevant for 1D topological SC wires supporting MZMs in which typically μ_N must be quite small, i.e. $|\mu_N| < \sqrt{V_x^2 - \Delta_{\text{ind}}^2}$ [46–49].

In the most recent realizations of 1D topological SC wires [9, 19–21] the SM and the interface between the SM and the SC are of very high quality so that very few

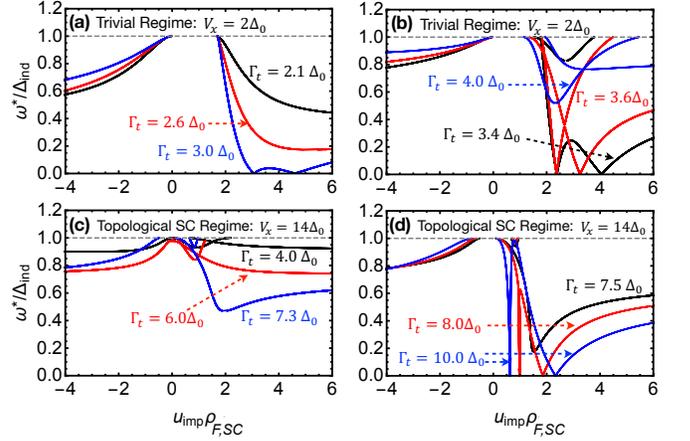


FIG. 3. (Color online) Spectrum of impurity-induced bound states as function of $u_{\text{imp}}\rho_{F,SC}$ for 1D N/SC heterostructure when the impurity is located in the SC in the trivial regime, (a) and (b), and topological regime (c) and (d). Here $k_{F,N}^2/(2m_N) = 1.5\Delta_0$, $\mu_N = 1.5\Delta_0$, $\alpha_{SO}k_{F,N} = 4.2\Delta_0$, $k_{F,N}/k_{F,SC} = 0.3$.

impurities are expected to be present in the SM or at the interface. On the other hand, the SC (i.e. aluminum) is disordered. Therefore, henceforth we consider the situation in which the impurities are located in the SC. In this case, using Eq. (9) one finds

$$T_{\text{SC}} = \frac{u_{\text{imp}}}{\tau_z \sigma_0 - u_{\text{imp}} \Sigma_{\text{SC,imp}}^{(0)}(\omega) - u_{\text{imp}} \Sigma_{\text{SC,imp}}^{(1)}(\omega)}. \quad (12)$$

For the case in which the SC is s-wave and the tunneling is such that $\hat{h}_T = t\delta(\mathbf{q}_{\parallel})\sigma_z\tau_0$ we obtain

$$\Sigma_{\text{SC,imp}}^{(0)}(\omega) = -\frac{\rho_{F,SC}}{\sqrt{\Delta_0^2 - \omega^2}} [\omega\sigma_0\tau_0 + \Delta_0\sigma_y\tau_y] \quad (13)$$

$$\Sigma_{\text{SC,imp}}^{(1)}(\omega) = \int d\mathbf{k}_{\parallel} \int d\mathbf{k}_{\perp} G_{\text{SC}}^{(0)}(\mathbf{k}_{\parallel}, \mathbf{k}_{\perp}, \omega) \Sigma_{\text{SC,t}}(\mathbf{k}_{\parallel}, \omega) G_{\text{SC}}(\mathbf{k}_{\parallel}, \mathbf{k}_{\perp}, \omega) \quad (14)$$

with $\Sigma_{\text{SC,t}}(\mathbf{k}_{\parallel}, \omega)$ given by Eq. (7). One can show that the strength of the second term $\Sigma_{\text{SC,imp}}^{(1)}(\omega)$ is proportional to the dimensionless parameter $\alpha_{\text{SWS}} = \frac{\Gamma_t}{E_{F,N}} \frac{k_{F,N}}{k_{F,SC}}$ (see [50] Sec.I for details) where $k_{F,N}$, $k_{F,SC}$ are the Fermi momenta in the N and SC, respectively.

Fig. 3 (a) shows the spectrum of the impurity-induced states as a function of $u_{\text{imp}}\rho_{F,SC}$ for the 1D case in which the N/SC heterostructure is in the topologically trivial phase, $V_x = 2\Delta_0 < V_x^c$, and different values of Γ_t . In the limit $\alpha_{\text{SWS}} \rightarrow 0$, $t \neq 0$ (i.e. $\Sigma_{\text{SC,imp}}^{(1)} \rightarrow 0$ and $\Delta_{\text{ind}} \neq 0$), we find bound states close to the gap edge. As α_{SWS} increases, the interplay between $\Sigma_{\text{SC,imp}}^{(0)}$ and $\Sigma_{\text{SC,imp}}^{(1)}$ may lead to low-lying subgap states as shown in Figs. 3 (a) and (b). The results of Fig. 3 (b) also show that as Γ_t increases the spectrum of the impurity-induced bound states becomes more asymmetric with respect to

$u_{\text{imp}} = 0$ as we have found for the case in which the impurity is located in the N. It is very interesting to notice that, contrary to the case when an impurity is located in the N, see Fig. 2 (a) in [50], an impurity in the SC may lead to low-lying subgap states with $\omega^* \rightarrow 0$ in the trivial regime.

Figs. 3 (c), (d) show the results when the N/SC heterostructure is in the topological phase, $V_x = 14\Delta_0 > V_x^{(c)}$. One can see that the spectrum is strongly asymmetric in this case even for relatively small values of Γ_t , Fig. 3 (c). For larger Γ_t we find that also in the topological phase the impurity can induce zero energy bound states for relatively small values of $u_{\text{imp}}\rho_{F,SC}$, Figs. 3 (d). These results suggest that in the topological phase the value of u_{imp} necessary to induce a zero-energy bound state decreases as Γ_t increases. Thus, there is an optimal value of Γ_t for which the induced gap is large and, at the same time, impurities in the SC do not result in significant subgap density of states.

The effect of V_x on the spectrum of the impurity-induced bound states is summarized by the results shown in Fig. 4. Fig. 4 (a), (c) show how, for fixed Γ_t , V_x affect the dependence of the spectrum on u_{imp} for the case when $V_x < V_x^{(c)}$, (a), and $V_x > V_x^{(c)}$ (c). As one can see there is a threshold value of V_x for the emergence of bound states with $\omega^* \rightarrow 0$ both in the trivial and topological regime. Fig. 4 (b), (d), show the evolution of ω^* with V_x for fixed u_{imp} for the same values of Γ_t and $k_{F,N}/k_{F,SC}$ used in (a) and (c), respectively. From the results of Fig. 4 we see that zero-energy impurity-induced bound states may appear in both the topological and the trivial regimes by tuning the magnetic field.

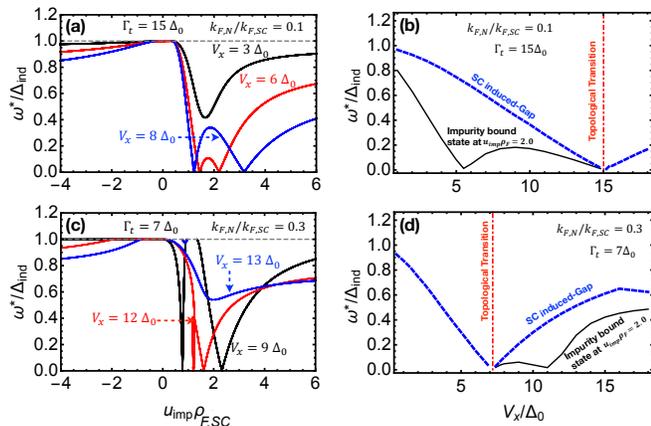


FIG. 4. (Color online) Effect of V_x on impurity-induced bound states spectrum. (a), (b): $\Gamma_t = 15\Delta_0$, $k_{F,N}/k_{F,SC} = 0.1$. In (a) $V_x < V_x^{(c)}$. (c), (d): $\Gamma_t = 7\Delta_0$, $k_{F,N}/k_{F,SC} = 0.3$. In (c) $V_x > V_x^{(c)}$. (b), (d) show the evolution of impurity-induced bound states (black solid line) for fixed $u_{\text{imp}}\rho_F = 2.0$.

Considering that V_x and Γ_t are two of the key parameters that can be controlled in experiments to realize

MZMs in proximitized nanowires, the knowledge of where in the (V_x, Γ_t) plane $\omega^* = 0$ is of great importance for the realization of topological qubits based on such systems [56–59]. Figs. 5 (a), (b) show in grey-blue (yellow) the regions in the (V_x, Γ_t) plane for which there exist a finite value of u_{imp} such that $\omega^* = 0$ ($\omega^* < 0.6\Delta_{\text{ind}}$). The red dashed line shows the boundary between trivial and topological regimes. The horizontal dashed line in Fig. 5 (a) (Fig. 5 (b)) identifies the values of Γ_t for which the results of Fig. 4 (a), (b) (Fig. 4 (c), (d)) were obtained. As follows from Fig. 5 (a), the area where $\omega^* = 0$ is rather large in the trivial regime and becomes smaller in the topological one when $k_{F,N}/k_{F,SC} \ll 1$. As the ratio $k_{F,N}/k_{F,SC}$ increases the area where $\omega^* = 0$ decreases in the trivial phase and increases in the topological phase, as shown by Fig. 5 (b). Thus, the ratio of $k_{F,N}/k_{F,SC}$ is an important parameter when trying to reduce disorder effects in superconducting heterostructures. For aluminum-based proximitized nanowires this parameter is quite small, $k_{F,N}/k_{F,SC} \ll 1$. The parameter α_{SWS} can be controlled experimentally by changing the back-gate voltage in proximitized nanowires [60, 61] so the propensity for the formation of impurity-induced bound states we predict, see Fig. 5, can be tested experimentally.

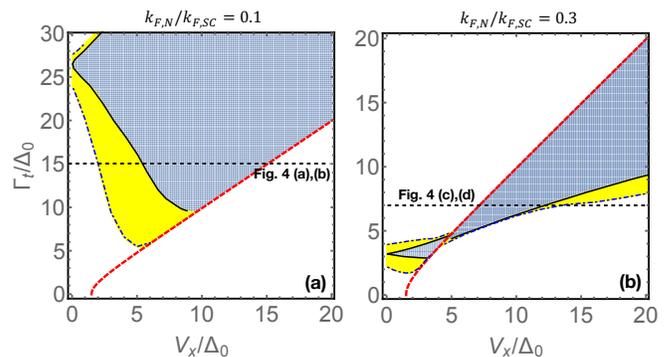


FIG. 5. (Color online) Phase diagram in (V_x, Γ_t) plane identifying the regions, shown in grey (yellow) for which $\omega^* = 0$ ($\omega^* < 0.6\Delta_{\text{ind}}$) for some finite value of u_{imp} (not for fixed value of u_{imp}). The red dashed line shows the boundary between trivial and topological regime. The horizontal dashed line is placed at the value of Γ_t for which the results of Fig. 4 were obtained. (an evolution of bound states for fixed u_{imp} is shown in [50] Sec.IV.) Here $k_{F,N}^2/(2m_N) = 1.5\Delta_0$, $\alpha_{SO}k_{F,N} = 4.2\Delta_0$.

Conclusions. We have studied impurity-induced subgap states in superconductor-based heterostructures. In the case of proximitized nanowires we find that in these structures there is a large region in parameter space for which the impurities in the superconductor can induce low energy states even when the superconductor is purely s-wave. Our work presents results for the spectrum of the bound states induced by a single impurity and so is complementary to the previous studies that considered the

case of many weak impurities [31–36, 38, 42, 44, 62] via disorder-averaging techniques. Our results are directly relevant to experimental situations in which the impurity density is low and disorder-averaging is not justified. In addition, they are instrumental to extend the study of the effect of many-impurities via disorder-averaging to the unitary limit, i.e. the limit of strong impurities, both for the case when the impurities are located in the SM and the case when they are located in the superconductor.

Our results provide guidance for the optimization of superconductor-semiconductor heterostructures: although a strong tunneling is beneficial to obtain a large gap it also enhances the effect of the impurities located in the s-wave superconductor on the superconducting state induced in the semiconductor. Therefore, we find that, when the effect of impurities is included, the optimal coupling to the superconductor is not strong but intermediate, i.e. $\Gamma_t \sim \Delta_0$.

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