Andreev and Majorana bound states in single and double quantum dot structures

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Abstract

We present a numerical study of the emergence of Majorana and Andreev bound states in a system composed of two quantum dots, one of which is coupled to a conventional superconductor, SC1, and the other connects to a topological superconductor, SC2. By controlling the interdot coupling we can drive the system from two single (uncoupled) quantum dots to double (coupled) dot system configurations. We employ a recursive Green’s function technique that provides us with numerically exact results for the local density of states of the system. We first show that in the uncoupled dot configuration (single dot behavior) the Majorana and the Andreev bound states appear in an individual dot in two completely distinct regimes. Therefore, they cannot coexist in the single quantum dot system. We then study the coexistence of these states in the coupled double dot configuration. In this situation we show that in the trivial phase of SC2, the Andreev states are bound to an individual quantum dot in the atomic regime (weak interdot coupling) or extended over the entire molecule in the molecular regime (strong interdot coupling). More interesting features are actually seen in the topological phase of SC2. In this case, in the atomic limit, the Andreev states appear bound to one of the quantum dots while a Majorana zero mode appears in the other one. In the molecular regime, on the other hand, the Andreev bound states take over the entire molecule while the Majorana state remains always bound to one of the quantum dots.

Keywords: topological superconductors, Andreev bound states, Majorana fermions

(Some figures may appear in colour only in the online journal)

1. Introduction

Nanosopic structures coupled to superconductors have attracted the attention of many researchers over the last two decades [1–9]. One interesting aspect of nanostructured systems such as quantum dots coupled to normal or superconducting contacts is their flexibility for studying many different phenomena, such as the Kondo effect [10], Andreev bound states (ABSs), etc. Due to confinement, quantum dot systems exhibit a discrete spectrum that can be modified by local gates, allowing for a fine control of their physical properties.

When a quantum dot is connected to a conventional superconductor, multiple Andreev reflections between the quantum dot and the superconductor give rise to ABSs in the dot [11, 12], with a signature visible in their transport properties [13, 14]. For example, by studying a graphene quantum dot coupled to normal and superconductor contacts, Dirks et al [13] have observed sharp in-gap conductance peaks attributed to individual ABSs in the system. Another interesting result is the interplay between the Kondo screening and the superconducting pairing in quantum dots observed by Pillet et al [6]. The interplay between Kondo and Andreev bound states has also been studied earlier by Franke and co-workers [9], in magnetic molecules on the surface of a superconductor.

More recently, quantum dots coupled to topological superconductor wires [15–18] supporting Majorana bound states (MBSs) in their ends have also attracted a lot of attention. Besides the interest in the fundamental concepts of Majorana state physics [19–21], it is also potentially useful for topologically protected quantum computation [22–27]. Despite the great effort of various researchers toward experimental observation [28–30], not much progress has been made lately. One of the most challenging tasks for a clear observation of MBS features in condensed matter systems is to tell apart...
features from other phenomena, as it has been argued that MBSSs may be confused with signatures from Kondo or ABSs. For instance, it has been shown by one of us that, under a certain regime, Majorana and Kondo physics can coexist in a quantum dot that is simultaneously coupled to a topological superconductor and to a metallic contact [17, 32]. Therefore, identifying features of a particular phenomenon can be experimentally puzzling. While the interplay between the Majorana and the Kondo effect has been investigated in some detail, very little attention has been devoted to MBSSs and ABSs together [33, 34]. For instance, do MBSSs and ABSs mix together? More importantly, if the MBS and ABS coexist in some regime, how can one distinguish them experimentally? The answers to these important questions remain unclear.

Aiming to address these questions, in this work we investigate the possible coexistence and interplay between ABSs and MBSSs in single and double dot systems. We consider a double quantum dot system in which one of the dots is coupled to a conventional s-wave superconductor while the other is coupled to a topological superconductor. The quantum dots are interconnected by a controllable tunneling barrier that allows us to drive the system from single to double dot configurations, providing a flexible structure to address the possible mixing of MBSSs and ABSs. For the sake of clarity, our system is schematically represented in figure 1. It resembles the one proposed by Pillet et al., in [6]. Here, however, while the left quantum dot (QD1) is coupled to a normal s-wave superconductor (SC1) the right one (QD2) is connected to a topological superconductor that provides the MBS. Furthermore, each of the quantum dots is coupled to individual metallic leads labeled (3) and (4) (see figure 1) that induce a natural broadening of the quantum dot levels. When the quantum dots are decoupled from each other, if SC2 is in its topological phase, a Majorana mode will appear in QD2, as predicted in [32], while in QD1 there will be a pair of ABSs.

To study the bound states we focus mainly on the spectral properties of the system, which is accessible via zero-bias differential conductance measurement as in the experiment reported in [6]. We employ the standard recursive Green’s function (GF) approach, from which we can obtain numerically exact results for the local density of states (LDOS) of the system. We first study the situation in which the quantum dots are fully decoupled from each other. In this configuration we monitor the local density of states of QD2 while driving SC2 from its trivial to its topological phase. We show that the MBSSs and the ABSs appear in two distinct regimes, which can be distinguished in tunneling spectroscopy measurements. We then go on and study the possible coexistence of MBSSs and ABSs in the double dot configuration. To do so we couple the two quantum dots by making the interdot coupling finite. We find that in the trivial phase of SC2 and in the atomic limit (small interdot coupling) the dot coupled to the normal superconductor exhibits the usual ABSs whereas the other one exhibits an atomic single particle peak. In the molecular regime (strong interdot coupling), the Andreev states take over the entire molecule, appearing clearly in the molecular orbitals. More interestingly, in the topological phase of SC2, in the atomic regime we see ABSs in QD1 and a Majorana zero mode in QD2. In the molecular regime, on the other hand, while the ABSs are seen over the entire molecule, the Majorana mode (seen only for spin down) is always bound to an atomic orbital.

The remainder of this paper is structured in the following way. In section 2 we describe the model and derive the main physical quantities and in section 3 we present our numerical results. Finally, we conclude our work in section 4.

2. Model and method

2.1. Hamiltonian model

For concreteness, our system is described by the following Hamiltonian:

\[ H = H_{\text{dots}} + H_{\text{SC}} + H_{\text{leads}} + H_{\text{dot-leads}} + H_{\text{dot-SC}} + H_T. \]  

(1)

Here \( H_{\text{dots}} \) and \( H_{\text{leads}} \) describe the isolated quantum dots and the normal leads, respectively, \( H_{\text{SC}} = H_1 + H_2 \) describes the normal and the topological superconductors, \( H_{\text{dot-leads}} \) connects the dot to the normal leads, \( H_{\text{dot-SC}} \) couples the dots to the superconductors and \( H_T \) describes the tunnel coupling between the dots. Explicitly, the various terms in the Hamiltonian (1) can be written as,

\[ H_{\text{dots}} = \sum_{i=1,2} \varepsilon_i d_i^\dagger d_i, \]  

(2)

\[ H_1 = \sum_{j=1,2} \left( \sum_{\mu=\downarrow,\uparrow} \tau_{\mu}^j c_{j,\mu}^\dagger c_{j,\mu} + \Delta c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger \right) + \text{H.c.}, \]  

(3)

\[ H_2 = \frac{1}{2} \sum_{j=1,2} \left( \sum_{\mu=\downarrow,\uparrow} \left( -\varepsilon_j + \frac{V_Z}{2} \sigma_{\mu}^{j,\mu} \right) c_{j,\mu}^\dagger c_{j,\mu} - i \tau_{\mu}^j c_{j,\mu}^\dagger c_{j,\mu} \right) + \Delta c_{j,\uparrow} c_{j,\downarrow}^\dagger + \text{H.c.}, \]  

(4)

\[ H_{\text{leads}} = \sum_{\ell=3,4} \varepsilon_{\ell,k} c_{\ell,k}^\dagger c_{\ell,k} \quad (\ell = 3,4), \]  

(5)

\[ H_{\text{dot-leads}} = \sum_{\ell=3,4} \left( V_{\ell,1} d_{1,k}^\dagger c_{\ell,k} + V_{\ell,2} d_{2,k}^\dagger c_{\ell,k} + \text{H.c.} \right), \]  

(6)

\[ H_{\text{dot-SC}} = \sum_{\ell=3,4} \left( V_{\ell,1}^2 d_{1,k}^\dagger d_{1,k} + V_{\ell,2}^2 d_{2,k}^\dagger d_{2,k} + \text{H.c.} \right). \]  

(7)
\[ H_{\text{dot-sc}} = -\sum_x (V_{1d}^{\dagger}_x c_{1,-1} + V_2 d_{2,x}^\dagger c_{1,x}) + \text{H.c.}, \]  
and  
\[ H_{\Gamma} = -V_2 \sum_x (d_{2,x}^\dagger d_{2,x} + d_{2,x}^\dagger d_{1,x}). \]

In equations (2)–(8), \( d_{i,x}^\dagger \) (\( d_{i,x} \)) creates (annihilates) an electron with energy \( \epsilon_{i,\alpha} \) and spin \( s \) in the quantum dot \( i = 1, 2 \). \( c_{j,k}^\dagger \) (\( c_{j,k} \)) creates (annihilates) an electron with spin \( s \) in the \( j \)th site of the superconductors and \( c_{i,k}^\dagger \) (\( c_{i,k} \)) creates (annihilates) an electron with energy \( \epsilon_{k,\alpha} \) with spin \( s \) in the \( i \)th lead. Note that besides the \( s \)-wave pairing potential \( \Delta_2 \) of \( H_2 \), it also contains a Rashba spin–orbit interaction characterized by \( t_{SO} \) and the effect of an external magnetic field that produces the Zeeman energy splitting \( V_2 \). These three ingredients are important for the topological regime of the superconductor [28, 31]. The coupling \( V_{34} \) is assumed to be \( k \)-independent, for simplicity, and the leads are considered to be identical and characterized by a flat density of states \( \rho_0(\omega) = (1/2\pi)\Theta(D - |\omega|) \), where \( D \) is their half bandwidth. In the wide band limit, the influence of the lead on the dots is just a broadening \( \Gamma = \pi V^2 \Delta/2D \) in the quantum dot levels, where \( V_2 = V_4 = V \). The wide band limit for the leads assumed here just simplifies the equations but it is not mandatory. In this limit, our calculation fully accounts for the effect of the leads.

The topological phase of SC2, described by the Hamiltonian (4), is obtained [35] for \( V_2 > V_4^* \), where \( V_4^* = \sqrt{\mu^2 + \Delta^2/4} \), with \( \mu = \mu + t \). In this phase, SC2 holds one Majorana mode at each of its ends. In our case, one of the ends of the topological wire is coupled to QD2 and the Majorana mode leaks into it, as we have shown in recent studies [32, 36]. On the other hand, for \( V_2 < V_4^* \) the wire is in its trivial phase and no Majorana will be present.

### 2.2. Electron GF

To study the LDOS of the quantum dots we employ the GF method. Using equation-of-motion techniques we obtain a recursive expression for the GFs. We follow a similar approach to that described in [36] and define the retarded GF matrix as
\[ G_{ij}(\epsilon) \equiv \langle \langle A_i; B_j \rangle \rangle, \]
where \( A_i \) and \( B_j \) (with \( i \) and \( j \) denoting any site of the system, including the quantum dots) are any of the operators \( c_{i,\alpha}^\dagger, c_{i,\alpha}, c_{j,\beta}^\dagger, c_{j,\beta} \) and the double bracket stands for the Fourier transform of the double time GF defined as [37]
\[ \langle \langle A_i; B_j \rangle \rangle = \int_{-\infty}^{\infty} (-i)\Theta(\tau) \langle [A_i(\tau), B_j(\tau')] \rangle e^{i\epsilon\tau} d\tau. \]

Here \( \tau = t - t' \) and \([\cdot, \cdot]_1 \) denotes the anticommutator between two fermion operators. The GF (9) defines a \( 4 \times 4 \) matrix that is determined via the energy space equation of motion for its elements
\[ \epsilon \langle \langle A_i, B_j \rangle \rangle = \langle [A_i, B_j]_1 \rangle + \langle [A_i, H], B_j \rangle \].  

Since there are no many-body terms in the Hamiltonian, equation (11) allows us to obtain numerically exact results including all the contacts (see details in [36]). Once we have the local GFs, we can compute the LDOS of the quantum dots’ sites,
\[ \rho_{ij}(\epsilon) = -\frac{1}{\pi} \text{Im} \left[ \langle \langle d_{i,\alpha}, d_{j,\alpha}^\dagger \rangle \rangle \right], \]
which can be readily extracted from the matrix GF (9).

As far as interdot coupling is concerned, it is well known that our double quantum dot system exhibits two distinct regimes: the atomic regime, for \( V_{12} \ll \Gamma \), and the molecular regime, for \( V_{12} \gg \Gamma \). In the atomic regime, because the electrons are more bound to the individual quantum dot orbitals, the spectral properties of the system are better understood in terms of the LDOS given by equation (12). On the other hand, in the molecular regime (in which electrons are shared between the quantum dots) the spectral properties can be better understood in terms of the molecular density of states. To analyze the latter regime we define two molecular orbitals,
\[ d_\pm,s = \frac{1}{\sqrt{2}} (d_{1,s} \pm d_{2,s}) \]
which provide us with the molecular density of states
\[ \rho_{\pm,s}(\epsilon) = -\frac{1}{\pi} \text{Im} \left[ \langle \langle d_{\pm,s}, d_{\pm,s}^\dagger \rangle \rangle \right]. \]
This expression can be written in terms of the local and non-local quantum dot GFs as
\[ \rho_{\pm,s}(\epsilon) = \rho_{\pm,1}^2 + \rho_{\pm,2}^2 + \frac{1}{2\pi} \text{Im}[\langle \langle d_{1,\alpha}, d_{1,\alpha}^\dagger \rangle \rangle + \langle \langle d_{2,\alpha}, d_{2,\alpha}^\dagger \rangle \rangle], \]
where the non-local GFs, \( \langle \langle d_{1,\alpha}, d_{1,\alpha}^\dagger \rangle \rangle \) and \( \langle \langle d_{2,\alpha}, d_{2,\alpha}^\dagger \rangle \rangle \) appearing on the rhs of this expression are easily obtained by our procedure. Note that the interdot GF vanishes as \( V_{12} \to 0 \). Therefore, in this case, the molecular density of states is just the average of the quantum dot (‘atomic’) density of states.

### 2.3. Majorana GF

From the theoretical point of view, it is useful to define the Majorana GF
\[ M_{\alpha,\alpha}^{\dag}(\epsilon) \equiv \langle \langle \gamma_{\alpha,\alpha}^{\dagger}, \gamma_{\alpha,\alpha}^{\dagger} \rangle \rangle \quad (\text{for } \alpha = A, B), \]
where
\[ \gamma_{\alpha}^{\dagger} = \frac{1}{2} (f_{\alpha,s} + f_{\alpha,s}^\dagger) \]
\[ \gamma_{\alpha} = -\frac{i}{2} (f_{\alpha,s} - f_{\alpha,s}^\dagger) \]
are the Majorana operators having the property
\[ \gamma_{\alpha}^\dagger = (\gamma_{\alpha}^{\dagger})^T \]
and obeying the anti-commutation relation
Once we have obtained the electron GF, the definitions of the Majorana operators (17) and (18) allow us to write the retarded Majorana GF in terms of the regular and the retarded Gorkov’s GF as

$$\left[ \gamma^\dagger_{\alpha \sigma} \gamma^{\sigma}_{\alpha \sigma} \right]_+ = 2 \delta_{\alpha \sigma} \delta_{\alpha \sigma}. \quad (20)$$

We can now compute the Majorana local spectral function (MLSF) as

$$D_{\alpha \sigma}(\epsilon) = -\frac{1}{\pi} \text{Im} [M^r_{\alpha \sigma, \alpha \sigma}]. \quad (23)$$

Here, $f_{\alpha \sigma}$ represents any regular fermion in the system. In particular, for the quantum dots, $f_{\alpha \sigma}$ stands for $d_{\alpha \sigma}$. Although the MLSF cannot be directly accessed in experiments, it will help us to tell whether the electron density of states is composed of two Majorana modes or a single one.

3. Numerical results

To obtain our numerical results we will set the hopping to $t_1 = t_2 = t = 10$ meV and $\Gamma = 5.0 \times 10^{-3}t$. We also set $\tilde{q}_i = \tilde{q}_0 = 0$. Following previous studies with realistic parameters [28, 38], we set $\Delta_1 = \Delta_2 = 0.025t$, $t_{SO} = 0.07t$.

3.1. Single dot configuration

We first want to show that in the case of a single quantum dot coupled to a superconductor, a regime in which there is an MBS in the system, the ABSs are suppressed. To this end, let us consider in our system the situation in which the two quantum dots are decoupled from each other, by setting $V_{12} = 0$. Here we will show the suppression of the ABS in QD2 as SC2 is driven from its trivial to its topological phase. We do it by setting $V_2 = 0.05t$ and varying $\mu$. The results are shown in figures 2(a) and (b), where we show the color map of the density of states at QD2 versus $\epsilon$ and $\mu$. Here, in particular, we set $V_2 = 0.008t$ so that the Andreev levels become very separated and, therefore, more visible. For $\mu = 0$ we clearly see the ABS symmetrically placed about $\epsilon = 0$ for both spin species. The small splitting in the ABS is due to the Zeeman effect. Now, observe that as $\mu$ decreases from 0 to $-t$ the upper branch of the ABS is progressively suppressed (also for both spins). This is because the strong electron–hole asymmetry induced by the change of the chemical potential suppresses the probability of creating a hole in SC2. Interestingly, we note that, after the upper branch of the ABS has faded out, within a small range of $\mu$ (of the order of $V_2$), we see the appearance of a peak at $\epsilon = 0$ for spin down only (figure 2(b)) (note that this feature is not seen for spin up). This region is precisely the topological phase of SC2, in which the MBS leaks out from SC2 into QD2 (see discussion below). For a further decrease of $\mu$, SC2 returns to its trivial phase, in which there is no MBS or ABS. The peaks of figures 2(a) and (b) would be interchanged if we chose the opposite sign of $V_2$.

The small range of $\mu$ for which SC2 is found in its topological phase can be readily understood from the topological condition $V_2^2 > \mu^2 + \Delta^2$, or $\mu \in [-t - (V_2^2 - \Delta^2)^{1/2}, -t + (V_2^2 - \Delta^2)^{1/2}]$.

For $V_2 = 0.05t$ and $\Delta = 0.025t$ we expect the MBS to appear only for $\mu$ approximately within the interval $[-0.043t, -0.057t]$ (or, equivalently, $-\mu H$ within [0.957, 1.043]) as seen in figure 2(b). Note that the zero mode is limited, precisely within the two vertical dashed lines delimiting the calculated interval. The discontinuities are consistent with the topological phase transition already predicted in [19].

Now that we have shown the suppression of the ABS by the chemical potential, let us show how the ‘surviving’ peak evolves with $V_2$ towards the MBS. In figures 2(c) and (d) (for spin up and down, respectively) we show the density of states for QD2 versus $\epsilon$ and $V_2$ for a fixed value of $\mu = -1.01t$, which is inside the region delimited by the two vertical lines in figure 2(b). Note that, essentially, nothing changes for the spin up density of states. When $V_2$ surpasses $V_2^*$ there is a transition from the single to the tree-peak structure, in which the zero-energy peak corresponds to the MBS. The satellite peaks separate very quickly because the level of QD2 is strongly coupled in resonance with the MBS from the wire. These peaks correspond to the Majorana state that is split off from the one that remains at zero energy. We will discuss this in the next section, when it will be more visible with smaller
values of \( V_2 \). These results show that, indeed, the ABS and the MBS cannot coexist in a single quantum dot.

As we have already mentioned above, experimentally, the signature of these features can be seen in the zero-bias differential conductance in spectroscopy tunneling measurements, which provide a probe of the LDOS at zero energy. To accomplish this, one can place an STM tip on top of QD2 to measure the zero-bias conductance from the normal contact into lead 2 into the tip. The observed conductance is no ABS.

This plot is quite different from that one found in figures 2(c) and is progressively changed as the density of states. These curves correspond to a cut along \( \varepsilon = 0 \) in the panels of figure 2. All the other parameters are the same as those of figure 2.

As we have seen above, the separation between the satellite peaks in QD2 for the topological phase of SC2 is much larger than the Andreev splitting; therefore, to make the results more visible, we now set the coupling between the dots and the superconductors \( V_1 = 0.008 \) and \( V_2 = 0.002 \). For these parameters and \( V_{12} = 0 \) we have the following situation: QD1 will always exhibit ABSs because it is coupled to a normal superconductor. On the other hand, QD2 will show a single particle peak if SC2 is in its trivial phase \( (V_2 < V_Z) \) and a zero mode corresponding to the Majorana mode leaked from SC2 in addition to two split peaks, for \( (V_2 > V_Z) \). This three-peak structure was extensively studied in our previous studies [32, 36].

In figure 4 we show a color map of the LDOS of the quantum dots as a function of the energy \( \varepsilon \) (vertical axis) and the interdot coupling \( V_{12} \) (horizontal axis). Let us start by analyzing these results in the normal phase of the superconductor SC2 \( (V_2 < V_Z) \) top panels). In this regime, \( \rho_2 \) (figure 4(c)) has just one peak at \( \varepsilon = 0 \) while \( \rho_1 \) (figure 4(a)) has two peaks located symmetrically about \( \varepsilon = 0 \). These two peaks correspond to the ABSs discussed earlier. The single particle peak at \( \varepsilon = 0 \) observed in \( \rho_2 \) shows that QD2 is not affected by the superconductors. The absence of Andreev states in QD2 for \( V_{12} = 0 \) is due to the fact that the particle–hole asymmetry in the superconductor SC2 suppresses Andreev scatterings. As \( V_{12} \) increases, this scenario remains roughly unchanged in the atomic regime \( V_{12} < \Gamma \) and is progressively changed as the system enters its molecular regime \( V_{12} > \Gamma \). In the molecular regime we note that \( \rho_2 \) exhibits a four-peak structure very much similar to those of \( \rho_1 \). These peaks correspond to the ABSs that

3.2. Double dot configuration

Since MBSs and ABSs exist in the system in different regimes of the single dot structure, it is still interesting to investigate the possible interplay between these bound states with MBSs in the double quantum dot configuration. Here, SC1 is treated as a conventional superconductor (i.e. no spin–orbit, or Zeeman field), whereas SC2 is considered either in its normal phase \( (V_2 < V_Z) \) or in its topological phase \( (V_2 > V_Z) \), with \( V_Z = \sqrt{\mu^2 + \Delta^2} \). Then we make the coupling \( V_{12} \) finite and study SC2 in the trivial and in the topological phase. Hereafter we set \( \mu = -0.01 \) so that \( V_Z \approx 0.027 \) and use \( V_2 = 0.021 < V_Z \) for the trivial phase and \( V_2 = 0.051 > V_Z \) for the topological phase of SC2. As long as \( V_2 \) is larger or smaller than \( V_Z \), the results we will show are quite independent of \( V_2 \).

As we have seen above, the separation between the satellite peaks in QD2 for the topological phase of SC2 is much larger than the Andreev splitting; therefore, to make the results more visible, we now set the coupling between the dots and the superconductors \( V_1 = 0.008 \) and \( V_2 = 0.002 \). For these parameters and \( V_{12} = 0 \) we have the following situation: QD1 will always exhibit ABSs because it is coupled to a normal superconductor. On the other hand, QD2 will show a single particle peak if SC2 is in its trivial phase \( (V_2 < V_Z) \) and a zero mode corresponding to the Majorana mode leaked from SC2 in addition to two split peaks, for \( (V_2 > V_Z) \). This three-peak structure was extensively studied in our previous studies [32, 36].

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\(^{1}\) Different values of \( V_1 \) and \( V_2 \) would essentially modify the positions and the intensity of the Andreev peaks.
are split by the interdot coupling. Note that while the inner peaks are weaker in \( \rho_1 \) they are stronger in \( \rho_2 \), as compared to the outer ones. This is because the inner (outer) peaks of \( \rho_1 \) (\( \rho_2 \)) correspond to the ABS in QD2 (QD1) projected onto QD1 (QD2). The peaks appearing for positive and negative energies correspond to Andreev states on the ‘+’ and ‘−’ molecular orbitals, defined in section 2.1. We will come back to this point and show the molecular density of states later in this section.

The results for the topological regime of the superconductor SC2 (\( V_2 > V'_2 \)) are shown in figures 4(b) and (d). We note in figure 4(b) that \( \rho_1 \) is almost unchanged from the previous case in the atomic regime, with two Andreev peaks in \( \rho_1 \). However, a completely different structure is seen in \( \rho_2 \). Note that even for \( V_{12} = 0 \) we see the three-peak structure known to be an indication of the leaking of the Majorana zero mode from the topological wire into QD2 [32]. This scenario also remains roughly unchanged for the entire atomic regime (\( V_{12} < \Gamma \)). Note that, because here the value of \( V_2 \) is smaller than in figure 2, the satellite peaks are closer to each other as compared to those of figure 2(d) for \( V_2 > V'_2 \). Moreover, the satellite peaks observed in \( \rho_2 \) correspond to a Majorana state that is not bound to QD2. Theoretically we can make it clear when we look at the Majorana spectral function as shown in figure 5 (shown only for \( V_2 > V'_2 \)). Observe that they appear only in \( D_{B2} \) (figure 5(d)) while the zero-energy peak is seen only for \( D_{A2} \) (figure 5(c)). This shows that the nature of these peaks is completely distinct from the ABS. We should also emphasize that the zero-energy peak seen in figure 4(c) corresponds to a regular fermion state whereas the one in figure 4(d) corresponds to an MBS. Experimentally, the distinction between them can be made just by measuring the zero-bias conductance through QD2 while changing the energy level of QD2 in the regime of \( V_{12} \rightarrow 0 \). One would see that the conductance due to the Majorana peak would remain constant while in the regular fermion case it would show a peak. In fact, this corresponds to a remarkable signature of the MBS as one of us has discussed in [32].

The situation in the molecular regime (\( V_{12} > \Gamma \)) is the opposite. In this regime, we see a three-peak structure in \( \rho_1 \) and two peaks in \( \rho_2 \). Note that as \( V_{12} \) surpasses \( \Gamma \), the Majorana zero-energy peak dies off in QD2 and arises in QD1 (compare the zero-energy peaks in figures 4(b) and (d)). This can be attributed to a second leaking of the Majorana from QD2 into QD1. To support this interpretation, we now use the theoretical advantage of defining the Majorana GF. In figures 5(a) and (b) we show the spectral function of the Majorana operators \( \gamma_{\uparrow A1} \) (\( D_{A1} \)) and \( \gamma_{\downarrow B1} \) (\( D_{B1} \)), respectively, for QD1 and in figures 5(c) and (d), we show the same for QD2. By comparing \( D_{A2} \) with \( D_{B2} \) from figures 5(c) and (d), respectively, we see that for \( V_{12} < \Gamma \) there is a zero-energy peak in \( D_{A2} \) but none in \( D_{B2} \). On the other hand, there is no zero-energy peak in \( D_{A2} \) or in \( D_{B2} \) for \( V_{12} > \Gamma \). This indicates that there is no single localized Majorana mode in QD2. Now, if we look at the QD1 Majorana spectral function (figures 5(a) and (c)) we can see that there is no Majorana zero mode for \( V_{12} < \Gamma \). However, as \( V_{12} \) becomes larger than \( \Gamma \), while the Majorana \( D_{A2} \) peak disappears from QD2 it emerges at QD1, as shown in \( D_{A1} \). This is the second leaking we have mentioned above.

The reader may ask what happens to the density of states for the spin up. To answer this question, in figure 6 we show the spin up density of states for the same set of parameters as in figure 4. Again, let us first look at the trivial phase of SC2 (\( V_2 < V'_2 \)) shown in figures 6(a) and (c) for QD1 and QD2, respectively. Comparing these plots with the corresponding ones in figure 4 we see that they are very much similar. This is because in the trivial phase, SC2 is overall gaped and the Zeeman effect has no effect on the rest of the system, as we have pointed out earlier. On the other hand, when we look at the topological phase of SC2, shown in figures 6(b) and (d), and compare it with figures 6(a) and (c), we see some small effect for finite energy even in the spin up electrons. This can be understood in the following

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**Figure 5.** Color map of the spin down Majorana spectral function (in unity of \( \Gamma \)) at QD1 (left) and QD2 (right) versus the energy and the interdot coupling \( V_{12} \). The top and lower panels show the results for the topological phase of wire 2, when we have an MBS. By comparing \( D_{A1} \) with \( D_{B1} \) for the same quantum dot at the same energy, a peak appearing in only one of those shows there is a single Majorana mode. See discussion in the text.

**Figure 6.** Color map of the spin up LDOS (in unity of \( \Gamma \)) of QD1 (left) and QD2 (right) as a function of the energy and the interdot coupling \( V_{12} \) for the same set of parameters as in figure 4.
way: because we have chosen $V_2$ to be positive, the topological wire is strongly polarized with spin down. Therefore, the coupling between electrons with spin up in the dot and the Majorana in SC2 is strongly suppressed. However, for finite $V_{12}$ QD2 is indirectly coupled to the normal superconductor SC2 via QD1 and an electron with spin up in the dot can couple to the Majorana mode via Andreev scatterings in SC1. The effect is rather small since this corresponds to very high order processes. This can also be seen in figure 7, where we show the spin up Majorana spectral functions. Note that the spin up Majorana spectral functions for the QD2 shown in figure 7(c) exhibit a signal of the zero mode coming from the spin down component.

To support our argument that in the molecular regime the Andreev states are bound to the molecule, while the Majorana mode is bound to a particular quantum dot (QD2, in our case), let us show the density of states for the molecular orbitals (defined in equation (15)). In figure 8 we show the molecular density of states for spin up (top) and down (bottom) and both molecular orbitals (left and right). Note that for $V_{12} < \Gamma$ we see (for both orbitals) three peaks for the spin up density of states and five peaks for the spin down. This is because in this regime, the molecular orbital corresponds, essentially, to the arithmetic mean value of the quantum dot density of states shown previously. The central peak for spin down, corresponding to the Majorana state bound to QD2, now appears on both molecular orbitals. The molecular density of states is more useful for $V_{12} \gg \Gamma$. In this regime, we note that for spin up (figures 8(a) and (c)) there are peaks only for negative energies in $\rho^\downarrow_s$, whereas only positive energy peaks appear in $\rho^\uparrow_s$. Similarly, $\rho^\uparrow_s$ and $\rho^\downarrow_s$ (figures 8(b) and (d), respectively) exhibit similar upper and lower branches of the peaks but with slightly more complex structures, because of the splitting of the central peak due to the interdot coupling, but the positive and negative energy peaks appear only in the ‘−’ and ‘+’ molecular orbitals, respectively. For $V_{12} \ll \Gamma$ their position in the energy increases almost linearly with $V_{12}$, which is characteristic of molecular orbitals. Interestingly, we note that there is a zero-energy peak that remains in both molecular orbitals. This indicates that this state is always bound to a quantum dot. Indeed, as we have seen previously, this zero-energy peak corresponds to the Majorana mode bound to QD2.

As we have done in the single dot configuration, we now discuss how these features of the double dot configuration could be observed within the currently available experimental technology. This has to be done via local $dI/dV$ measurement as in [6]. This is because in this configuration, the transport measurement between our lead 3 and 4 would not provide a local spectroscopy of the density of states of the quantum dots, individually. Therefore, as with the single dot configuration, the STM tip can be placed on top of an individual quantum dot. The zero-energy feature of our plots could be obtained experimentally by fixing the gate voltage of the dots and controlling the interdot coupling, while measuring $dI/dV$ from the leads into the STM tip. Figure 8 shows the zero-energy LDOS versus the interdot coupling for both the trivial and topological phases of SC2 for each quantum dot, individually. The features seen in this figure were already present in the previous one but here, some of them are more apparent and deserve to be discussed. First, as we already noted earlier, we see that in the trivial regime ($V_2 < V_2^*$), even though $V_2$ is finite the density of states is degenerate for spin up and down. This is because the application of a small Zeeman field in SC2 does not affect the LDOS of the dots since there are no in-gap states of SC2 that couple to the dot. This is not the case in the topological phase of SC2 in which there is an MBS. Further, note the difference between the LDOS of QD1 and QD2. Note that for $V_{12} \ll \Gamma$, $\rho^\uparrow_s(0) \ll \rho^\downarrow_s(0)$ (top panels). The suppression of $\rho^\downarrow_s(0)$ for $V_{12} < \Gamma$ results from the presence of ABSs in QD1. For $V_{12} \gg \Gamma$, we see that both $\rho^\uparrow_s(0)$ (both spins) decrease as the ABSs take over the entire molecule. In the topological regime (bottom), the presence of the MBS leaked into QD2 is manifested for $V_2 = 0$ as $\pi \Gamma \rho^\uparrow_s(0) = 1/2$, in agreement with what some of us have reported in [32]. As $V_{12}$ increases, we see...
that $\rho^\uparrow_2(0)$ decreases while $\rho^\downarrow_1(0)$ increases, approaching $1/2$, because the MBS leaks into QD1. Finally, as a remarkable signature of the MBS, when we look only into QD1 we note that as $\rho^\downarrow_1(0)$ decreases, $\rho^\uparrow_1(0)$ also decreases for $V_{12} \gg \Gamma$, which produces strong polarization that could be detected using a spin-polarized STM tip.

Another interesting point is that the signature of the topological quantum phase transition is still seen in the LDOS in the double dot configuration. To show this, in figure 10 we show the zero-energy density of states of the individual quantum dots versus $V_z$ for both the atomic ($V_{12} = \Gamma/2$) and the molecular regime ($V_{12} = 5\Gamma$) in the top and lower panels, respectively. In the atomic regime (top panels) we see a jump in $\rho^\downarrow_1(0)$ at $V_z = V_2$. On the other hand, in the molecular regime (lower panels) the jump is overwhelmingly more pronounced in $\rho^\downarrow_1(0)$ (figure 10(b)) than the one observed in $\rho^\uparrow_2(0)$ (figure 10(d)). For the spin up LDOS (diamonds (blue)), for both regimes and in both QDs we do not see any substantial change. The small jump in $\rho^\downarrow_1(0)$ noted in figure 10(d) (diamond (blue) line) results from a weak mixture of spin up and down in the molecular regime due to Andreev scatterings. The results shown in figure 10 tell us that the topological quantum phase transition, well discussed in the single dot case, manifests itself even when MBSs and ABSs coexist in the double dot configuration. Moreover, as in the single dot system, these features can be experimentally accessed in a simple spectroscopic tunneling measurement.

4. Conclusion

In summary, we have studied the appearance of ABSs and MBSs in a double quantum dot system. By studying the decoupled quantum dot configuration, we have shown that the MBS and the ABS cannot coexist in a single dot. This is because in the low-density regime (necessary for the topological phase of the superconductor) the electron–hole asymmetry suppresses the ABS. In the coupled dot configuration, one of the quantum dots (QD1) is coupled to a conventional superconductor that provides ABSs while the other (QD2) is coupled to a topological superconductor, providing the MBS in its topological phase. We show that in the trivial phase of SC2, in the atomic limit of the system—where the interdot coupling is much smaller than the level broadening of the quantum dots ($V_{12} \ll \Gamma$)—QD1 exhibits ABSs while QD2 exhibits a regular fermion state broadened by $\Gamma$. When the system is brought into its molecular regime ($V_{12} \gg \Gamma$), the ABSs take over the entire molecule. More interesting behavior occurs in the topological phase of SC2. In this situation, we show that for $V_{12} \ll \Gamma$ there are ABSs in QD1 for both spin components, while in QD2 we find an MBS for spin down and ABSs for spin up. In the molecular regime, on the other hand, the MBS leaks from QD2 into QD1, while the ABS can be seen in the entire molecule for the spin up component. These results reveal that, in contrast to the single dot case, the MBSs and ABSs coexist; while ABSs can appear in molecular orbitals, MBSs are always bound to an atomic orbital. Another important feature that merits being highlighted here is the remarkable signature of the topological quantum phase transition, manifested as a sharp jump in the zero-energy LDOS of the quantum dots, and persisting even in the double dot case, in which the MBSs and ABSs coexist. Finally, we believe our results are relevant from both the theoretical and experimental viewpoints and should stimulate future spectral tunneling measurements to detect the signatures of MBSs and ABSs in the double dot system proposed here.

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