Majorana molecules and their spectral fingerprints

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We introduce the concept of a Majorana molecule, a topological bound state appearing in the geometry of a double quantum dot (QD) structure flanking a topological superconducting nanowire. We demonstrate that, if the Majorana bound states (MBSs) at opposite edges are probed nonlocally in a two probe experiment, the spectral density of the system reveals the so-called half-bowtie profiles, while Andreev bound states (ABSs) become resolved into bonding and antibonding molecular configurations. We reveal that this effect is due to the Fano interference between pseudospin superconducting pairing channels and propose that it can be caught by a pseudospin resolved Scanning Tunneling Microscope (STM)-tip.

I. INTRODUCTION

The recent decade witnessed the increasing interest of the condensed matter community in Majorana physics. In particular, the concept of Majorana bound states (MBSs) as promising building blocks for topologically protected and fault-tolerant quantum computing received special attention [1–6]. MBSs are zero-modes appearing at topological boundaries of condensed matter systems with spinless $p$-wave superconductivity, as it was first predicted by A. Y. Kitaev in his seminal work [7]. They manifest themselves via zero-bias peak (ZBP) signature in local conductance measurements [8]. As candidates for hosting nonlocal MBSs, such material platforms as ferromagnetic atomic chains [9–11] and semiconductor hybrid nanowires [8, 20–23] were proposed. Isolated MBSs are also supposed to be attached to cores of superconducting vortices [24, 25].

Interestingly enough, the Majorana quasiparticle detection can be done by determining transport quantities through a single quantum dot (QD) [26–30]. As examples of such, we highlight the electrical shot-noise [31, 32] and the thermoelectric properties [33–36]. Although the former cannot fully trace the QD density of states (DOS), it is specially helpful in introducing a full counting statistics of charge tunneling events, which is unique for Majorana systems [30]. Further, the shot-noise allows in distinguishing a nontopological ZBP from the corresponding topological [31]. It also reveals that the fractional value of the effective charge, by means of current fluctuations, thus depends on the system bias-voltage [32]. Additionally, the differential quantum noise shows that the photon absorbed spectra by a MBS shows a universal behavior, being frequency and bias-voltage independent [33]. Similarly, the zero-bias limit of the thermoelectric properties present striking features. The thermopower enhancement [34, 35] and according to some of us, the possibility of a tuner of heat and charge assisted by MBSs [36], are just few examples of such.

Astonishingly, upon attaching an extra QD, the control of the MBS leakage [27] into QDs becomes feasible [37, 38]. According to Jesus D. Cifuentes et al. [37], in several geometric arrangements of QDs, known as “parallel”, “in-series” and “T-shaped”, the spatial manipulation of a MBS is allowed. On the grounds of the pseudospin, this switching is revealed as the cornerstone for the Majorana fermion qubit cryptography, as proposed in Ref. [39] by some of us. This cryptography arises from the delicate interplay between Fano interference [39, 40] and topological superconductivity.

Noteworthy, the pseudospin has been guided the interpretation of the transport through spinless two-level QD and double-QD systems [41–43]. Specially in the latter, the Kondo effect is induced by an interdot Coulomb correlation [43]. It is worth mentioning that, the pseudospin consists of mapping the system orbital degrees of freedom into those equivalent to the spin components of its spin-1/2 counterpart, i.e., by projecting them along the quantization of the pseudospin axis [41]. We highlight that these peculiar degrees of freedom are experimentally detectable by the pseudospin resolved transport spectroscopy [44].

Concerning the Fano interference in the presence of MBSs and QDs with a plethora of intriguing characteristics [45–54], special attention should be paid to the findings of Ref. [47] by J.-J. Xia et al.. Their results reveal that the conductance through two QDs obeys in an elegant manner, and within the low bias-voltage limit, a Fano-like expression [39, 40]. Surprisingly, this expression is dressed by the QD-wire couplings and a Fano parameter of interference, which is dependent upon the MBSs overlapping. Therefore, such an analysis offers an attractive experimental strategy, clearly supported by the Fano effect, in recognizing MBSs far apart in superconducting wires, as well as in estimating how topological these MBSs are.

In this work, distinct from Refs. [37, 38, 47], by including the nonlocality degree of MBSs [28], we propose the concept of a Majorana molecule within the pseudospin.
dospin framework \[41-43\]. It is worth citing that, such a nonlocality feature is a key ingredient for reproducing experimental results \[23-28\]. Then, this molecule appears in the configuration similar to those considered in the end of Ref. \[23\], but with spectral fingerprints probed by a dospin resolved Scanning Tunneling Microscope (STM)-tip, similarly to Ref. \[29\] and schematically shown in Fig.1(a) of the current paper. It consists of a one-dimensional (1D) topological superconductor (TSC) hosting MBSs at the edges, which hybridize with normal fermionic states of a pair of QDs flanking the TSC wire, placed in the strong longitudinal magnetic field. If the latter is strong enough, so that Zee- man splitting becomes much larger than all other characteristic energies of the system, the spinless condition is fulfilled. In this case, the tuning of the parameters of the system leads to a crossover between the well-known regime of individual Andreev bound states (ABS) \[24\] (The Majorana molecule turned-off), and the regime in which one witnesses the splitting of the ABS into bonding and antibonding molecular configurations (The Majorana molecule turned-on). The formation of these states can be described in terms of the so-called pseudospins \((\uparrow, \downarrow)\), which determine the structure of the QDs orbitals by means of superconducting parings in these channels. Note that, contrary to the single QD geometry considered before \[23,28\], in our setup the QDs act as a nonlocal two-probe detector which catches the Fano interference effects between various tunneling paths, including those involving the MBSs.

We demonstrate that, similar to what happens in the system of a pair of QDs placed within a semiconductor \[55\] or a Dirac-Weyl semimetal host \[55,57\], the Fano effect in the considered system defines the novel type of molecular binding of QD orbitals, and leads to the formation of a Majorana molecule, characterized by the so-called half-bowtie profiles in the spectral density of states.

II. THE MODEL

The geometry we consider is shown in the Fig.1(a). The system under study consists of an STM-tip perturbatively coupled to the 1D-TSC nanowire with nonlocal MBSs formed at its edges and flanked by a pair of QDs, where the latter are attached to metallic leads. We suggest that the external magnetic field applied along the direction of the wire is large enough, so that only spin up states lie below the Fermi energy, and spin down states can be just totally excluded from the consideration \[23,27,36\]. We account for the possible coupling between MBSs localized at the opposite edges of the TSC wire, which can change their nonlocality degree and lead to the crossover between highly nonlocal MBSs and more local ABSs.

The Hamiltonian of the system reads:

\[\mathcal{H} = \sum_{\alpha k} \varepsilon_{\alpha k} \hat{c}_{\alpha k}^\dagger \hat{c}_{\alpha k} + \sum_{\alpha} \varepsilon_{\alpha} \hat{d}_{\alpha}^\dagger \hat{d}_{\alpha} + t_c (\hat{d}_{L}^\dagger \hat{d}_{R} + H.c.) + \mathcal{V} \sum_{\alpha k} (\hat{c}_{\alpha k}^\dagger \hat{d}_{\alpha} + H.c.) + \lambda_{L1} (\hat{d}_{L}^\dagger - \hat{d}_{L}) \Psi_1 + \lambda_{L2} (\hat{d}_{L} + \hat{d}_{L}^\dagger) \Psi_2 + \lambda_{R1} (\hat{d}_{R} + \hat{d}_{R}^\dagger) \Psi_2 + \lambda_{R2} (\hat{d}_{R}^\dagger - \hat{d}_{R}) \Psi_1 + i \varepsilon_M \Psi_1 \Psi_2, \]

where the operators \(\hat{c}_{\alpha k}, \hat{d}_{\alpha}\) correspond to electrons in the right and left metallic leads \(\alpha = L,R\) having momentum \(k\) and energy \(\varepsilon_{\alpha k} = \varepsilon_k - \mu_{\alpha}\), with \(\mu_{\alpha}\) the corresponding chemical potential. The operators \(\hat{d}_{\alpha}^\dagger, \hat{d}_{\alpha}\) describe the localized orbitals in the right and left QDs with energies \(\varepsilon_{\alpha}\), \(t_c\) is the hopping term corresponding to the normal direct tunneling between the QDs, which can lead to the formation of usual molecular orbitals \[55\] and \(\mathcal{V}\) describes the strength of the coupling between the QDs and the leads (we take it equal for right and left QDs). At the edges of the TSC wire, the nonlocal MBSs described by the operators \(\Psi_j = \Psi_j^\dagger\) couple to the QDs with the amplitudes \(\lambda_{\alpha j}\) with \(j = 1,2\) (the ratio \(\eta_\alpha = |\lambda_{\alpha 1}/\lambda_{\alpha 2}|\) defines the nonlocality degree) and to each other via the overlap term \(\varepsilon_M\).
forms a regular fermionic state.

Performing the rotation in the pseudospin space $\sigma = \pm 1 (\uparrow, \downarrow)$, with the two leads at the same chemical potential $\mu_L = \mu_R = 0$ [23], corresponding to R and L states, $d_L^\dagger = \cos \theta_{d_L} - \sin \theta_{d_L}$, $d_R^\dagger = \sin \theta_{d_R} + \cos \theta_{d_R}$, $\tilde{c}_{kL} = \cos \theta_{ckL} - \sin \theta_{ckL}$, $\tilde{c}_{kR} = \sin \theta_{ckR} + \cos \theta_{ckR}$ with

$$\theta = \frac{\pi}{4} + \frac{1}{2} \arcsin \frac{\Delta \varepsilon}{\sqrt{4(t_c)^2 + (\Delta \varepsilon)^2}}$$

(3)

and $\Delta \varepsilon = \tilde{\varepsilon}_L - \tilde{\varepsilon}_R$, the Hamiltonian of the system can be rewritten as:

$$\mathcal{H} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} \varepsilon_{d\sigma} d_{\sigma}^\dagger d_{\sigma} + \sum_{\sigma} V \varepsilon_{\sigma} (c_{k\sigma}^\dagger d_{\sigma} + \text{H.c.})$$

$$+ \varepsilon_M (f^\dagger f - \frac{1}{2}) + \sum_{\sigma} (\nu_{d\sigma} d_{\sigma}^\dagger f + V_{d\sigma} f d_{\sigma} + \text{H.c.}),$$

(4)

where $\varepsilon_{d\sigma} = \frac{\delta_{L,R} \varepsilon_{e\sigma}}{2} - \frac{\varepsilon_{e\sigma}}{2} \sqrt{4(t_c)^2 + (\Delta \varepsilon)^2}$, $\nu_{d\sigma} = \frac{1}{\sqrt{2}} [(\lambda_{R2} \mp \lambda_{L1}) \sin \theta + (\lambda_{L1} \mp \lambda_{R2}) \cos \theta]$ and $\nu_{d\sigma} = \frac{\varepsilon_{e\sigma}}{2} [(\lambda_{R2} \mp \lambda_{L1}) \cos \theta - (\lambda_{L1} \mp \lambda_{R2}) \sin \theta]$.

The Hamiltonian given by Eq. (4) corresponds to the mapping of the original problem to one equivalent to a single spinor QD coupled to fermionic state $\mu$ and characterized by the following mixture of states: the amplitudes $\nu_{\uparrow\downarrow}$ correspond to the formation of delocalized Cooper pairs $(d_{\sigma} f)$, while the terms $\nu_{\uparrow\downarrow}$ give the normal couplings between the effective QD and $f (d_{\sigma} f^\dagger)$.

By making explicit the pseudospin basis, we recognize the symmetric $d_L^\dagger = \sin \theta_{dL} + \cos \theta_{dL}$ and antisymmetric $d_L^\dagger = \cos \theta_{dL} - \sin \theta_{dL}$ superpositions as the bonding and antibonding molecular states, respectively, due to the linear combination of atomic orbitals (LCAO) between $d_L^\dagger$ and $d_R^\dagger$. Strictly for $t_c = 0$, note that from Eq. (4), $\theta = \frac{\pi}{4} (\theta = 0)$ when $\Delta \varepsilon \to 0^+ (\Delta \varepsilon \to 0^-)$ leading to the breaking down of the LCAO. As we are interested in the pairing dominated by the MBSs, in the following discussion, we will consider then the case of identical QDs weakly coupled. It corresponds to $\tilde{\varepsilon}_L = \tilde{\varepsilon}_R = \varepsilon_{d}$ and $t_c \to 0$, but finite as in Ref. [58], thus giving rise to $\theta = \frac{\pi}{4}$ as shown in Fig. 2(a) of Sec. III, where we present the profile of Eq. (3) as a function of $\Delta \varepsilon$ for several $t_c$ values.

The QD states corresponding to the opposite pseudospins are now simply symmetric and antisymmetric combinations between the orbitals of right and left QDs:

$$d_{\uparrow} = \frac{d_R + d_L}{\sqrt{2}}$$

$$d_{\downarrow} = \frac{d_R - d_L}{\sqrt{2}},$$

(5)

which represent the bonding and antibonding molecular states with the energies $\varepsilon_{d\uparrow} = \varepsilon_{d} - \sigma t_c$, respectively.

Moreover,

$$V_{\uparrow\dagger} = \frac{\lambda_R - \lambda_L \pm (\lambda_{R1} + \lambda_{L2})}{2}$$

(6)

and

$$V_{\dagger\dagger} = \frac{\lambda_R - \lambda_L \pm (\lambda_{R1} - \lambda_{L2})}{2}.$$
the system energy scale) and low bias-voltage $eV \rightarrow 0$ ($eV \ll \Gamma$), $\mathcal{G} \propto \int d\omega \text{LDOS}(\omega) \left\{ -\frac{1}{\pi} n_F(\omega - eV) \right\} \approx \text{LDOS}(eV)$, with $n_F$ as the Fermi-Dirac distribution and $\left\{ -\frac{\partial}{\partial \omega} n_F(\omega - eV) \right\} \approx \delta(\omega - eV)$. This means that the conductance becomes ruled by the Local Density of States (LDOS) evaluated at the tip chemical potential $\mu_{\text{tip}} = eV = \omega$. For the STM-tip placed over the left (right) QD, the LDOS behavior will be determined by pseudospin becomes naturally resolved. Noteworthy, we clarify that the quantitative evaluation of the LDOS spatial dependence along the 1D-TSC is not the focus of the current work, once it requires to adopt the Kitaev chain explicitly in the approach.

To evaluate $\langle \langle d_\text{l}, d_\text{r}^\dagger \rangle \rangle$, we apply the equation-of-motion method \cite{60} to Eq.\,(4), which gives:

$$ (\omega + i0^+) \langle \langle d_\text{l}, d_\text{r}^\dagger \rangle \rangle = \delta_{\sigma\sigma'} + \langle \langle [d_\text{l}, \mathcal{H}] ; d_\text{r}^\dagger \rangle \rangle. $$

(13)

The last term in the Eq.\,(13) will generate the anomalous Green functions $\langle \langle d_\text{l}, d_\text{r}^\dagger \rangle \rangle$. As the Hamiltonian is quadratic, the system of equations can be closed and written in the matrix form as

$$ A^\sigma(\omega) \langle \langle d_\text{l}^\dagger ; d_\text{r}^\dagger \rangle \rangle \langle \langle d_\text{l} ; d_\text{r}^\dagger \rangle \rangle \langle \langle d_\text{l}^\dagger ; d_\text{r} \rangle \rangle = (1 \ 0 \ 0 \ 0)^T, $$

$$ A^\sigma(\omega) = \begin{bmatrix} a_\sigma(\omega) & -k_2^\sigma(\omega) & k_1^\sigma(\omega) & k_2^\sigma(\omega) \\ -k_2^\sigma(\omega) & a_\sigma(\omega) & k_1^\sigma(\omega) & k_2^\sigma(\omega) \\ k_1^\sigma(\omega) & k_1^\sigma(\omega) & b_\sigma(\omega) & -k_2^\sigma(\omega) \\ k_2^\sigma(\omega) & -k_2^\sigma(\omega) & b_\sigma(\omega) & (\omega + i0^+) \end{bmatrix}, $$

(14)

where $a_\sigma(\omega) = -\sigma k_1^\sigma(\omega) = \nu_\sigma \nu_\sigma^+(\omega + \epsilon_\text{M})^{-1} + \nu_\sigma^+ \nu_\sigma^-(\omega + \epsilon_\text{M})^{-1}, k_2^\sigma(\omega) = \nu_\sigma \nu_\sigma^+ \nu_\sigma \nu_\sigma^-(\omega + \epsilon_\text{M})^{-1} + \nu_\sigma^+ \nu_\sigma \nu_\sigma^+ \nu_\sigma^-(\omega + \epsilon_\text{M})^{-1}, a_\sigma(\omega) = -\epsilon_d - k_2^\sigma(\omega) + i\Gamma$ and $b_\sigma(\omega) = \omega - \epsilon_d - k_2^\sigma(\omega) + i\Gamma$.

III. RESULTS AND DISCUSSION

We assume $\Gamma = 40\mu eV$ \cite{27} as the energy scale of the model parameters of the system. In Fig.\,(2a) we present Eq.\,(3) as a function of $\Delta \omega$, which shows that the pseudospin mapping is applied to $\theta = \frac{\pi}{2}$, when $t_c \rightarrow 0$, but finite for the experimental condition $\Delta \omega = 0$. This point defines the scenario adopted in this work for the evaluation of the spectral analysis.

Our aim is to investigate the spectral function of the considered system defined by the Eq.\,(3). To better understand the situation qualitatively, we start from the geometry wherein only the left QD is strongly coupled to MBSs, i.e., from the Majorana molecule turned-off scenario. We present the results for both the case of highly nonlocal MBSs \cite{27} (Fig.\,(2b)) and the case of overlapping MBSs (Fig.\,(2f)). For both cases we present the 2D plots of the spectral functions in the $\omega$ and $\epsilon_d$ axes.

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Figure 2. (Color online) The Majorana molecule turned-off scenario. Color maps of the spectral density of the QDs spanned by $\omega$ and $\epsilon_d = \epsilon_d = \epsilon_d$. Panel (a) shows Eq.\,(3) for $\theta$ as function of $\Delta \omega$, which points out that for two identical weakly coupled QDs ($t_c \rightarrow 0$, but finite as in Ref.\,[58]), Eq.\,(4) should be evaluated at $\theta = \frac{\pi}{2}$. Panels (b)-(e) correspond to the case of a right QD weakly coupled to the MBSs, $\lambda_{\text{L1}} = 3\Gamma$ and $t_c = \lambda_{\text{L2}} = \lambda_{\text{R1}} = \lambda_{\text{R2}} = \epsilon_d = 10^{-5}\Gamma$. In panel (b) the density plot of $\tau_{\text{LL}}(\omega)$ demonstrates clearly visible horizontal bright line, corresponding to the ZBP due to the coupling with the MBS $\Psi_1$, which is robust against changes in $\epsilon_d$ \cite{27}. In panel (c) the spectral density $\tau_{\text{RR}}(\omega)$ reveals solely the resonant level of the right QD, weakly coupled to the MBSs at $\omega = \epsilon_d$. In this regime, Fano interference between the QDs is absent and $\tau_{\text{LR}}(\omega) = \tau_{\text{RL}}(\omega) = 0$. Panels (d) and (e) show $\tau_{\text{RR}}(\omega) \rightarrow \tau_{\text{L1}}(\omega)$ and $\tau_{\text{RL}}(\omega) \rightarrow \tau_{\text{L1}}(\omega)$ respectively, which reveal clear signatures of constructive and destructive Fano interference. Panel (f) accounts for the coupling of the left QD to the overlapping MBSs ($\lambda_{\text{L1}} = 3\Gamma$, $\lambda_{\text{L2}} = 0.001\Gamma$, $t_c = \lambda_{\text{R1}} = \lambda_{\text{R2}} = 10^{-5}\Gamma$ and $\epsilon_d = 2\Gamma$). In this case the density plot of $\tau_{\text{LL}}$ reveals the transformation of the horizontal bright line, corresponding to the ZBP, into a bowtie profile, characteristic for split ABSs \cite{29}.
Majorana molecule is not formed.

Now, we can consider the symmetric case sketched in Fig.1(a) with $t_c = 10^{-5}\Gamma$, $\lambda_{L1} = \lambda_{R1} = 3\Gamma$, $\lambda_{L2} = \lambda_{R2} = 1.5\Gamma$ and $\varepsilon_M = 0.05\Gamma$, corresponding to The Majorana molecule turned-on scenario: both QDs are coupled to both MBSs, and thus interfere with each other through the 1D-TSC. In this situation, a bowtie-like signature emerges in the spectral density $\tau_{LR(RR)}(\omega)$, as it can be seen from Fig.3(a). Moreover, the features characteristic to usual molecular binding can be seen, as upper and lower arcs provided by the coupling of the QD states, visible in Fig.2(f), become split in Fig.3(b) due to the TSC-mediated overlap of the states of right and left QDs. Naturally, this leads to $\tau_{RL}(\omega) = \tau_{LR}(\omega) \neq 0$ (see Fig.3(b)), which, according to the Eqs. (11) and (12), means that $\tau_{\uparrow\downarrow}(\omega) \neq \tau_{\downarrow\uparrow}$ and $\tau_{\downarrow\uparrow}(\uparrow\downarrow)(\omega) = 0$.

Physically, this means that spin up and spin down channels become decoupled in the pseudospin basis and a Majorana molecule, which is a bonding or antibonding superposition of ABSs is formed. The latter manifest themselves in the spectral profiles of $\tau_{\uparrow\downarrow}(\omega)$ and $\tau_{\downarrow\uparrow}(\omega)$ shown in Figs.3(c) and (d), respectively as half-bowtie signatures. They are consequences of the Fano interference between $\tau_{LR}(\omega)$ and $\tau_{RL}(\omega)$, shown in Fig.3(b). Note that the latter contains both peaks and pronounced Fano dips, which interfere constructively or destructively depending on the sign in the Eqs. (11) and (12), with the peaks in the spectral densities of $\tau_{\uparrow\downarrow}(\omega)$ and $\tau_{\downarrow\uparrow}(\omega)$, which gives in the end the mentioned half-bowtie profiles.

In terms of the effective Hamiltonian [Eq. (11)], the considered regime corresponds to the case when $|V_{\downarrow\uparrow}^-| \neq 0$, $|V_{\uparrow\downarrow}^-| = 0$, $|V_{\downarrow\uparrow}^+| = 0$ and $|V_{\uparrow\downarrow}^+| \neq 0$. This means that only the pseudospin Cooper pairing $d_\uparrow f$ and normal electron tunneling $d_\downarrow f^\dagger$ contribute to the transport assisted by the formation of Majorana molecules.

IV. CONCLUSIONS

In summary, we have proposed the concept of a Majorana molecule, a bonding or antibonding state appearing in the system of a pair of QDs flanking a 1D-TSC nanowire. The coupling between QDs is achieved via the channel provided by the presence of MBSs. It is demonstrated that these states manifest themselves via half-bowtie spectral fingerprints in the spectral density of states, which are qualitatively different from full bowtie profiles, characteristic to the case of a single QD. Such features can be measured by an STM-tip, which becomes naturally pseudospin resolved, once the QDs behave as a nonlocal two-probe detector of the Fano interference assisted by the MBSs.

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