Can Caroli-de Gennes-Matricon and Majorana vortex states be distinguished in the presence of impurities?

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Majorana zero modes states (MZMs) are predicted to appear as bound states in vortices of topological superconductors. MZMs are pinned at zero energy and have zero charge due to particle-hole symmetry. MZMs in vortices of topological superconductors tend to coexist with other subgap states, named Caroli-de Gennes-Matricon (CdGM) states. The distinction between MZMs and CdGM is limited since current experiments rely on zero-bias peak measurements obtained via scanning tunneling spectroscopy. In this work, we show that a local impurity potential can push CdGM states to zero energy. Furthermore, the finite charge in CdGM states can also drop to zero under the same mechanism. We establish, through exploration of the impurity parameter space, that these two phenomena generally happen in consonance. This means that energy and charge shifts in CdGM may be enough to imitate spectroscopic signatures of MZMs.

Introduction. Braiding of non-Abelian anyonic quasiparticles is a possible platform for topological quantum computation [1]. Currently, Majorana zero modes [2] (MZMs) are the leading candidates for implementing topological quantum computing protocols, and several proposals for the realization of MZMs in condensed matter systems were proposed [3, 4]. Particularly, MZMs were predicted to exist as zero-energy states in the interior topological superconductor vortices [5–8].

An irrefutable observation of MZMs remains elusive [9–14]. Since MZMs are zero-energy states, the typical experiments aiming to detect them in vortices rely on the observation of a zero-bias conductance peak via scanning tunneling spectroscopy [10, 15–18]. However, MZMs belong to a class of low-energy excitations in superconductors known as Andreev bound states [19]. This class include a variety of topologically trivial states, such as Yu-Shiba-Rusinov states, bound states in superconducting weak links, and Caroli-de Gennes-Matricon states (CdGM) [19–24]. Under the right conditions, e.g. in the presence of disorder or external fields, these trivial states may appear as zero-energy excitations as well [14, 16, 19, 24, 25]. Thus, spectroscopic measurements are necessary but insufficient signature of Majorana quasiparticles [9, 10].

In particular, CdGM states are trapped in vortices are predicted to co-exist with Majorana zero modes in topological superconductors [19]. In a trivial superconductor, these in-gap excitations have a spectrum given by [20] (see Fig. 1 (a, b)): 

\[ E_m = \frac{m\Delta_0^2}{\mu}, \]  

with \( m \in \mathbb{Z}^* \), \( \mu \) the chemical potential, and \( \Delta_0 \) the bulk superconducting pairing potential of the system. Hence, trivial CdGM states are predicted to appear as finite-energy excitations in the measured spectrum. Therefore, it is often assumed that, with adequate experimental precision, it is possible to differentiate these trivial states

![FIG. 1. Sketch of the spectrum of states inside the vortex for a (a) clean \( p \)-wave system and (b) a \( s \)-wave system with and without a screen charge impurity. The blue line shows the position dependency of the superconducting order parameter, the dashed lines schematically show the energy of in-gap CdGM states, and the black arrow indicates the energy shift cause by the impurity potential. In panel (b), red dashed lines indicate the CdGM spectrum in the absence of a charge impurity, whereas the spectrum with a impurity is shown in black. Density of states (black) and charge (red) for (c) \( p \)-wave system and (d) \( s \)-wave system with impurity.](image-url)
from Majorana excitations with tunneling spectroscopy measurements [26–28]. It seems unreasonable, however, to believe that the phenomenology of vortex states is so different to Majorana nanowires, for which it was already theoretically shown that zero-bias conductance peaks can appear due to non-topological reasons [25].

Thus far, several experiments observed zero-bias conductance peaks in vortex cores, in addition to trivial CdGM states at finite energy [12–17, 29–31]. Nevertheless, these zero-bias signals are not observed in all vortices, but often stabilized by magnetic [31] or scalar [13] impurities. While it was shown that the former can happen for non-topological reasons, it remains an open question whether scalar impurities can have a similar effect [32].

Besides tunneling spectroscopy, non-local measurements were predicted to reveal information on the topological nature of superconducting systems [33]. As a consequence, recent efforts have focused on combining local and non-local probes to identify topological phase transitions [11, 34–36]. Non-local transport in vortex states was recently proposed as a way to extract the Bardeen-Cooper-Schrieffer (BCS) charge of in-gap vortex excitations [26]. The charge of CdGM states are also non-zero, in contrast to the Majorana charge, which is zero due to particle-hole symmetry [3].

In this paper, we show how CdGM states located inside topological superconductor vortices can mimic and essentially become indistinguishable from MZMs when in presence of screened charged impurities. We find that the two states cannot be uniquely identified by experimentally accessible quantities such as energy and BCS charge. Our results show that local electrostatic changes are capable of shifting the lowest CdGM state energy arbitrarily close to zero, as schematically shown in Figs. 1 (a, b).

We compare vortex states in trivial s-wave superconductors with an added impurity with topological chiral p-wave superconductors. It is also relevant to note that the impurity, although modeled as a screened charge, brings to light the general issue of the modification of typical CdGM energies and charges due to fluctuations in the chemical potential.

Our main findings are summarized by Figs. 1 (c, d): we compare the density of states and the charge spectral density of a clean p-wave superconductor (Fig. 1(c)) with an s-wave superconductor in the presence of a charge impurity (Fig. 1(d)) – the quantities are computed as prescribed by Eqs. 9 and 11. We show that there is no qualitative difference between Figs. 1(c, d), suggesting that the current experiments cannot distinguish MZMs from CdGM states, as further discussed in the text.

**Model.** We consider a two-dimensional electron gas in a square lattice:

\[ H_0 = -t \sum_{\langle i,j \rangle} \psi_i^\dagger \tau_z \psi_j , \]

(2)

where \( t \) is the hopping constant, \( \tau_z \) is a Pauli matrix acting on particle-hole spinors \( \psi_i = (c_i, c_i^\dagger)^T \), and \( c_i^\dagger (c_i) \) is a creation (annihilation) operator at site \( i \). The tight-binding calculations were implemented using Kwant [37].

Superconductivity is added in two different flavours: with s-wave, and chiral p-wave order parameters. In both cases, we add a vortex at \( \mathbf{r} = 0 \). The superconducting pairing potential for the s-wave system is:

\[ H_{s\text{-wave}} = \sum_i \Delta_i \psi_i^\dagger \tau_z \psi_i^\dagger + h.c., \]

(3)

\[ \Delta_i = \Delta_0 e^{i\phi_i} \tanh\left( \frac{r_i}{\xi} \right) , \]

(4)

where \( \Delta_0 \) is the amplitude of the bulk order parameter, \( r_i \) the distance from \( \mathbf{r} = 0 \) to the atomic position \( i \), \( \xi \) the vortex radius, and \( \phi_i = \tan^{-1}(y_i/x_i) \) the order

![FIG. 2. Superconducting order parameter magnitude (a) and phase (b) implemented in the tight-binding calculations for both order parameters. The BCS charge-resolved spectrum of in-gap vortex states in clean (c) s-wave and (d) p-wave superconductors.](image)
parameter phase. For chiral $p$-wave pairing, the lack of rotational symmetry renders a superconducting term to the Hamiltonian given by:

$$H_{p\text{-wave}} = \sum_{\langle i,j \rangle} \psi_i^\dagger (\mathcal{R}\{\Delta_{\langle i,j \rangle}\} \tau_x + i\mathcal{I}\{\Delta_{\langle i,j \rangle}\} \tau_y) \psi_j^\dagger + h.c.,$$

$$\Delta_{\langle i,j \rangle} = \Delta_0 e^{i\phi_{\langle i,j \rangle}} \tanh \left( \frac{r_{\langle i,j \rangle}}{\xi} \right), \quad r_{\langle i,j \rangle} = \frac{r_i + r_j}{2},$$

where $\langle i,j \rangle$ denotes nearest-neighbor hoppings. In this expression, all parameters have the same definition to the $s$-wave case, except for the order parameter phase, which takes the form

$$\phi_{\langle i,j \rangle} = \arctan \left( \frac{y_{\langle i,j \rangle}}{x_{\langle i,j \rangle}} \right) + \frac{\pi}{2} r_{\langle i,j \rangle} \cdot \mathbf{e}_y,$$

with $r_{\langle i,j \rangle} = (x_{\langle i,j \rangle}, y_{\langle i,j \rangle})$. The Fig. 2 (a, b) shows the superconducting order parameter amplitude and phase in real space. For the remaining of this paper, we will use $\Delta_0 = t/2$.

Figures 2(c, d) show the spectrum and the respective charge expectation values, $Q := \langle \Psi | \tau_z | \Psi \rangle$, of in-gap vortex states for $s$-wave and chiral $p$-wave systems, as a function of the vortex radius $\xi$. In both cases, finite energy levels approach zero as $\xi$ increases, as expected for quantum confined levels. The spectrum for the chiral $p$-wave model reveals the existence of a zero-energy state corresponding to a Majorana mode as confirmed by Majorana polarization calculations shown in Fig. 5 (see discussion below).

Given the Majorana condition $\gamma = \gamma^\dagger$, MZMs in topological superconductors must be composed by equal combinations of electron and hole states. Thus, due to particle-hole symmetry, MZMs (i) are robust zero-energy modes, and (ii) have zero charge [3, 5, 19]. Both properties are shown in Figure 2(d) for a clean, chiral $p$-wave system.

**Impurity potential in an $s$-wave superconductor.** As reported in recent experiments [13], dilute impurities appear to favor the formation of MZMs inside vortex cores in iron-based superconductors. Generally, isolated charged impurities introduce local fluctuations in the chemical potential and modify the energy spectra. In particular, for superconductors with undetermined (or unknown) pairing order parameter, local impurities can produce states at zero energy and modify the local charge distribution, suggesting the presence of MZMs. However, local energy and charge modulations should happen in trivial (non-topological) superconductors under the same circumstances as well. Hence, one expect similar signatures for topological and trivial states under the presence of impurities.

To confirm this expectation we investigate the effect of a screened charged impurity on the $s$-wave Hamiltonian by incorporating an onsite modulation term as follows:

$$H_{\text{imp}} = \delta \mu \ e^{-|r|^2/4\eta^2} \tau_z,$$

where $\delta \mu$ is the potential strength and $\eta$ is the screening length. With this model we calculate the energy spectra and the charge of the Andreev quasiparticles (BCS charge), $Q$.

Figure 3 shows the resulting low-lying energy spectrum for a vortex in an $s$-wave superconductor pinned at an impurity site, as a function of $\xi$ and $\delta \mu$ for $\eta = 2a$. Notice that both charge and energy of the lowest state may be arbitrarily close to zero, as it occurs in the chiral $p$-wave case (Fig. 2(d)). The fact that the spectrum of an impurity-laden but trivial system is indistinguishable from that of a topological $p$-wave system is one of the central results of this paper.

The effects of the vortex size and impurity screening length interplay on the ground state energy and charge are shown in Fig. 4. Indeed, these calculations clearly show that a suppression of $E_1$ and $Q$ on large regions of the $\eta$, $\delta \mu$ parameter space, indicating the above results hold beyond the highly-localized impurity regime, $\eta \ll \xi$.

Due to the underlying particle-hole symmetry of the system, there is a correlation between the BCS charge and $E_1$, and these two quantities approach zero simultaneously. As a consequence, the distinction of trivial states from MZMs using local probes might become increasingly difficult. The extensive region of parameter space showing trivial excitations with small values of $E_1$ and $Q$, suggests that smooth fluctuations in the electrostatic potential can mimic Majorana signatures.

**Experimental relevance.** To show the significance of our results for experimental data, we compute the density of states $n_{\mathcal{R}}$ and spectral charge density $C_{\mathcal{R}}$ inside the vortex. The density of states is correlated to scanning tunneling spectroscopy, while the spectral charge
density correlates with non-local conductance measurements [36]. In Fig. 1(c) we observe the zero-energy peak in the density of states due to the presence of an MZM at the center inside the vortex. The corresponding spectral charge density at the same energy is zero, as expected for a zero-energy Majorana state. In Fig. 1(d), however, the same calculation for a s-wave superconductor with a charge impurity at the center of the vortex shows the same quantitative features: a zero-energy peak in density of states with corresponding negligible spectral charge density.

These observations suggest that recent experiments claiming impurity-assisted formation of MZMs [13] must be interpreted carefully. At the same time that local changes in the chemical potential could lead to a topological phase transition, trivial CdGM states can also be shifted arbitrarily close to zero energy. Thus, zero-bias peak signatures in the vicinity of scalar impurities are ambiguous to distinguish MZM and CdGM states. Moreover, even in combination with non-local scanning tunneling microscopy signatures, the distinction between trivial and non-trivial zero-energy states is unclear since the spectral charge density value is arbitrarily small in both cases.

Conclusions. Several claims of Majorana zero modes in vortices are justified by the presence of a zero bias peak in scanning tunneling spectroscopy measurements. However, most of these observations do not show zero bias peaks for all vortices probed. Moreover, in many works the presence of zero-energy states is correlated to the presence of magnetic or scalar impurities. We studied the behavior of CdGM states in superconducting vortices pinned to scalar impurity sites. Our results show that local scalar perturbations in the vicinity of the vortex center lower the energy of CdGM states and suppress their BCS charge. Particularly, the energy and charge of CdGM modes can be shifted arbitrarily close to zero. These results are particularly relevant to experimental works that often rely on the fact that CdGM states have finite energy. Furthermore, we also argue that recent theoretical proposals to distinguish trivial CdGM states to Majoranas based on their BCS charge might be impossible in the presence of impurities. Therefore, we argue that, even combined, these two quantities are insufficient to unveil the Majorana nature of zero-energy states.

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Data availability. All the scripts and resulting data used to prepare this manuscript are freely available on Zenodo [38].

Authors’ contributions. LGDS and NS formulated the initial project goal and was later refined with contributions from all authors. BSM and ALRM carried the numerical simulations, and analyzed the data with input from the other authors. ALRM identified the role of scalar impurities on the in-gap spectrum. NS and LGDS supervised the project. BSM wrote the initial draft of the manuscript. All authors contributed to writing the manuscript.

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SUPPLEMENTARY MATERIAL

Computation of spectral quantities

To provide a qualitative prediction of the behavior expected from scanning tunneling microscopy experiments, we compute the density of states and the charge spectral density in a region \( R \) defined as a disk with radius \( \xi \) centered at \( r = 0 \). Due to the exponential localization of in-gap vortex states, the region above should contain most of the wavefunction. With this definition, we get rid of edge states' contributions in the \( p \)-wave case.

The density of states \( n_R(\omega) \) is defined as

\[
n_R(\omega) = \frac{1}{\pi} \text{Im} \left\{ \text{Tr} \int_R d^2r \ G_R(\omega) \right\},
\]

\[
G_R(\omega) = [\omega - \mathcal{H} + i0^+]^{-1},
\]

whereas the charge spectral density is given by

\[
C_R(\omega) = \frac{1}{\pi} \text{Im} \left\{ \text{Tr} \int_R d^2r \ G_R(\omega) \tau_z \right\}.
\]

Majorana polarization in the presence of impurities.

As an additional quantitative check of the topological character of the zero-energy states of the \( p \)-wave superconductor in the presence of impurities, we calculate the Majorana polarization (MP) [39] defined by:

\[
\langle M \rangle_R = \frac{\left| \sum_{i \in R} \langle \Psi_i | \tau_z \mathcal{K} | \Psi_i \rangle \right|}{\sum_{i \in R} \langle \Psi_i | \Psi_i \rangle},
\]

where \( \tau_z \mathcal{K} \) is the particle-hole operator. Majorana states obey \( \langle \Psi_i | \tau_z \mathcal{K} | \Psi_i \rangle = 1 \), thus \( \langle M \rangle_R \to 1 \) over a region indicates the presence of a Majorana state.

Figures 5(a) and (b) show the MP intensity for the low-lying states for clean and single-impurity cases, respectively. We note that the zero-energy state retains the topological character (\( \langle M \rangle_R = 1 \)), irrespective of the vortex size (quantified by the coherence length, \( \xi \)) or the impurity potential strength \( \delta \mu \), as expected.

FIG. 5. Majorana polarization-resolved spectrum of in-gap vortex states for (a) a clean \( p \)-wave superconductor as a function of the vortex size \( \xi \) and (b) a \( p \)-wave superconductor with a single impurity as a function of the impurity strength \( \delta \mu \).