Entangled end states with fractionalized spin projection in a time-reversal-invariant topological superconducting wire

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We study the ground state and low-energy subgap excitations of a finite wire of a time-reversal-invariant topological superconductor (TRITOPS) with spin-orbit coupling. We solve the problem analytically for a long chain of a specific one-dimensional lattice model in the electron-hole symmetric configuration and numerically for other cases of the same model. We present results for the spin density of excitations in long chains with an odd number of particles. The total spin projection along the axis of the spin-orbit coupling $S_z = \pm 1/2$ is distributed with fractions $\pm 1/4$ localized at both ends, and shows even-odd alternation along the sites of the chain. We calculate the localization length of these excitations and find that it can be well approximated by a simple analytical expression. We show that the energy $E$ of the lowest subgap excitations of the finite chain defines tunneling and entanglement between end states. We discuss the effect of a Zeeman coupling $\Delta_Z$ on one of the ends of the chain only. For $\Delta_Z < E$, the energy difference of excitations with opposite spin orientation is $\Delta_Z/2$, consistent with a spin projection $\pm 1/4$. We argue that these physical features are not model dependent and can be experimentally observed in TRITOPS wires under appropriate conditions.

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I. INTRODUCTION

Topological materials including topological superconductors (TS) are a subject of great interest recently in condensed matter physics. This field of research had a burst after the observation by Kitaev that a one-dimensional model of spinless fermions with $p$-wave BCS pairing has a topological phase with zero-energy subgap excitations that are described by Majorana fermions.\textsuperscript{1} The non-abelian statistics obeyed by these quasiparticles is an appealing property for implementing quantum computing protocols. Since then, several proposals for realizing this phase in concrete physical systems were formulated. In particular, quantum superconducting wires with spin-orbit coupling and magnetic field\textsuperscript{2–8} edge states of the quantum spin Hall state in proximity to superconductors and in contact to magnetic moments,\textsuperscript{9} and Shiba states induced by magnetic adatoms on superconducting substrates.\textsuperscript{10} All these mechanisms to generate the topological superconducting phase contain ingredients breaking time-reversal symmetry.

In contrast, there is another family of TS, the time-reversal-invariant topological superconductors (TRITOPS) where the zero-mode edge excitations appear in Kramers pairs.\textsuperscript{11–20} This property has interesting implications which can be relevant for their detection and manipulation.\textsuperscript{21,22} In particular, Zhang et al.\textsuperscript{12} proposed to engineer one- and two-dimensional TRITOPS via proximity effect between nodeless extended $s$-wave iron-based superconductors and semiconducting systems with large Rashba spin-orbit interactions. A sketch of a one-dimensional (1D) setup is shown in Fig. 1. At each end of a long TRITOPS wire, there is a Kramers pair of Majorana edge states at zero energy. For a finite wire, there is a mixing of the end states and the four states of zero energy split in two pairs with energy $\pm E$. One of the interesting properties of this family is the fact that subgap excitations were argued to have fractional spin projection along the direction of the spin-orbit coupling.\textsuperscript{13} This has consequences in the physical behavior of these systems when put in contact to magnetic systems. An example is the quench of the $0-\pi$ transition in the
Josephson current of a quantum dot embedded in a TRITOPS junction\textsuperscript{23}

In this work we study these low-energy end states of a finite chain. By using a method presented recently by Alase et al.\textsuperscript{24,25} we analytically calculate the zero-energy eigenstates of an infinite chain of the model introduced by Zhang et al. in Ref. \textsuperscript{12} in the particle-hole symmetric configuration of the normal system (which means that the chemical potential $\mu = 0$). This corresponds to the explicit solution of the Kramers pairs of Majorana edge states. We calculate the localization length of the low-energy excitations for arbitrary $\mu$. We also find analytical explicit expressions for these states in the case of finite chains with $\mu = 0$ and complement our study with some numerical results for other values of $\mu$. In finite chains with an odd number of particles, there is an effective tunneling which entangles the end states. This stabilizes a ground state in which the total spin projection at each end is $S^z = \pm 1/4$ [or $e = L$ (right) or $e = R$ (right)]. Instead, for systems with an even number of particles, the total spin is zero. We show that the parameter characterizing the tunneling is, precisely, the energy $E$ of the lowest subgap excitations. We also calculate the distribution of $S_z$ along the chain. In addition, we analyze the response to Zeeman coupling $\Delta_Z$ induced by a weak magnetic field or an Ising coupling with a magnetic moment, acting on one of the edges of the wire, as sketched in Fig. 1. We show that for very large wires, where the zero modes are completely decoupled, the effect of an arbitrary small magnetic field breaks the fractionalization of $S_z$ of the subgap excitations. Instead, in short enough chains where the excitations at both ends are entangled, the fractionalization of $S_z$ manifests itself in a Zeeman splitting of half the amplitude of the usual one for spin $1/2$. The condition to observe this fractional Zeeman response is $\Delta_Z < E$. Importantly, although we solve a specific model, the physical behavior related to the distribution of $S_z$ and response is generic of any TRITOPS wire.

The finite energy of these odd parity states might be detected in experiments where capacitance effects permit to control the charge in small superconducting islands.\textsuperscript{29} In these systems also the chemical potential $\mu$ can be controlled by a gate voltage. The Zeeman splitting can also be detected by scanning tunneling spectroscopy experiments akin to those performed to observe Shiba states induced by magnetic adatoms in superconducting substrates.\textsuperscript{18,29} Finally also microwave excitations,\textsuperscript{27,28} in a finite chain with odd number of particles might detect the anomalous (half) Zeeman splitting of the low-energy excitations.

The paper is organized as follows. In Sec. \textsuperscript{I} the model is described. In Sec. \textsuperscript{II} we present the approach to analytically diagonalize it for $\mu = 0$. In Sec. \textsuperscript{III} we show the dependence on the localization length with $\mu$ and compare with a simple analytical approximation. Sec. \textsuperscript{IV} contains analytical and numerical results for the spin projection $S^z_i$ at each site $i$ for a finite wire with odd number of particles. In Sec. \textsuperscript{VII} we calculate the effect of a magnetic field at one end of the chain. In Sec. \textsuperscript{VIII} we present a summary and a brief discussion.

\section{Model}

The TRITOPS chain is described by the Hamiltonian proposed in Ref. \textsuperscript{12}

\begin{equation}
H = \sum_{j=1}^{L} \sum_{\sigma} \left[ -tc_{j+1\sigma}^\dagger c_{j\sigma} - \mu c_{j\sigma}^\dagger c_{j\sigma} + i\lambda \sigma c^\dagger_{j+1\sigma} c_{j\sigma} + (\Delta_{\sigma} e^{i\phi} c^\dagger_{j+1\sigma} c^\dagger_{j\bar{\sigma}} + \text{h.c.}) \right],
\end{equation}

where $\lambda_{\uparrow,\downarrow} = \pm \lambda$, $\Delta_{\uparrow,\downarrow} = \pm \Delta$ and $\uparrow = \downarrow$, $\downarrow = \uparrow$. The first term corresponds to nearest-neighbor hopping, $\mu$ is the chemical potential, and $\lambda$ and $\Delta$ are the strengths of Rashba spin-orbit coupling and extended s-wave pairing, respectively.

For completeness, we include in the Hamiltonian the phase $\phi$, which is important when the chain is coupled in a Josephson circuit, although it does not play an important role in the behavior of the spin excitations.\textsuperscript{12,23,24,55} For $\phi = 0$, the Hamiltonian is invariant under time reversal symmetry. In addition, in absence of superconductivity ($\Delta = 0$), for $\mu = 0$, the Hamiltonian is invariant under the electron hole transformation $c_{j\sigma} \rightarrow (-1)^j c_{j\bar{\sigma}}$.

While $H$ supports topological and nontopological phases, in our work we are interested in the topological phase that takes place for $|\mu| < 2|\Delta|$. In Ref. \textsuperscript{12} a local s-wave pairing $\Delta_0$ was also considered. Since the topological phase exists for dominant nearest-neighbor pairing ($|\Delta_0| < |\Delta|$), for simplicity we focus on the case $\Delta_0 = 0$. In this phase when the number of sites $L \rightarrow \infty$, there is a Kramers pair of Majorana fermions at each end with energy $E = 0$. For a finite chain the end states mix as described in the following Sections.

\section{Diagonalization of the Chain with Arbitrary Boundary Conditions}

In this Section, we discuss the application of the method presented in Refs. \textsuperscript{27,28} by Alase et al. to diagonalize a 1D non-interacting homogeneous Hamiltonian with arbitrary boundary conditions. Then, we study the particular case of an electron-hole symmetric band ($\mu = 0$) for which an analytical result for the zero-energy eigenstates for $L \rightarrow \infty$ is derived. Finally we also obtain analytically the low-energy eigenstates for $\mu = 0$ and a long finite chain. Those readers who are not interested in the derivation can skip this section, and go directly to the analytical results for $\mu = 0$: Eq. (18) and the following for the zero-energy modes of the infinite chain, and Eq. (38) and the following for the low-energy modes of the finite chain.
A. Formalism for the general case

Here we discuss the application of the method of Alase et al. to the model of Eq. (1). For those readers who are more familiar with Nambu notation, an alternative version of the procedure is presented in Appendix A.

To simplify the use of the method of Alase et al. it is convenient to map the model with $M$ spin-orbitals $\alpha$ ($M = 2L$ in our case) to one expressed in terms of $2M$ kets associated with the annihilation ($a$) and creation ($c$) operators

$$c_\alpha \leftrightarrow |a\alpha\rangle, \ c_\alpha^\dagger \leftrightarrow |a^\dagger\alpha\rangle. \ (2)$$

The ensuing Hamiltonian is

$$\hat{H} = \sum_{\beta} (A_{\beta a}|\beta a\rangle \langle a\alpha| + B_{\beta a}|\beta c\rangle \langle a\alpha| - \bar{A}_{\beta a}|\beta c\rangle \langle a\alpha| + \bar{B}_{\beta a}|\beta a\rangle \langle a\alpha|), \ (3)$$

with $\bar{A}_{\beta a} = A_{\beta a}^*$ and $\bar{B}_{\beta a} = B_{\beta a}^*$. These matrix elements are defined from the equations

$$[c_\alpha, H] = \sum_{\beta} (A_{\beta a} c_\beta + B_{\beta a} c_\beta^\dagger). \ (4)$$

Hence

$$\hat{H}|\alpha a\rangle = \sum_{\beta} (A_{\beta a}|\beta a\rangle + B_{\beta a}|\beta c\rangle),$$
$$\hat{H}|\alpha c\rangle = -\sum_{\beta} (A_{\beta a}|\beta c\rangle + B_{\beta a}|\beta d\rangle). \ (5)$$

Thus, we see that solving Eq. (5) is equivalent to solving Eq. (1).

In this notation we define projection operators over bulk ($P_B$) and boundary ($P_{\text{bou}}$) states with $P_B + P_{\text{bou}} = 1$. The projector $P_B$ is over all those sites in which all the hopping terms are contained in the chain. In our case

$$P_B = \sum_{j=2}^{L-1} P_j,$$
$$P_{\text{bou}} = P_1 + P_L,$$
$$P_j = \sum_{\sigma}(j \sigma a)\langle j \sigma a| + |j \sigma c\rangle\langle j \sigma c|. \ (6)$$

Following again Alase et al., we construct generalized Bloch functions which permit to solve the bulk eigenvalue problem $P_B \hat{H}|e\rangle = E P_B |e\rangle$ for certain roots $z(E)$. Finally the equation $P_{\text{bou}} \hat{H}|e\rangle = P_{\text{bou}} E|e\rangle$ determines the allowed energies $E$ and the eigenstates $|e\rangle$. Specifically, for our problem the four generalized Bloch states can be written as

$$|z \sigma a\rangle = w_z \sum_{j=1}^L z^{j-1} |j \sigma a\rangle, \ (7)$$

where $a = a$ or $c$, $\sigma = \uparrow$ or $\downarrow$, $w_z$ is the coefficient of $|j \sigma a\rangle$ and $z$ is a complex number to be determined later.

Using Eqs. (1), (4), (5), (6) and (7) and some algebra we get

$$P_B \hat{H}|z \uparrow a\rangle = [-\mu - t \left(z + \frac{1}{z}\right)] |z \uparrow a\rangle + i \lambda \left(z - \frac{1}{z}\right) |z \downarrow c\rangle,$$
$$P_B \hat{H}|z \downarrow c\rangle = [\mu + t \left(z + \frac{1}{z}\right)] |z \downarrow c\rangle - i \lambda \left(z - \frac{1}{z}\right) |z \uparrow a\rangle + \Delta e^{i\phi} \left(z + \frac{1}{z}\right) P_B |z \uparrow a\rangle + \Delta e^{-i\phi} \left(z + \frac{1}{z}\right) P_B |z \uparrow a\rangle. \ (8)$$

Similar equations are obtained interchanging $\uparrow$ and $\downarrow$ and simultaneously changing the sign of both, $\lambda$ and $\Delta$.

Using Eqs. (5), and the ansatz $|e\rangle = u|z \uparrow a\rangle + v|z \downarrow c\rangle$, the bulk eigenvalue problem $P_B (\hat{H} - E)|e\rangle = 0$ takes the form

$$\begin{pmatrix} a(z) - E & b(z) e^{-i\phi} \\ b(z) e^{i\phi} - a(z) - E \end{pmatrix} \begin{pmatrix} u(z) \\ v(z) \end{pmatrix} = 0, \ (9)$$

where

$$a(z) = -\mu - t \left(z + \frac{1}{z}\right) + i \lambda \left(z - \frac{1}{z}\right),$$
$$b(z) = \Delta \left(z + \frac{1}{z}\right). \ (10)$$

Vanishing of the determinant of the matrix implies

$$E^2 = \mu^2 + (t^2 + \Delta^2) \left(z + \frac{1}{z}\right)^2 - \lambda^2 \left(z - \frac{1}{z}\right)^2 + 2 \mu t \left(z + \frac{1}{z}\right) - 2 i \lambda \left[\mu \left(z - \frac{1}{z}\right) + t \left(z^2 - \frac{1}{z^2}\right)\right]. \ (11)$$

For each energy $E$, there are four solutions $z_k(E)$ of this equation, which lead to four eigenstates $|e_k\rangle$ of the bulk equation with $u_k > 0$ and

$$\frac{v_k}{u_k} = \frac{e^{i\phi} (E - a_k)}{b_k}. \ (12)$$
with the definitions

\[ a_k^\uparrow = w_k (-\mu - tz_k + i\lambda z_k), \]
\[ a_k^\downarrow = w_k (-\mu - t z_k - i\lambda z_k) z_k^{-1}, \]
\[ b_k^\uparrow = w_k \Delta z_k, \quad b_k^\downarrow = w_k \Delta z_k^{-1}. \]}

Interchanging \( \uparrow \) and \( \downarrow \) and simultaneously changing the sign of both, \( \lambda \) and \( \Delta \), or directly applying the time reversal operator for \( \phi = 0 \), eigenstates (degenerate with the previous ones) which involve linear combinations of the form \( u|z \downarrow a \rangle + v|z \uparrow c \rangle \) are obtained.

\section*{B. Solution for \( \mu = 0 \), \( L \to \infty \), \( E \to 0 \)}

In general, for finite wires, the chemical potential \( \mu \) can be adjusted using a gate voltage. For \( \mu = 0 \), Eq. \( (11) \) can be solved analytically. In fact, for \( \mu = 0 \) the odd powers of \( z \) in Eq. \( (11) \) disappear and the ensuing equation is quadratic in \( z^* \). This value of the chemical potential is within the topological phase, which is characterized by Kramers pairs of Majorana zero modes localized at the ends of the chain. These states are exactly at \( E = 0 \) only in the limit of an infinitely long chain, where they are completely decoupled. We discuss this limit here since this solution sheds light on the structure and properties of these states. In particular for \( t \to 0 \), \( |\Delta| = |\lambda| \) a very simple solution is found, which involves operators at sites \( 1 \) and \( L \) only. We postpone the discussion of the effect of the finite length of the chain for the next subsection.

Note that for any \( \mu \), Eq. \( (11) \) is invariant under the simultaneous change of sign of \( \lambda \) and \( z \leftrightarrow 1/z \). In addition, if \( z \) is a solution of \( (11) \), its complex conjugate \( \bar{z} \) is a solution of the same equation for the opposite sign of \( \lambda \). Combining both properties one realizes that if \( z \) is a solution of \( (11) \), \( 1/\bar{z} \) is also a solution. For \( \mu = 0 \), if \( z \) is a solution, \( -z \) is also a solution. This implies that knowing one solution of Eq. \( (11) \), which we call \( z_1 \), the others are related to it as follows

\[ z_2 = -z_1, \quad z_3 = \frac{1}{z_2}, \quad z_4 = -z_3. \]

For \( E = 0 \) two solutions have \( |z| < 1 \) and the other two \( |z| > 1 \). Choosing \( z_1 \) as one of the solutions satisfying \( |z_1| < 1 \), we obtain after some algebra

\[ z_1^2 = z_2^2 = -t^2 + (|\Delta| - |\lambda|)^2 \Delta^2 + (t - i\lambda)^2. \]

Then, the amplitude of \( |j\sigma_o \rangle \) in the states \( |e_k \rangle \) with \( k = 1, 2 \) (\( k = 3, 4 \)) decrease (increase) exponentially as \( j \) increases. In the limit where \( L \to \infty \) we can separate the states localized at each end. For the left one (low \( j \)) only \( k = 1, 2 \) matter. Using Eq. \( (12) \) we obtain

\[ \frac{v_1}{u_1} = \frac{v_2}{u_2} = p, \]

where we define

\[ p = ie^{i\phi} \text{sign}(\Delta\lambda). \]

We also define \( w_k = 1/u_k \) and normalize the states at the end of the calculation. With this choice, the last two Eqs. \( (13) \) lead to \( a_2^\uparrow = -a_1^\downarrow, b_2^\downarrow = -b_1^\uparrow \), and the first two Eqs. \( (13) \) lead to \( a_2 = a_1 \). In terms of the original fermionic operators, the normalized solution for the zero-energy \( \uparrow \) spin excitation localized at the left end reads

\[ \gamma_\uparrow = N \sum_{n=0}^{\infty} z_1^{2n} \left( c_{2n+1\uparrow} + pc_{2n+1\downarrow}^\dagger \right), \]
\[ N = \left( 1 - |z_1|^4 \right)^{1/2}. \]

Similarly, interchanging \( \uparrow \) and \( \downarrow \) and inverting the signs of \( \lambda \) and \( \Delta \) we have

\[ \gamma_\downarrow = N \sum_{n=0}^{\infty} z_1^{2n} \left( c_{2n+1\downarrow} + pc_{2n+1\uparrow}^\dagger \right), \]

which corresponds to the Kramers partner of Eq. \( (19) \). Surprisingly, the even sites do not enter these Eqs. In addition, note that

\[ \gamma_\downarrow = \bar{p} \gamma_\uparrow, \quad \gamma_\uparrow = \bar{p} \gamma_\downarrow. \]
\[
\eta_1 = \gamma_\uparrow + \gamma_\uparrow, \quad \eta_2 = i(\gamma_\uparrow - \gamma_\uparrow), \quad (22)
\]
such that \(\eta_1^\dagger = \eta_1\).

A particular simple case is \(t \to 0, |\Delta| = |\lambda|\), for which \(z \to 0\) [see Eq. (10)] and then Eqs. (19), (20) reduce to
\[
\gamma_\sigma = \frac{1}{\sqrt{2}} \left( c_{1\sigma} + pc_{1,\sigma}^\dagger \right). \quad (23)
\]

It can be verified directly that for these parameters, \([\gamma_\sigma, H] = 0\).

We can proceed in a similar way to derive the zero-energy excitations localized at the right end. Using Eqs. (14), the right-end eigenstates of zero energy can be expressed in terms of fermionic operators as
\[
\begin{align*}
\hat{\gamma}_\uparrow &= \sum_{n=0}^\infty z_{2n}^2 \left( c_{L-2n\uparrow} - pc_{L-2n\downarrow}^\dagger \right), \\
\hat{\gamma}_\downarrow &= \sum_{n=0}^\infty z_{2n+1}^2 \left( c_{L-2n\downarrow} - pc_{L-2n\uparrow}^\dagger \right). \quad (25)
\end{align*}
\]

Similarly to the left-end excitations, they are related by
\[
\hat{\gamma}_\uparrow = -\bar{p}\hat{\gamma}_\downarrow, \quad \hat{\gamma}_\downarrow = -\bar{p}\hat{\gamma}_\uparrow. \quad (26)
\]

C. Properties of the end excitations of the infinite chain

The relations given by Eqs. (21) and (26) imply
\[
\{\gamma_\uparrow, \gamma_\downarrow\} = p, \quad \{\hat{\gamma}_\uparrow, \hat{\gamma}_\downarrow\} = -p. \quad (27)
\]

Denoting by \(\hat{\gamma}_\sigma\) any of the two operators \(\gamma_\sigma, \hat{\gamma}_\sigma\), it is easy to verify that
\[
[\hat{\gamma}_\sigma, S_z] = (s/2)\hat{\gamma}_\sigma, \quad (28)
\]
where \(s = 1\) (-1) for \(\sigma = \uparrow (\downarrow)\) and \(S_z = \sum (c_{1\uparrow}c_{1\downarrow} - c_{1\downarrow}c_{1\uparrow})/2\) is the total spin projection in the Rashba direction \(z\). Using Eq. (28) it is easy to see that rotating the operator \(\hat{\gamma}_\sigma\) an angle \(\varphi\) around \(z\) one obtains
\[
\exp(-i\varphi S_z)\hat{\gamma}_\sigma \exp(i\varphi S_z) = \exp(isi\varphi/2)\hat{\gamma}_\sigma. \quad (29)
\]

Then \(\hat{\gamma}_\uparrow (\hat{\gamma}_\downarrow)\) transforms like a spin with \(S_z = -1/2\) (1/2) under rotations around \(z\). Note however that due to the Rashba spin-orbit coupling, the total spin is not conserved. For example one has
\[
[\gamma_\uparrow, S_x] = \frac{N}{2} \sum_{n=0}^{\infty} z_{2n} (c_{2n+1\downarrow} - pc_{2n+1\uparrow}^\dagger), \quad (30)
\]
and the second member anticommutes with all low-energy operators \(\hat{\gamma}_\sigma\). This is also true for \(S_y\) and the rest of the \(\hat{\gamma}_\sigma\) operators.

The end excitations described by \(\gamma_\sigma, \hat{\gamma}_\sigma\) satisfy the usual Pauli exclusion principle \(\gamma_\sigma^2 = \hat{\gamma}_\sigma^2 = 0\). Hence, taking into account the relations of Eqs. (21) and (26), we can characterize the end states by two operators, \(\gamma \equiv \gamma_\uparrow\) and \(\hat{\gamma} \equiv \hat{\gamma}_\downarrow\). These operators define q-bit states \(|L0\rangle, |L1\rangle\), localized at the left edge and \(|R0\rangle, |R1\rangle\), localized at the right, satisfying
\[
\begin{align*}
\gamma|L0\rangle &= 0, \quad |L1\rangle = \gamma^\dagger|L0\rangle, \\
\hat{\gamma}|R0\rangle &= 0, \quad |R1\rangle = \hat{\gamma}^\dagger|R0\rangle. \quad (31)
\end{align*}
\]

Eqs. (16), (19), (20) and (25) define the zero-energy excitations of the infinite chain. For finite odd \(L\), the corresponding operators continue to commute with the Hamiltonian. This means that the zero energy excitations persist. This is a particular property of the case \(\mu = 0\). For even finite \(L\), the states \(\gamma_\sigma\) and \(\hat{\gamma}_\sigma\) mix as described in the next section.

D. Extension to finite large even \(L\)

For finite odd \(L\), as long as \(\mu = 0\), the edge states have the same properties as those of \(L \to \infty\). Namely, they have exactly energy \(E = 0\), and they can be expressed as in Eqs. (16), (19), (20), and (25). For finite even \(L\), the left and right zero modes discussed in the previous section hybridize and the resulting subgap eigenstates have finite energy \(\pm E\), which decreases exponentially with \(L\). For even \(L\), the first correction to the solution presented in the previous section is of order \(E \sim |z_1|^L\). From Eq. (11) we see that the first correction to the roots \(z_1\) is of order \(E^2\). Then, to linear order in \(E\), the \(z_1\) are not modified. On the other hand, Eqs. (10), (12) are linear in \(E\). Explicitly, after substituting the solution of Eq. (16) and the definition of Eq. (18) they read
\[
\begin{align*}
\frac{v_1}{u_1} &= p + \frac{e^{i\varphi} E}{\Delta (z_1 + \frac{1}{z_1})}, \\
\frac{v_2}{u_2} &= -p + \frac{e^{i\varphi} E}{\Delta (z_1 + \frac{1}{z_1})}, \\
\frac{v_3}{u_3} &= -p + \frac{e^{i\varphi} E}{\Delta (z_1 + \frac{1}{z_1})}, \\
\frac{v_4}{u_4} &= -p - \frac{e^{i\varphi} E}{\Delta (z_1 + \frac{1}{z_1})}. \quad (32)
\end{align*}
\]
As we know from the previous Section, for \( L \to \infty, E = 0 \), the two ends are decoupled and Eqs. \([13, 14]\) give \( \alpha_2 = \alpha_1, \alpha_4 = \alpha_3 \) for the coefficients of the eigenstate \( \sum \alpha_k | e_k \rangle \). We define two deviations from this limit, linear in \( E \), \( \beta_1 = \alpha_2 - \alpha_1, \beta_3 = \alpha_4 - \alpha_3 \). Choosing \( w_k = 1/u_k \) for \( k = 1, 2 \) (weight 1 for \( c_{11} \)) and \( w_k = z_1^{-L}/u_k \) for \( k = 3, 4 \) (weight 1 for \( c_{1L} \)), the linear corrections in \( E \) to Eqs. \([13]\) lead to the following relations: \[ 0 = 2\alpha_1 E \left[ \frac{z_1}{z_1 + \frac{1}{z_1}} \right] - 1 \]

\[ + 2\alpha_3 z_1^{L-2} \left[ -t + i\lambda - pe^{-i\phi} \Delta \right] + \beta_1 z_1 \left[ t - i\lambda - pe^{-i\phi} \Delta \right], \tag{33} \]

\[ 0 = -2\alpha_1 E \left[ p + \frac{(-t + i\lambda) e^{i\phi} z_1}{\Delta \left( z_1 + \frac{1}{z_1} \right)} \right] \]

\[ + 2\alpha_3 z_1^{L-2} \left[ (-t + i\lambda) p + e^{i\phi} \Delta \right] - \beta_1 z_1 \left[ p (t - i\lambda) + e^{i\phi} \Delta \right]. \tag{34} \]

From these expressions, \( \beta_1 \) can be eliminated leaving an equation that relates \( \alpha_1 \) and \( \alpha_3 \). In fact \( \beta_1 \) turns out to be exponentially small and we neglect it. More precisely, performing the operation Eq. \([33] + Eq. \ [34]/p \) and substituting Eq. \([13]\), results in the following relation between \( \alpha_1 \) and \( \alpha_3 \):

\[ E \gamma_1 \alpha_1 + x \alpha_3 = 0, \tag{35} \]

where

\[ y = 1 + \text{sign}(\Delta \lambda)(t - i\lambda) z_1^2 + \Delta \left( z_1^2 + 1 \right) \Delta, \]

\[ x = z_1^{L-2} \varepsilon, \quad \varepsilon = \frac{2}{\Delta} [t - i\lambda + \text{sign}(\Delta \lambda) \Delta]. \tag{36} \]

We can follow a similar procedure to evaluate the linear corrections in \( E \) to Eqs. \([14]\). The result is

\[ \bar{E} \gamma_1 \alpha_1 + E \bar{\gamma} \alpha_3 = 0. \tag{37} \]

From Eqs. \([35]\) and \([37]\) we finally obtain the desired energy and the ratio \( \alpha_3/\alpha_1 \) which has modulo 1. For the energy, we get

\[ E = \pm \left| \frac{x}{y} \right| = \pm \frac{z_1^{L-2} \varepsilon}{y}, \tag{38} \]

which explicitly defines a relation between the finite length of the chain and the non-zero energy of the excitations. For positive \( E \) we define \( \theta \) from

\[ \frac{\alpha_3}{\alpha_1} = - \frac{x}{y} = e^{i\theta}. \tag{39} \]

We recall that \( \alpha_1 (\alpha_3) \) is the amplitude of the quasiparticle excitation at the left (right) end of the chain. The corresponding excitations are described by \( \gamma_\sigma, \bar{\gamma}_\sigma \) given by Eqs. \([19, 25]\). In the case of the finite chain we are analyzing here, the exact subgap eigenstate with energy \( E > 0 \) given by Eq. \([33]\), is a linear combination of the latter ones. It can be described in terms of the annihilation operator of a quasiparticle with this energy as

\[ \Gamma_\uparrow = \frac{1}{\sqrt{2}} (\gamma_\uparrow + e^{i\theta} \bar{\gamma}_\uparrow), \tag{40} \]

where \( \gamma_\uparrow \) and \( \bar{\gamma}_\uparrow \) have the same form as in Eqs. \([19, 25]\), except for the fact that for the finite chain the sum in these equations extends up to \( L \) instead of \( \infty \), and then the normalization changes to

\[ N = \left[ \frac{1 - |z_1|^4}{2 (1 - |z_1|^2 L)} \right]^{1/2}. \tag{41} \]

As before, a degenerate solution is obtained interchanging spin up and down and changing the sign of both \( \Delta \) and \( \lambda \) (or by time reversal operation if \( \phi = 0 \))

\[ \Gamma_\downarrow = \frac{1}{\sqrt{2}} (\gamma_\downarrow + e^{-i\theta} \bar{\gamma}_\downarrow). \tag{42} \]

Using Eqs. \([21, 26]\), it can be easily checked that the low-energy eigenstates with negative energy given by Eq. \([38]\) coincide except for an irrelevant factor with the operators \( \Gamma_\uparrow, \Gamma_\downarrow \), transpose conjugate of those defined by Eqs. \([40]\) and Eqs. \([42]\). This can be expected since taking the transpose conjugate of the equation

\[ [\Gamma_\sigma, H] = E \Gamma_\sigma, \tag{43} \]

implies \( [\Gamma_\sigma, H] = -E \Gamma_\sigma^\dagger \).

Here and in what follows, when an operator \( O \) satisfies \( [O, H] = EO \), with \( E \neq 0 \), implying \( [O^\dagger, H] = -EO^\dagger \) we choose as annihilation operator \( O \) for positive \( E \) and \( O^\dagger \) for negative \( E \), so that the vacuum \( |0\rangle_O \) of all these annihilation operators \( (O|0\rangle_O = 0) \) is the ground state.

IV. LOCALIZATION LENGTH OF THE END STATES

To define the localization length \( \lambda_\sigma \) of the end states, it suffices to consider a chain of infinite length. In this case the energy of the low energy states is \( E = 0 \) and it is not necessary to solve the boundary equation to obtain \( E \). The four complex roots of Eq. \([11]\) provide the decay
along the chain of the components of the eigenstates of the Hamiltonian, as illustrated in Sec. 111. We choose the eigenstates localized at the left end for the following discussion (of course the results are the same choosing the right end). From the four solutions of Eq. (11), only those two with \(|z_i| < 1\) contribute to the states localized at the left end. Let us denote as \(|z_i|\) the largest of these two absolute values. Clearly this is the one that determines the localization length because at large distances, the probability \(p(n)\) of finding a particle at site \(n\) is proportional to \(|z_i|^{2n}\). Defining as usual the localization length \(\lambda_e\), from \(p(n) \sim \exp(-n/\lambda_e)\) we obtain

\[
\lambda_e = \frac{-1}{2 \ln|z_i|}.
\]  

(44)

For \(\mu = 0\) both roots with \(|z_i| < 1\) are given by Eq. (16) and replacing in Eq. (44), \(\lambda_e\) is derived. In general, one has to solve the quartic equation (11) and choose the largest \(|z_i|\) with the condition \(|z_i| < 1\) to obtain the localization length. Following this procedure we derived the results shown in Fig. 2 where the localization length as a function of the chemical potential \(\mu\) is represented. Note that if \(z\) is a solution of Eq. (11), \(-z\) is a solution for the opposite value of \(\mu\). This and other properties listed above Eq. (11) allows us to restrict the calculations and discussions to all parameters assumed positive, and extend later the result for all signs using the symmetry properties of Eqs. (11) and (44). Starting from \(\mu = 0\) and increasing \(\mu\), the localization length increases and diverges as the transition to the non-topological phase at \(\mu = 2\lambda\) is approached, as expected. In fact for \(\mu = 2\lambda\) there is a double root \(z = -i\) of Eq. (11) for \(E = 0\). The other two roots are given by

\[
z = i \left( t^2 + \Delta^2 + \lambda^2 \pm 2\Delta \lambda \right) \frac{i t^2 + \Delta^2 - \lambda^2 - 2it\lambda}{t^2 + \Delta^2 - \lambda^2 - 2it\lambda}.
\]  

(45)

It is easy to see that for positive \(\Delta\) and \(\lambda\), one of these two roots has \(|z| > 1\) and the other \(|z| < 1\). Then for \(\mu \to 2\lambda\), \(|z_i| \to 1\), and \(\lambda_e \to +\infty\).

In order to find an analytical expression for the localization length near the topological transition, we expand Eq. (11) up to total second order in \(y = z + i\) and \(\epsilon = 2\lambda - \mu > 0\) around the point \(y = \epsilon = 0\), to obtain after some algebra

\[
4(t^2 + \Delta^2)y^2 - 4ty + \epsilon^2 = 0.
\]  

(46)

Solving this equation, using Eq. (44) and extending the results to other signs of \(\mu\) and \(\lambda\) we get

\[
\lambda_e \approx \frac{t^2 + \Delta^2}{|\Delta|^2 |\lambda^2 - |\mu||}.
\]  

(47)

While this equation is expected to be valid only near the topological transition, it is a good approximation for the whole range of chemical potential within the topological phase defined by \(2|\lambda| > |\mu|\) and \(\Delta \neq 0\), as indicated in Figs. 2 and 3. Note that \(\lambda_e\) diverges not only at the boundary \(|\mu| \to 2|\lambda|\) of the topological phase, but also for \(\Delta \to 0\), which is of course also a boundary of the topological phase and in addition to superconductivity.

For a chain of finite length \(L\), on general physical grounds one expects that the energy \(E\) of the low-energy excitations is proportional to \(\exp(-L/\lambda_e)\). This is supported by the analytical results of the previous section for \(\mu = 0\).
V. SPIN DISTRIBUTION ALONG A FINITE CHAIN

In this Section, we calculate the density of spin projection along the Rashba direction $z$ at each site of a finite long chain. We show that for subgap excitation with an odd number of particles, the ground state has a localized spin projection $S_z = \pm 1/4$ at each end.

For an even number of particles, the ground state $|g_e\rangle$ can be constructed by applying to the vacuum $|0\rangle_c$ of the $c_{j\sigma}$ operators $(c_{j\sigma}|0\rangle_c = 0)$ a product of all annihilation operators of excitations that satisfy

$$[\Gamma_{ij}, H] = E_{ij} \Gamma_{ij},$$

with positive $E_{ij}$. Denoting $\Gamma_{ij} = \Theta \Gamma_i \Theta^\dagger$, where $\Theta$ is the time reversal operator, the ground state can be written in the form

$$|g_e\rangle = N \prod_i \Gamma_{ij} |0\rangle_c,$$

where $N$ is a normalization factor.

The $z$ component of the spin operator at site $j$ is

$$S_j^z = \frac{c_{j\uparrow}^\dagger c_{j\downarrow} - c_{j\downarrow}^\dagger c_{j\uparrow}}{2}.$$ 

Therefore

$$\langle S_j^z \rangle = \langle g_e|S_j^z|g_e\rangle = \langle g_e|\Theta^\dagger \Theta S_j^z \Theta^\dagger \Theta |g_e\rangle = -\langle g_e|S_j^z|g_e\rangle = 0,$$

hence, the expectation value of the spin projection at each site vanishes in the ground state of a chain with an even number of particles.

The ground state for an odd number of particles, corresponds to creating the one-particle excitation of lowest energy to $|g_e\rangle$. The energy cost is rather large for all $\Gamma_i^\dagger$ except for the subgap states close to $E = 0$ calculated in the previous Section (or their generalization for finite $\mu$). The latter have energy $E \sim |z_i|^L - 2$ decaying exponentially with $L$. In order to split the spin degeneracy we assume that a small magnetic field is applied, so that the ground state becomes

$$|g_o\rangle = \Gamma_i^\dagger |g_e\rangle,$$

where

$$\Gamma_i = \sum_j \left( u_j c_{j\uparrow} + v_j c_{j\downarrow}^\dagger \right),$$

with the coefficients given by Eqs. (19), (25) and (40) for $\mu = 0$. Then

$$\langle S_j^z \rangle = \langle g_o|\Gamma_i S_j^z \Gamma_i^\dagger |g_o\rangle = \langle g_o|\Gamma_i S_j^z \Gamma_i^\dagger |g_c\rangle,$$

where we have used Eq. (54) in the last equality. From Eqs. (50) and (53) we get

$$[\Gamma_i, S_j^z] = \frac{u_j c_{j\uparrow} + v_j c_{j\downarrow}^\dagger}{2}.$$ 

Using $\langle g_e|\Gamma_i^\dagger = 0$ we can write Eq. (54) in the form

$$\langle S_j^z \rangle = \langle g_e|[[\Gamma_i, S_j^z], \Gamma_i^\dagger]|g_e\rangle,$$

and calculating the anticommutators using Eqs. (53) and (55) we finally obtain

$$\langle S_j^z \rangle = \frac{|u_j|^2 + |v_j|^2}{2}.$$

A. Examples

In Fig. 4 we show $\langle S_j^z \rangle$ for an odd number of particles and total spin projection $S_z = \sum_j S_j^z = 1/2$, obtained from the analytical solution, as described in the previous Section. We also checked the result by numerical diagonalization of the finite chain. The results are practically identical. The energy of the excitation (which coincides with the difference in energy of the ground state for odd an even particles) is $E = 6.314 \times 10^{-4}$. The numerical
energy is higher by \( \sim 2 \times 10^{-8} \) which can be ascribed to terms of order \( E^2 \) neglected in the analytical treatment.

Clearly half of the total spin projection is localized at each end of the chain and \( \langle S_i^z \rangle \) is practically zero in the middle of the chain. Although the physics is different, this is reminiscent of the spin 1/2 excitations at the ends of the \( S = 1 \) antiferromagnetic chain. In addition, there is a marked even-odd oscillation. While \( \langle S_i^z \rangle \) decays exponentially as the distance from the ends increase, \( \langle S_i^z \rangle \) vanishes exactly at distances equal to an odd number of lattice constants from the ends. This is a particular property of the case \( \mu = 0 \), but the oscillations remain for finite \( \mu \) as shown in Figs. 5 and 6.

In Fig. 5 we show \( \langle S_i^z \rangle \) as a function of the site, derived form the numerical solution of the chain for the same parameters as before, except for the fact that \( \mu \) is increased but not too much, in order that the system is kept within the topological region \( |\mu| < 2|\lambda| \). In this case, according to the calculations of the previous section, the localization length of \( \langle S_i^z \rangle \) at the ends of the chain increases from \( \lambda_c \approx 6.4 \) to 12.7. This is consistent with the increase in the magnitude of the energy by nearly an order of magnitude to \( E = 5.51 \times 10^{-3} \). In contrast to the case \( \mu = 0 \) for which the energy vanishes for chains of odd length, the energy is similar for one site less \( (E = 5.71 \times 10^{-3}) \) or one site more \( (E = 5.28 \times 10^{-3}) \). For the chosen length of the chain \( L = 80 \), with order of magnitude comparable to \( \lambda_c \approx 12.7 \), the spin excitations at the ends are not well separated. However, the overall trend is similar to the previous case, with larger \( \langle S_i^z \rangle \) at the ends and even-odd oscillations. Curiously, while for \( i \leq 10 \), \( \langle S_i^z \rangle \) is larger for odd sites, the situation is reversed for \( 11 \leq i \leq 30 \). A similar situation takes place at the other end replacing \( i \) by \( L + 1 - i \).

![Figure 5](image)

**FIG. 5:** Same as Fig. 4 for \( \mu = 0.2 \).

As shown in Fig. 6 if the length of the chain is increased while keeping the same energy parameters, \( \langle S_i^z \rangle \) near the ends is practically not affected. However it is now clear that the spin excitations at both ends are well separated. In this case, the excitation energy is \( E = 2.335 \times 10^{-4} \).

**VI. GENERAL PROPERTIES OF THE END STATES**

In this section, we would like to summarize some properties that are generally valid for the subgap excitations of any 1D TRITOPS system. In particular Eqs. (27) which we reproduce here for the ease of the reader

\[
\{\gamma_\uparrow, \gamma_\downarrow\} = p, \quad \{\tilde{\gamma}_\uparrow, \tilde{\gamma}_\downarrow\} = -p, 
\]

where \( p \) is defined in Eq. (18) have been demonstrated using a continuum formulation in Section II of the supplemental material of Ref. 23 for \( \phi = 0 \). We expect them to be generally valid. Extension for \( \phi \neq 0 \) is trivial using a gauge transformation.

These operators obey the commutation rules with the operator \( S_z \) (with \( z \) being the direction of the spin-orbit interaction) that were given in Eq. (28).

In the case of a finite chain with length \( L \), the exact subgap eigenstate with energy \( E > 0 \) given by Eq. (38), is a linear combination of the form given in Eq. (10),

\[
\Gamma_\uparrow = \frac{1}{\sqrt{2}} \left( \gamma_\uparrow + e^{i\theta} \tilde{\gamma}_\uparrow \right),
\]

which satisfies \( \{\Gamma_\uparrow, \Gamma_\downarrow\} = 0 \). The time-reversal partner is the operator defined in Eq. (12),

\[
\Gamma_\downarrow = \frac{1}{\sqrt{2}} \left( \gamma_\downarrow + e^{-i\theta} \tilde{\gamma}_\downarrow \right),
\]
The result is of generating two quasiparticles with \( \Gamma \) magnetic field (or Ising type interaction) energy of these excitations under the effect of a weak ground state and low-energy excitations, as well as the \( V \)

VII. EFFECT OF A MAGNETIC FIELD AT ONE END

A. Quasiparticles

In this Section we calculate the spin projection along the Rashba direction at the ends of the chain \( S_z^e \) of the ground state and low-energy excitations, as well as the energy of these excitations under the effect of a weak magnetic field (or Ising type interaction) \( B > 0 \) applied at one end only, parallel to the Rashba direction \( z \). Without loss of generality we assume that the field is applied at the right end of the chain and includes all sites for which \( \langle S_z^e \rangle \) is significantly different from 0 for \( B = 0 \), which means that the length of the region subject to the magnetic field is much larger than the localization length \( \lambda_c \) of the low-energy quasiparticles (see Sec. IV). In particular it can include the right half of the chain. For concreteness, we assume the latter option and write the Hamiltonian for the superconducting wire in the presence of the external magnetic field \( B \), described by a Zeeman coupling \( \Delta_Z = g\mu_B B \) as

\[
H_{\text{tot}} = H - \Delta_Z S_z^e, \tag{62}
\]

where \( S_z^R = \sum_{j=L/2}^{L} S_j^z \) is the operator of the total spin projection at the right half of the chain. A sketch is shown in Fig. 1 (see bottom left). Similarly for the left end \( S_L^z = S_z^e - S_j^e \). Alternatively, we can also consider a magnetic island or a magnetic adatom with classical magnetic moment \( M \) close to the right end of the chain coupled with the spin through an Ising interaction \( H_B = -JS_z^e M \). This is equivalent to the Hamiltonian of Eq. (62) upon identifying \( JM \equiv \Delta_Z \). In the case of the magnetic field we assume that its magnitude is much smaller than the critical field of the superconductor. In the case of the magnetic moment, we assume a weak coupling \( J \), such that it interacts with the subgap edge-state excitation but it does not induce low-energy Yu-Shiba-Rusinov states inside the superconducting gap. This assumption implies that we can restrict the effect of the magnetic field to the low-energy in-gap states.

Taking for the moment our analytical solution for \( \mu = 0 \) using Eqs. (40), (42), (21), and (26) we obtain

\[
[\gamma_\sigma, H_{\text{tot}}] = E\epsilon^{i\theta}\tilde{\gamma}_\sigma, \tag{63}
\]

where \( s = 1 \) (1) for spin \( \uparrow \) (\( \downarrow \)). For our model with \( \mu = 0 \), the explicit values of \( E \) and \( \epsilon^{i\theta} \) are given by Eqs. (58) and (39). However, we want to stress that the form of Eqs. (63) is generally valid for any TRITOPS chain: the zero modes of the infinite chain \( \gamma_\sigma \) at the left and \( \tilde{\gamma}_\sigma \) and the right become mixed and split in the finite chain by an effective hopping \( E\epsilon^{i\theta} \) whose detailed value depends on the particular system) for spin up, and time reversal symmetry implies a hopping \( E\epsilon^{-i\theta} \) for spin down. In addition, it can be easily seen from our analytical solution for \( \mu = 0 \) [see Eq. (30) and the sentence below it], that to linear order in \( B \) the end states of the infinite chain do not split if the magnetic field is applied perpendicular to the direction of the Rashba field (as in our notation). For general TRITOPS models a splitting for all directions of the magnetic field is expected, but with a strong anisotropy.

Using a Bogoliubov transformation, two annihilation operators can be defined such that

\[
[\Gamma_{B,\sigma}, H_{\text{tot}}] = E_\sigma \Gamma_{B,\sigma}, \tag{64}
\]

with \( E_\sigma > 0 \). Specifically

\[
\Gamma_{B,\sigma} = \alpha_\sigma \gamma_\sigma + \beta_\sigma \epsilon^{i\theta} \tilde{\gamma}_\sigma, \\
E_\sigma = r - \frac{\Delta_Z}{4}, \tag{65}
\]

\[\text{where } \theta \text{ depends on the model. Generally, going from the infinite chain to the finite one introduces a tunneling between the operators of both ends which can be written as } E\epsilon^{i\theta} \text{ with } E \text{ real. This point will be further discussed in the next Section [see Eqs. (63)], whose results are also generic. For the particular model of Section II, } \theta \text{ is given by Eq. (39).}

The operators \( \Gamma_\sigma \) annihilate two degenerate excitations (corresponding to \( \sigma = \uparrow, \downarrow \)) with energy \( E \). Let us also highlight that the structure of the operators \( \Gamma_\sigma \) defined in Eqs. (40) and (42) imply entanglement of the excitations localized at the left and the right ends of the chain. In fact, we can define two q-bit states in the basis of Eq. (31) \( \langle l, r \rangle \equiv \langle L, R \rangle \), with \( l, r = 0, 1 \) and analyze the effect of generating two quasiparticles with \( \Gamma_\sigma \) on these states. The result is

\[
\Gamma_\sigma^\dagger \Gamma_\sigma^\dagger |0, 0\rangle = \Gamma_\sigma^\dagger \Gamma_\sigma^\dagger |1, 1\rangle = 0, \\
\Gamma_\sigma^\dagger \Gamma_\sigma^\dagger \frac{1}{\sqrt{2}} [\langle 0, 1 \pm | 1, 0 \rangle] = \frac{B}{2\sqrt{2}} \left[ (e^{-i\theta} | 0, 0 \rangle - (1 \mp e^{-i\theta}) | 0, 1 \rangle \right]. \tag{61}
\]

We see that \( \Gamma_\sigma^\dagger \Gamma_\sigma^\dagger \) does not act on the subspace of product states of single qubits. On the other hand, since the phase \( \theta \) resulting from Eq. (39) is in general different from 0, \( \pi \), this operator maps Bell states into combinations of Bell states. Notice that this construction relies on the fact that for finite wires, the energy of the subgap states is finite. In contrast, in the limit of \( L \to \infty \), the four two-qubit states are exactly degenerate at \( E = 0 \) and two-quasiparticle excitations can be constructed with any linear combination of these states. These operators, obey the commutation rules with the Hamiltonian given by Eq. (43).
being
\[ r = \sqrt{(\Delta_Z/4)^2 + E^2}, \]
\[ \alpha_\uparrow^2 = \beta_\uparrow^2 = \frac{1}{2} + \frac{\Delta_Z}{4r}, \]
\[ \alpha_\downarrow^2 + \beta_\downarrow^2 = 1, \alpha_\sigma, \beta_\sigma > 0. \] 

Using Eqs. (27) and (66) one can verify that the operators \( \Gamma_{B,\sigma} \) and \( \Gamma_{B,\sigma}^\dagger \) obey canonical anticommutation rules.

### B. Zeeman splitting

The previous equations make explicit the fact that the finite energy \( E \) of the excitations in chains of finite length has associated an hybridization of the localized zero modes. This implies a degree of entanglement between modes localized at opposite ends. Our goal is to analyze the impact of this entanglement in the magnetic response.

The behavior of the quasiparticle excitations given by Eq. (65) have two important limits, which correspond to \( \Delta_Z \gg E \) and \( \Delta_Z \ll E \).

#### 1. \( \Delta_Z \gg E \)

This corresponds to strongly localized end states with energy \( E \sim 0 \). This situation is achieved for very long chains, where the end modes are almost completely decoupled. In this case we can expand \( r \) defined in Eq. (66) as \( r \sim (\Delta_Z/4) [1 + (4E/\Delta_Z)^2/2] \) and we get
\[ E_\uparrow = \frac{2E^2}{\Delta_Z}, \]
\[ E_\downarrow = \frac{2E^2}{\Delta_Z} + \frac{\Delta_Z}{2}. \] 

In this limit, the operator \( \Gamma_{B,\uparrow} \) that corresponds to the one-particle excitation with energy \( E_\uparrow \) [see Eq. (65)] tends to the quasiparticle \( \gamma_\uparrow \) localized at the left end of the chain \([\alpha_\uparrow^2 \sim 1\), see Eq. (66)], and is not affected by the magnetic field. In turn, the excitation with energy \( E_\downarrow \), related to \( \Gamma_{B,\downarrow} \sim \gamma_\downarrow \) with energy \( E_\downarrow \) corresponds to annihilating a quasiparticle at the right end of the chain with spin down for creating one with spin up since \( \gamma_\downarrow^\dagger = -\gamma_\uparrow^\dagger \), see Eq. (26). This leads to a decrease of the total energy in \( E_\downarrow \sim \Delta_Z/2 \), for annihilating an ordinary electron with spin down or creating one with spin up, which is the expected result for an ordinary spin 1/2.

Naturally, the complete spectrum of one-particle excitations also contains those corresponding to the Hermitian conjugate of the above described operators, in particular \( \gamma_\uparrow^\dagger \sim \gamma_\uparrow \) with an energy loss \( E_\uparrow \), so that an ordinary Zeeman splitting is \( 2E_\downarrow \sim \Delta_Z \) can be inferred from the magnetic-field dependence of the total spectral density of an ordinary electron observed in scanning tunneling spectroscopy, particularly if the STM tip is located near the end of the chain where the magnetic field is applied.

#### 2. \( \Delta_Z \ll E \)

This case corresponds to a sizable hybridization and entanglement of the end modes. In this other limit we consider \( r \sim E [1 + (\Delta_Z/4E)^2/2] \). Hence
\[ E_\uparrow = E \left[ 1 + \frac{1}{2} \left( \frac{\Delta_Z}{4E} \right)^2 \right] - \frac{\Delta_Z}{4}, \]
\[ E_\downarrow = E \left[ 1 + \frac{1}{2} \left( \frac{\Delta_Z}{4E} \right)^2 \right] + \frac{\Delta_Z}{4}. \] 

All low-energy quasiparticles have nearly equal weight at both ends \([\alpha_\uparrow^2 \sim 1/2, \beta_\uparrow^2 \sim 1/2], \) see Eq. (66)]. As a consequence, the effect magnetic field at only one end is reduced by a factor 1/2 with respect to the application of the field in the whole sample. The Zeeman splitting between the one-particle excitations of positive energy (corresponding to annihilation of quasiparticles) is \( E_Z = E_\downarrow - E_\uparrow = \Delta_Z/2 \), which is half the Zeeman splitting of a spin 1/2.

We believe that this splitting might be observed not only by an STM which senses the one-particle spectral density but also with microwave radiation which induces transitions conserving the number of electrons\(^{33,34}\). While the light does not couple directly with the spin, the spin-orbit coupling couples it with the orbital degrees of freedom and circularly polarized light induces transition between states with angular momentum projection 1/2 and -1/2. As before, the full spectrum of one-particle excitations also contains negative energies with the same moduli as the positive ones described above.

### C. Spin polarization

As in section \( \nabla \) the ground state \( |g_\sigma\rangle \) for an even number of particles is constructed by applying all annihilation operators to the vacuum of the \( c_{i\sigma} \). Following a similar procedure as in Section \( \nabla \) and Eqs. (65), we obtain for this state \( \sum_{i=1}^L \langle S_i^\sigma \rangle = \sum_{i=1}^L \langle g_i | S_i^\sigma | g_e \rangle = (\beta_\uparrow^2 - \beta_\downarrow^2)/2 = \Delta_Z/(4r) \). For odd number of particles, the ground state is \( |g_\sigma\rangle = \Gamma_{B,\uparrow}^\dagger |g_e\rangle \), with excitation energy \( E_\uparrow \), and the expectation value of the spin projection at the right is \( \sum_{i=L/2}^L \langle S_i^\sigma \rangle = \beta_\uparrow^2/2 \). Then, using Eqs. (66) depending on the number of particles \( N \), the expectation value of the spin projection at the right end (where the magnetic field is applied) is
\[
\langle S^z_R \rangle = \frac{1}{4} + \frac{\Delta_Z}{4\sqrt{(\Delta_Z)^2 + 4E^2}}, \quad N \text{ odd},
\]
\[
\langle S^z_R \rangle = \frac{\Delta_Z}{2\sqrt{(\Delta_Z)^2 + 4E^2}}, \quad N \text{ even}
\]

In Fig. 7 we show this spin projection for an odd number of particles and the difference between the ground state energies for odd and even number of particles \(E(B)\) as a function of the magnetic field. For \(B = 0\), \(E(0) = E\) and \(\langle S^z_R \rangle = 1/4\), consistent with the fact that the total spin-1/2 excitation is identically distributed among the left and right halves of the chain, as discussed in previous sections. In general \(1/4 \leq \langle S^z_R \rangle \leq 1/2\) and \(0 \leq E(B) = E_\uparrow \leq E\), and for \(\Delta_Z \gg E\), \(E(B) \to 0\) and \(\langle S^z_R \rangle \to 1/2\), implying a fully polarized state for sufficiently large values of the magnetic field. Concomitantly, the spin projection at the left half of the chain \(\langle S^x_L \rangle = 1/2 - \langle S^z_R \rangle\) decreases from 1/4 at \(B = 0\) to vanishing small values for high magnetic field. Thus a finite chain with positive \(E\) is necessary to observe manifestations of a fractional \(S^z_e\).

![Graph](image_url)

**FIG. 7:** (Color online) Spin projection at the right end of the chain (left scale dashed line) and excitation energy of the ground state (right scale full line) for an odd number of particles as a function of magnetic field applied to the right end.

**VIII. SUMMARY AND DISCUSSION**

We have calculated the low-energy eigenstates of a finite chain of a time-reversal-invariant topological superconductor numerically and in the particular case of an electron-hole symmetric band \((\mu = 0)\) also analytically. The analytical solution allows one to gain insight on the main features of the Majorana zero-energy excitations at the ends of the topological chain and how the end states mix in the finite chain giving rise to low-energy excitations with finite energy.

Using these solutions we have calculated spin projection for each site \(i\) of the chain \(\langle S^z_i \rangle\) along the Rashba direction \(z\) in finite chains. We show that excitations with total spin projection \(S_z = \pm 1/2\) fractionalize in two pieces with \(S^z_e = \pm 1/4\) localized at each end of the chain. \(\langle S^z_i \rangle\) displays oscillations with an exponential envelope. The decay length of \(\langle S^z_i \rangle\) at each end can be calculated solving a quartic equation with complex coefficients for any \(\mu\) and is well approximated by a simple analytical formula [Eq. (17)].

Although we presented results for a specific model Hamiltonian, all the physical behavior discussed in the present work is generic of TRITOPS wires.

The finite energy excitation \(E\) in chains with an odd number of particles with respect to those with even number of particles should be experimentally detectable. In ordinary superconductors, this energy is of order of the superconducting gap and has been measured in experiments in small islands in which capacitance effects allow researchers to control the number of electrons in small superconducting systems\(^{33,34}\). Furthermore, these experiments permit to tune the chemical potential \(\mu\) changing the localization length of the states at the end of the chain and the excitation energy \(E\) of the quasiparticles entangling both ends. In the present case, \(E\) lies deep inside the superconducting gap. Alternatively, scanning tunneling microscope measurements\(^{35,36}\) could also detect these subgap excitations.

An application of a magnetic field opens other interesting possibilities. The excitation energy \(E\) is split by the magnetic field. Applying the field only to one end of the chain would open the possibility of analyzing the response of the fractional \(S^z_e\) for an odd number of particles. We identify two possible scenarios, depending on the amplitude of the Zeeman energy \(\Delta_Z\) relative to the energy of the excitations without magnetic field \(E\). In the case of \(\Delta_Z \gg E\), which can be easily achieved for very long chains, the end excitations are almost uncorrelated. The magnetic response is basically that of a single spin 1/2 which can accommodate parallel or antiparallel to the magnetic field as well as in the opposite end without coupling to the magnetic field. On the other hand, for \(\Delta_Z \ll E\), the entanglement between left and right end excitations manifests itself in the magnetic response. In this case, there is a Zeeman splitting of the excitations equal to \(\Delta_Z/2\). This is precisely half the magnitude of the one expected for a ordinary spin 1/2 and reflects the fact that \(S_z\) is fractionalized, with \(S^z_e = \pm 1/4\) at the ends. Scanning tunneling microscope measurements akin to those used to investigate Yu-Shiba-Rusinov excitations induced by magnetic impurities should be able to detect these features in the subgap spectrum of TRITOPS wires\(^{37}\). We believe that also microwave radiation\(^{38,39}\) can produce transitions between the quasiparticles split...
by $\Delta z/2$ for a small magnetic field.

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Appendix A: Summary of the method by Alase et al in the Nambu formalism

We start by expressing the Hamiltonian of Eq. (1) in terms of Nambu spinors $\psi_j^\dagger = \left( c_{j \uparrow}^\dagger, c_{j \downarrow}^\dagger, c_{j \uparrow}, -c_{j \downarrow}^\dagger \right)$. The result is

$$H = \sum_{j=1}^{L} \psi_j^\dagger h_0 \psi_j + \sum_{j=1}^{L-1} \left( \psi_j^\dagger h_1 \psi_{j+1} + H.c. \right), \quad (A1)$$

with

$$h_0 = \frac{\mu}{2} \sigma_0 \otimes \tau_z,$$

$$h_1 = -\frac{t}{2} \sigma_0 \otimes \tau_z + i\frac{\lambda}{2} \sigma_z \otimes \tau_z + \Delta \tau_z. \quad (A2)$$

Here $\sigma_j$ and $\tau_j$ are Pauli matrices acting on the spin and particle-hole degrees of freedom, respectively, while $\sigma_0$ and $\tau_0$ are $2 \times 2$ unit matrices. We define the state $|j\rangle$ associated to the Nambu operator $\psi_j$ such that

$$H = \sum_{j=1}^{L} h_0 |j\rangle \langle j| + \sum_{j=1}^{L-1} \left( h_1 |j\rangle \langle j+1| + H.c. \right). \quad (A3)$$

In this notation we define projector operators over bulk ($P_B$) and boundary ($P_{bou}$) as follows

$$P_B = \sum_{j=2}^{L-1} |j\rangle \langle j|, \quad P_{bou} = |1\rangle \langle 1| + |L\rangle \langle L|. \quad (A4)$$

The projector $P_B$ is over all the sites in which all the Hamiltonian matrix elements are contained in the chain, while $P_{bou}$ contains the sites at the left and right ends of the chain. They satisfy $P_B + P_{bou} = 1$.

Following Alase et al, we aim to solve the bulk-boundary eigenvalue problem

$$P_B H |\Psi\rangle = E P_B |\Psi\rangle, \quad P_{bou} H |\Psi\rangle = E P_{bou} |\Psi\rangle. \quad (A5)$$

We construct a generalized Bloch state expanding in powers of a complex number $z$ as follows

$$|\psi^B(z)\rangle = w_z \sum_{j=1}^{L} z^{j-1} |j\rangle. \quad (A6)$$

The latter is represented with a spinor of the form $|\psi^B(z)\rangle = (u_\uparrow(z), u_\downarrow(z), v_\uparrow(z), -v_\downarrow(z))^T$. The coefficients $(u_\sigma(z), v_\sigma(z))$ are determined in order to satisfy

$$P_B [H - E(z)] |\psi^B(z)\rangle = 0. \quad (A7)$$

The rest of the calculation continues in Eq. (9) to Eq. (11). The four eigenstates corresponding to the solution of the bulk problem (A7) are Nambu states $|\psi^B_k\rangle \equiv |\psi^B(z_k)\rangle$ of the bulk Hamiltonian with $u_{\sigma,k} > 0$ given by Eq. (12) for $\sigma = \uparrow$ and the same equation changing the sign of both $\Delta$ and $\lambda$ for $\sigma = \downarrow$.

The last step is to find the solution of the full eigenvalue equation $(H - E) |\Psi\rangle = 0$. To this end we express the state $|\Psi\rangle$ as a linear combination of the bulk eigenstates $|\psi^B_k\rangle$,

$$|\Psi\rangle = \sum \alpha_k |\psi^B_k\rangle. \quad (A8)$$

The coefficients $\alpha_k$ and the energy $E$ are determined in order to satisfy

$$P_{bou} [H - E] |\Psi\rangle = 0. \quad (A9)$$

The corresponding coefficients are given by Eqs. (13) and (14).

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