Phase diagram of a model for topological superconducting wires

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We calculate the phase diagram of a model for topological superconducting wires with local s-wave pairing, spin-orbit coupling $\hat{\lambda}$ and magnetic field $\vec{B}$ with arbitrary orientations. This model is a generalized lattice version of the one proposed by Lutchyn et al. [Phys. Rev. Lett. 105 077001 (2010)] and Oreg et al. [Phys. Rev. Lett. 105 177002 (2010)], who considered $\hat{\lambda}$ perpendicular to $\vec{B}$. The model has a topological gapped phase with Majorana zero modes localized at the ends of the wires. We determine analytically the boundary of this phase. When the directions of the spin-orbit coupling and magnetic field are not perpendicular, in addition to the topological phase and the gapped nontopological phase, a gapless superconducting phase appears.

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I. INTRODUCTION

The study of topological superconducting wires, which host Majorana zero modes (MZMs) at their ends, is a field of intense research in condensed matter physics, not only because of the interesting basic physics involved, but also because of possible applications in decoherence-free quantum computing.

In 2010, Lutchyn et al. and Oreg et al. proposed a model for topological superconducting wires describing a system formed by a semiconducting wire with spin-orbit coupling (SOC) and proximity-induced s-wave superconductivity under an applied magnetic field perpendicular to the direction of the SOC. This yields a topological superconducting phase with MZMs localized at its ends. The observation of these MZMs in these types of wires was reported in different experimental studies.

The search for different models and mechanisms leading to topological superconducting phases continues being a very active avenue of research theoretically and experimentally.

More recently, there has been experimental research as well as theoretical studies in similar models, including those for time-reversal invariant topological superconductors, of the effects of MZMs in Josephson junctions, in particular because the dependence on the applied magnetic flux introduces an additional control knob.

In particular, it has been recently proposed that the current-phase relation measured in Josephson junctions may be used to find the parameters that define the MZMs. A possible difficulty in these experiments is the slow thermalization to the ground state in the presence of a gap. A way to circumvent this problem is to rotate the magnetic field slowly from a direction not perpendicular to the SOC in which the system is in a gapless superconducting phase, in which thermalization is easier. Therefore, it is convenient to know the phase diagram of the system and the extension of this gapless phase.

In this work we calculate the phase diagram of the lattice version of the model and discuss in particular the gapless phase. The paper is organized as follows. In Sec. II we describe the model. The topological invariants used to define the phase diagram are presented in Sec. III. In Sec. IV we show the numerical results, analytical expressions for the boundaries of the topological phase and discuss briefly the Majorana zero modes. We summarize the results in Sec. V.

II. MODEL

The model for topological superconducting wires studied in this work is the lattice version of that introduced by Lutchyn et al. and Oreg et al. The Hamiltonian can be written as

$$H = \sum_{\ell} \left[ c_{\ell}^\dagger \left( -t \sigma_0 - i\hat{\lambda} \cdot \vec{\sigma} \right) c_{\ell+1} + \Delta c_{\ell\uparrow}^\dagger c_{\ell\downarrow}^\dagger + \text{H.c.} \right] - c_{\ell}^\dagger \left( \vec{B} \cdot \vec{\sigma} + \mu \sigma_0 \right) c_{\ell},$$

(1)

where $\ell$ labels the sites of a chain, $c_{\ell} = (c_{\ell\uparrow}, c_{\ell\downarrow})^T$, $t$ is the nearest-neighbor hopping, $\hat{\lambda}$ is the SOC, $\Delta$ represents the magnitude of the proximity-induced superconductivity, $\vec{B}$ is the applied magnetic field and $\mu$ is the chemical potential. As usual, the components of the vector $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and $\sigma_0$ is the 2x2 unitary matrix. The pairing amplitude $\Delta$ can be assumed real. Otherwise, the phase can be eliminated by a gauge transformation in the operators $c_{\ell\sigma}^\dagger$, that absorbs the phase.

Without loss of generality, we choose the $z$ direction as that of the magnetic field ($\vec{B} = B\hat{z}$) and $x$ perpendicular to the plane defined by $\hat{\lambda}$ and $\vec{B} = (\lambda_y \hat{y} + \lambda_z \hat{z})$. After Fourier transformation, the Hamiltonian takes the form $H = \sum_k H_k$, with
Using the four-component spinor \((c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger, c_{-k\uparrow}, c_{-k\downarrow})\) the contribution to the Hamiltonian for wave vector \(k\) can be written in the form

\[
H_k = -(\mu + 2t \cos(k))(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{k\downarrow}^\dagger c_{k\downarrow}) - B(c_{k\uparrow}^\dagger c_{-k\downarrow} - c_{k\downarrow}^\dagger c_{-k\uparrow}) + 2\lambda_2 (c_{k\uparrow}^\dagger c_{k\downarrow} - c_{-k\uparrow}^\dagger c_{-k\downarrow}) + \Delta (c_{k\uparrow}^\dagger c_{-k\downarrow} + c_{-k\uparrow}^\dagger c_{k\downarrow}).
\]

In addition, a \(\mathbb{Z}_2\) invariant \(I\) can be defined from the relative sign of \(\text{Det}(A)\) (which is real for \(k = 0\) and \(k = \pi\)) between the points \(k = 0\) and \(k = \pi\):

\[
I = (-1)^W = \left\lfloor \frac{\text{Det}(A(\pi))}{\text{Det}(A(0))} \right\rfloor.
\]

III. TOPOLOGICAL INVARIANTS

In this section we define the topological invariants we use to characterize the topological phases. In general, the Hamiltonian belongs to topological class D with a \(\mathbb{Z}\) topological invariant corresponding to a winding number \(\gamma\). In this case, the calculation of the topological invariant is simpler, as shown by Tewari and Sau.

Following this work, we perform a rotation in \(\pi/2\) around the \(y\) axis in particle-hole space, which transforms \(\tau_x\) to \(\tau_y\): \(H'_{k} = UH_kU^\dagger\) with \(U = \text{exp}(-i\pi/4)\tau_y\).

Taking \(z = 0\), this rotation yields an off-diagonal (chiral symmetric) Hamiltonian. This allows us to define a winding number \(W\) (a topological \(\mathbb{Z}\) invariant) from the phase of the determinant of the \(2 \times 2\) matrix \(A(k)\), which is the upper right corner of Eq. (5) from which the Berry phase \(\gamma = -\text{Im} \int_{0}^{2\pi} \frac{d\theta}{\theta} \langle u(k)| \frac{\partial}{\partial k} | u(k) \rangle\).
In our model, $H_k$ has four eigenvalues $E(k)$. The lowest one $E_1(k)$ is always negative and the corresponding eigenvector has always a Berry phase 0. From the above mentioned charge-transfer symmetry, the fourth eigenvalue (the highest one) has energy $E_4(k) = -E_1(-k) > 0$. Therefore, the Berry phase of the second eigenvalue (which is equal to that of the third one) determines the $\mathbb{Z}_2$ invariant. We have calculated the Berry phase $\gamma$ of each of the four bands (and particularly the second one) from the normalized eigenvectors $|u_j⟩ = |u(k_j)⟩$ of the $4 \times 4$ matrix obtained numerically at $M$ wave vectors $k_j = 2\pi(j - 1)/M$, using a numerically invariant expression\cite{26,33}. This expression is derived in the following way. Discretizing Eq.\cite{9} and approximating $\partial|u(k)/\partial k = (M/2\pi)(|u(k_{j+1})⟩ - |u(k_j)⟩)$, one obtains

$$\gamma = -\text{Im} \sum_{j=1}^{M} [⟨u_j| (|u_{j+1}⟩ - |u_j⟩)]. \quad (10)$$

If $M$ is large enough so that $k_j$ and $k_{j+1}$ are very close, then $x = ⟨u_j|u_{j+1}⟩ - 1$ is very small and one can retain only the first term in the Taylor series expansion $\ln(1 + x) = -x^2/2 + ...$ Replacing in Eq. (10) one obtains

$$\gamma = -\text{Im} [\ln(P)], \quad \text{where}$$

$$P = ⟨u_1|u_2⟩⟨u_2|u_3⟩...⟨u_{M-1}|u_1⟩ \quad (11)$$

It is easy to see that Eq. (10) is gauge invariant. This means that the result does not change if $|u(k)⟩$ is replaced by $e^{i\varphi(k)}|u(k)⟩$, where $\varphi(k)$ is a smooth function with $\varphi(2\pi) = 0$. Similarly, the product $P$ is independent of the base chosen by the numerical algorithm to find the eigenstates $|u_j⟩$. Therefore, Eq. (11) is numerically gauge invariant. Analyzing the change in the results with increasing $M$, we find that $M \sim 250$ is enough to obtain accurately all phase boundaries shown below. A further increase in $M$ leads to changes that are not visible in the scale of the figures.

This $\mathbb{Z}_2$ topological invariant defined by the Berry phase of the second (or third) state can be trivially extended to the gapless case if the energies of the second and third state do not cross as a function of $k$. Even if the energies cross the Berry phases can be calculated switching the states at the crossing. However, this case is not of interest here.

**IV. RESULTS**

**A. Phase diagram**

We start by discussing the simplest case of perpendicular $\vec{\lambda}$ and $\vec{B}$. In Fig. 1 we display the resulting phase diagram for some parameters, showing the possible different shapes. There are two gapped phases, the trivial (white region II) and the topological one (light gray I), separated in general by two circular arcs defined by Eqs. (8). For simplicity we discuss the case $t, B > 0$. The topological character is independent of the sign of the different parameters. If $B < 2t$, the region of possible values of $|\mu|$ inside the topological sector extends from $2t - B$ to $2t + B$ for $\Delta \to 0$ and shrinks for increasing $\Delta$ until it reduces to the point $|\mu| = 2t$ for $\Delta \to B$. If $B = 2t$, the semicircle touches the point $\mu = 0$. For larger $B$, the region $|\mu| < \sqrt{B^2 - 2} - 2t$ for $\Delta^2 < B^2 - 4t^2$ is excluded from the topological region.

![FIG. 1. Phase diagram in the $\mu, \Delta$ plane for perpendicular $\vec{\lambda}$ and $\vec{B}$, $t = 1$, $\lambda = |\vec{\lambda}| = 2$, and several values of $B$. Gray region I denotes the topological sector and white region II the non topological one.](image)

![FIG. 2. (Color online) Phase diagram in the $\mu, \Delta$ plane for $t = 1$, $\lambda = 2$, $B = 4$ and several values of the angle $\beta_{AB}$ between $\vec{\lambda}$ and $\vec{B}$. Regions I and II as in Fig. 1. Region III (IV) in dark gray (black) corresponds to the gapless phase with Berry phase $\pi$ $(0)$. The red points at the top left corresponds to numerical calculations which detected localized states at the ends.](image)
for general angles $\beta_{AB}$ between both vectors, there is a
finite region in the $\mu$, $\Delta$ plane for which the gap vanishes,
in particular for $|\Delta| < \Delta_c$, where $\Delta_c$ is a critical value,
independent of $\mu$, determined analytically below. Before
presenting the analytical calculation, we describe the
general features of each phase in the phase diagram, as
shown in Fig. 2. The gapped regions in the figure are de-
denoted by I and II. The remaining two regions are gapless.
We separate them by the trivial (topological) character of
the Berry phases of the second and third eigenstate, indicat-
ing the corresponding regions with black (dark gray)
color and roman number IV (III). In spite of the topolog-
ic phase to the gapless phases, we represent in Fig. 3 the
finite region in the $\mu$, $\Delta$ plane.

We have also checked the boundaries of the topological
phase solving numerically finite chains and searching for
localized states at their ends and the presence of the finite
gap. The localized states are described in Sec. [14,13]. For
convenience, we discuss first the case $z = 0$ (perpendicular $\hat{\lambda}$ and $\vec{B}$) and later consider the general case $\lambda = \lambda_x \hat{x} + \lambda_z \hat{z}$ with $\lambda_z \neq 0$. For
$\lambda_z = 0$, the determinant $D_0(k)$ of $H_k$ [see Eqs. (11) or (13)]

$$D_0(k) = C^2 + 4\Delta^2y^2,$$

$$C = a^2 + \Delta^2 - B^2 - y^2,$$  

(12)
is positive semidefinite. It can vanish only for $y = 0 \implies$k = 0 or $k = \pi$. For $k = 0$ ($k = \pi$), $C = 0 \implies |\mu + 2t| = r$ ($|\mu - 2t| = r$). Comparing with Eqs. (8), one realizes that
the gap vanishes in general only at one wave vector and
only at the transition between topological and non-topological
gapped phases, as expected. The exception is the case $|t| = r$ and $\mu = 0$, for which
the gap vanishes at both wave vectors.

In the general case with $z = 2\lambda_z \sin(k)$ non zero, the
determinant of $H_k$ is [see Eq. (8)]

$$D(k) = D_0 + 2z^2(\Delta^2 + y^2 - a^2 - B^2) + z^4$$  

(13)

We can consider $D(k)$ as a function of $x = \cos(k)$. For
large enough $|\lambda_x|$, it turns out that, at the wave vector
$k = 0$, and parameters for which $C = y = z = 0$ [imply-
ing $D(0) = 0$, $dD(x)/dx > 0$ and as a consequence for
small positive $k$ ($x < 1$) the determinant becomes neg-
ave signaling the instability of the gaped phase. For
$\lambda_x = 0$, as in the previous case the derivative is negative,
but $x$ cannot be increased beyond 1, so that $D(k) \geq 0$. A
similar reasoning with the corresponding changes in the
sign can be followed for $k = \pi$. An explicit calculation of
the derivative using the conditions $C = \sin(k) = 0$ gives

$$\frac{dD}{dx} = 32[B^2\lambda_x^2 - \Delta^2(\lambda_x^2 + \lambda_y^2)]x.$$  

(14)

This implies that to have a gap one needs that $|\Delta| > \Delta_c$
where

$$\Delta_c = B^2\frac{\lambda_x^2}{\lambda_x^2 + \lambda_y^2} = B^2\cos^2(\beta_{AB}).$$  

(15)

This condition has been found before for a model similar
to ours in the continuum with quadratic dispersion.

After some algebra, the determinant in the general case

$$D = (C - x^2)^2 + 16(\lambda_x^2 + \lambda_y^2)(\Delta^2 - \Delta_c^2)(1 - x^2),$$  

(16)
is again positive semidefinite for $|\Delta| > \Delta_c$ and
positive definite for $0 \neq k \neq \pi$, indicating a gaped gap.
Since $x = 1$ implies $y = z = 1$, the remaining boundaries
of the topological phase remain the same as for perpen-
dicular $\lambda$ and $\vec{B}$. For $|\Delta| = \Delta_c$ (as in Fig. 4), the values of $k$ for which the determinant vanishes are given by the solutions with $|x| \leq 1$ of the following quadratic equation

$$0 = 4(t^2 + \lambda^2)x^2 + 4t\mu x$$

$$+ \mu^2 + \Delta_c^2 - B^2 - 4\lambda^2,$$  

(17)

where $\lambda = |\lambda|$.  

C. Transition from the topological phase to the gapless phases

To gain insight into the transition from the topological
phase to the gapless phases, we represent in Fig. 6
the second and third eigenvalues of $H_k$ [$E_2(k)$ and $E_3(k)$,
respectively] for different values $\beta_{AB}$ of the angle between
$\lambda$ and $\vec{B}$. The parameters are such that, for $\lambda \cdot \vec{B} = 0$,
the system is in the topological phase with a finite
gap. As the angle is changed (in either direction) the
gap between the second and third eigenvalue decreases
until at a certain critical angle [given by the solution of
Eq. (17)] $E_2(k_c) = E_3(k_c) = 0$ at one particular wave
vector $k_c$ (0.3613\pi in the figure), denoting the onset of the
-gapless phase. Further turning $\lambda$ and $\vec{B}$ to the parallel
(or antiparallel) direction, both eigenvalues vanish at two
different wave vectors.
If keeping the other parameters fixed, the chemical potential $\mu$ is changed towards one border $\mu_c$ of the topological phase for $\vec{\lambda} \cdot \vec{B} = 0$ [given by Eq. (8)]; the critical wave vector $k_c$ is displaced either to $k_c = 0$ or to $k_c = \pi$ depending on the border. This is illustrated in Fig. 4. At the corresponding border $\mu = \mu_c$, one has $E_2(k_c) = E_3(k_c) = 0$, indicating a crossing of the levels which is also accompanied by a change in the Berry phases of the corresponding eigenvectors. Further displacing $\mu$ the system enters the non topological gapped phase. Therefore, the point $\mu = \mu_c$, $\Delta = \Delta_c$, is at the border of the topological phase, the nontrivial gapless phase with Berry phase $\pi$, and the non-topological gapped phase. In fact also the trivial gapless phase reaches this tetracritical point in the phase diagram (see Fig. 2).

**D. Majorana modes**

The topological phase is characterized by the presence of Majorana modes zero modes at the ends of an infinite chain. For a finite chain, the modes at both ends mix, giving rise to a fermion $\Gamma$ and its Hermitian conjugate with energies $\pm E$ which decay exponentially with the length $L$ of the chain. We have obtained $\Gamma$ numerically in chains of $L \sim 200$ sites. The probability $p(i)$ of finding a fermion at site $i$ (adding both spins and creation and annihilation) is shown in Fig. 5. The main feature of the top figure is a decay of $p(i)$ as the distance from any of the ends increases. We have chosen a case with a rather slow decay to facilitate visualization. In addition to this decay, some oscillations are visible with a short period. In order to quantify the decay length of the localization of the end modes, we have fit the probability with an exponentially decaying function $p(i) \sim A \exp(-i/\xi)$ at the left end. At the bottom of Fig. 5 we show the dependence of $\xi$ inside the topological phase I as one of the parameters is varied. As expected, $\xi$ diverges at the boundary with the non topological gapped phase II, which has a different $\mathbb{Z}_2$ topological invariant (at $\Delta_{c_3} = 3.872983346$ in the figure). We also find that $\xi$ diverges at the boundary with the gapless phase III (at $\Delta_{c_3} = 0.694592711$ in the figure), a phase with the same topological invariant but gapless. These facts allow us to obtain numerically the transitions from the localization of the end states (see top left panel of Fig. 2).

**FIG. 3.** (Color online) Second (black thin lines) and third (red thick lines) eigenvalues of $H_0$ as a function of wave vector for $t = 1$, $\lambda = \Delta = 2$, $B = \mu = 5$, and several values of the angle $\beta_{AB}$ between $\vec{\lambda}$ and $\vec{B}$.

**FIG. 4.** (Color online) Same as Fig. 3 for $t = 1$, $\lambda = \Delta = 2$, $B = 5$, $\beta_{AB} = 66.42^\circ$ and several values of $\mu$.

**FIG. 5.** Top: probability of finding a fermion at each site of a chain for the eigenstate of lowest positive energy for $t = 1$, $\lambda = 2$, $B = 4$, $\beta_{AB} = 80^\circ$, $\mu = 3$, and $\Delta = 0.75$. Bottom: inverse of the localization length as a function of $\Delta$. The transition between phases I and III is at $\Delta_{c_1} = 0.694592711$ and the transition between phases I and II is at $\Delta_{c_2} = 3.872983346$. 

\[ \beta_{AB} = 0^\circ \quad \beta_{AB} = 20^\circ \]

\[ \beta_{AB} = 40^\circ \quad \beta_{AB} = 66.42^\circ \]

\[ \beta_{AB} = 80^\circ \quad \beta_{AB} = 90^\circ \]
V. SUMMARY AND DISCUSSION

Using numerical and analytical methods, we calculate the phase diagram of a widely used model for topological superconducting wires, the essential ingredients of which are local s-wave pairing $\Delta$, spin-orbit coupling $\lambda$ and magnetic field $B$. We determine the boundary of the gapped topological phase analytically. This phase contains robust Majorana zero modes at both ends that are of great interest. We expect that this result will be relevant for future studies in the field.

The optimal situation for topological superconductivity is when $B$ is perpendicular to $\lambda$. In this case, both the topological and non-topological phases are gapped. If instead $B$ has a component in the direction of $\lambda$, a gapless superconducting phase appears for certain parameters. This phase can also be separated in two phases differing in a $\mathbb{Z}_2$ topological invariant. However, due to the absence of a gap, we do not find Majorana zero-modes at those present in the gapped topological phase.

Tilting the magnetic field to enter the gapless phase might be used as a trick to relax the system to the ground state in some measurements, like Josephson current. In the gapped topological phase, in the absence of low-frequency phonons or other excitations, the physics is dominated by a few bound states inside the gap, completely isolated from the continuum, and the current would oscillate, without reaching a steady state. One way to avoid this problem would be to use a magnetic field so that the system is in the gapless phase, with low-energy excitations available for thermalization, and then rotate adiabatically the field to the desired value so that the system remains in the ground state.

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