Polynomial description of inhomogeneous topological superconducting wires

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Abstract
We present the universal features of the topological invariant for p-wave superconducting wires after the inclusion of spatial inhomogeneities. Three classes of distributed potentials are studied, a single-defect, a commensurate and an incommensurate model, using periodic site modulations. An analytic polynomial description is achieved by splitting the topological invariant into two parts; one part depends on the chemical potential and the other does not. For the homogeneous case, an elliptical region is found where the topological invariant oscillates. The zeros of these oscillations occur at points where the fermion parity switches for finite wires. The increase of these oscillations with the inhomogeneity strength leads to new isolated non-topological phases. We characterize these new phases according to each class of spatial distributions. Such phases could also be observed in the XY model, to which our model is dual.

Keywords: topological phase transition, 1D p-wave superconductor, disorder

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

1. Introduction

Topological phases arising in superconducting materials have become a major research topic in condensed matter physics in the recent years [1–3]. Indeed, the search for Majorana zero modes observation in labs has already begun [4–6]. The potential application of these quantum phases is sustained by their robustness against a weak disorder, suggesting its realization in fault tolerant quantum computing [7–9]. Hence, it is important to survey the effect of disorder in such topological phases.

A paradigmatic model in this context is the Kitaev chain [10], a lattice version of a spinless p-wave superconducting wire, whose topological phase has a bulk gap protected by time-reversal and particle-hole symmetries. The properties of this model, including spatial modulations, have been broadly and intensely studied [11–19]. Moreover, complex cases including symmetry breaking interactions, like spin-orbit or quartic fermionic terms, have been proposed to study recent experiments [20–23]. Yet, the key ingredients of the Kitaev free model can deal with the essential aspects of the topology with or without interactions, since all strongly interacting topological phases can be represented by noninteracting systems [24–26].

There are some previous works dedicated to study the Kitaev chain with modulated chemical potentials [11–17], while other works deal with a modulated hopping [18, 19]. They found, exploiting among other tools a scaled chemical potential [12, 13], that the spatial distributions strongly modify the original topological phase diagram of the Kitaev model. Here, we are able to explain the origin of those changes by introducing a topological invariant which is characterized by an oscillatory polynomial delimited by two values. We took the strategy of separately modulate the chemical potential and the hopping amplitude to compare with previous works, as well as to pinpoint qualitatively the differences of these two cases. We also took three representative classes of distributions to predict general trends of the modulations.

In particular, we can predict how new non-topological isolated phases emerge with the inhomogeneities and characterize all changes induced on the phase diagram. For example, in the homogeneous case the zeros of the oscillatory function

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of our approach are exactly at the positions where the fermion parity of the ground state for finite wires switches, positions that were previously obtained by other approaches [15, 16]. We therefore propose that our method can be further used to describe the fermion parity switches in the general inhomogeneous case. We also propose to use this method to detect and map new paramagnetic phases in the ferromagnetic region of the phase diagram of the one-dimensional XY model, when the transverse field or any other exchange coupling constant are equally modulated. The latter is achievable because the Kitaev chain can be mapped exactly onto the XY model through a non-local Jordan-Wigner transformation [27, 28].

The paper is organized as follows: in section 2, we introduce the model, present the different site distributions we use and indicate the symmetry properties that classify it in the BDI symmetry class. The Z-type topological invariant is constructed using the Zak phase. We also present here our main results, where new non-topological regions appear in the phase diagram due to the modulations. In section 3, we introduce our approach of separating the topological invariant into two parts, one involving the chemical potential and the other does not. We further compare two examples, the homogeneous case and a site-distributed case, to unveil the origin of the new non-topological phases obtained in this work. In section 4, we present some physical insights and summarize the main results, where new non-topological regions appear in the phase diagram due to the modulations. In section 5, we present some physical insights and summarize our results. An appendix compiles useful information about the polynomials.

2. The model

Consider a periodically modulated Kitaev model, with site-dependent chemical potentials and hopping amplitudes through an enlarged unit-cell—of size $q$—repeated along the chain, while using periodic boundary conditions. Generically, for a system with $N$ sites we can write such model Hamiltonian as $\mathcal{H} = \sum_{\ell=1}^{N/q} \mathcal{H}_\ell$, where

$$\mathcal{H}_\ell = \sum_{s=x,y,z=1}^q \mu_s \hat{c}_{s,\ell}^\dagger \hat{c}_{s,\ell} + \sum_{s=x,y,z=1}^q \left( -t_s \hat{c}_{s,\ell}^\dagger \hat{c}_{s,\ell+1} + \Delta \hat{c}_{s,\ell}^\dagger \hat{c}_{s,\ell+1} \right) + \text{H.c.}$$

$\mathcal{H}_\ell$ is a tight-binding model of spinless fermions with a site-dependent chemical potential ($\mu_s$), a site-dependent hopping amplitude ($t_s$), and a triplet $p$-wave superconducting pairing ($\Delta$). For the site modulations we use either

$$\mu_s = \mu (1 + \lambda w_s),$$

$$t_s = t (1 + \lambda w_s),$$

for the chemical potential or for the hopping amplitude, respectively, while $\Delta$ is kept real and constant. The additional parameter $\lambda$ provides the strength of the inhomogeneity and $w_s$ are the spatial distributions, which are taken as

$$w_s = \begin{cases} \delta_{s,1}, & \text{a single-defect (S)} \\ \cos(2\pi s/q), & \text{commensurate (C)} \\ \cos(2\pi s/3), & \text{incommensurate (I)} \end{cases}$$

where $\beta = (3 + 1)/2$ is the golden ratio. The first of these distributions (S) needs no justification, while the others two (C,I) are in the class of Aubry-André or Harper potentials, useful for studying the interrelation of disorder and superconductivity [17, 29–31].

Upon using the Fourier transformation in each unit cell, $\hat{c}_{s,\ell}^\dagger = \sqrt{q/N} \sum_k \hat{c}_{s,k} e^{i\beta k}$, with $k \in (-\pi/q, \pi/q]$, the reduced Brillouin zone, and through the well-known Bogoliubov-de Gennes (BdG) transformation [32],

$$\hat{\Psi}_k^{\dagger} = (\hat{c}_{1,k}^\dagger, \ldots, \hat{c}_{q,k}^\dagger, \hat{c}_{-1,k}^\dagger, \ldots, \hat{c}_{-q,k}^\dagger),$$

we can write down the Hamiltonian in momentum space as

$$\mathcal{H} = \frac{1}{2} \sum_k \hat{\Psi}_k^\dagger \mathcal{H}_k \hat{\Psi}_k = \frac{1}{2} \sum_k \hat{\Psi}_k^\dagger \left( V_k M_k - V_k^\dagger \right) \hat{\Psi}_k,$$ (5)

where $V_k$ and $M_k$ are $q \times q$ matrices whose non-zero elements are: $V_k^{s,s'} = \mu_s$ for $s = 1, \ldots, q$; $V_k^{s,s+1} = V_k^{s+1,s} = -t_s$ and $M_k^{s,s+1} = M_k^{s+1,s} = -\Delta$ for $s = 1, \ldots, q - 1$; while $V_k^{1,q} = (V_k^{q,1})^* = -t_q e^{i\beta q}$ and $M_k^{1,q} = (-M_k^{q,1})^* = -\Delta e^{i\beta q}$ (see also Gao et al [18]).

As long as the values of $\mu_s$, $t_s$ and $\Delta$ are real, this model has a time-reversal symmetry $\mathcal{T} = K$ ($K$ takes the complex conjugate) that satisfies $\mathcal{T} H k \mathcal{T}^{-1} = -H_k$, while the BdG transformation evinces a particle-hole symmetry of the model, characterized by $\mathcal{P} = \tau_z K$ (where $\tau_z$ is the Pauli matrix acting on the particle-hole space) that satisfies $\mathcal{T} H_k \mathcal{P}^{-1} = -H_{-k}$. With these two operators, we can build a chiral operator $\mathcal{C} = \mathcal{T} \mathcal{P} = \tau_z$ that satisfies $\mathcal{C} H_k \mathcal{C}^{-1} = -H_{-k}$. For the operators described above, we have $\mathcal{T}^2 = \mathcal{P}^2 = \mathcal{C}^2 = I$, classifying this 1D system into the BDI symmetry class [33, 34], whose topological invariant is characterized by a $Z$-index.

The topological invariant can be built from the Zak phase [35–37], which is the Berry phase for periodic fermion systems. To implement it, we first rotate the Hamiltonian (5) into a purely off-diagonal form

$$\Omega H_k \Omega^\dagger = \begin{pmatrix} 0 & A_k \\ A_k^\dagger & 0 \end{pmatrix}, \quad A_k = V_k + M_k,$$ (6)

where $\Omega = e^{-i\pi \tau_z}$ is the unitary transformation and $\tau_z$ is the Pauli matrix acting on the particle-hole space. The topological index is thus the winding number of the eigenstates in the reduced Brillouin zone, which for this kind of off-diagonal (chiral) matrix is given by [36]

The pairing $\Delta$, which comes from an effective mean-field approach, was kept real and constant to compare with previous works. Another aspect would be to consider a pairing of the form $\Delta = |\Delta| e^{i\phi}$, with a phase constant, which can be eliminated by a gauge transformation. See [10].
\[ \mathcal{W} = -\frac{i}{\pi} \int_{k=0}^{\pi} \frac{d\xi}{z_k}, \quad \text{where} \quad z_k = \frac{\text{Det}(A_k)}{\text{det}(A_k)}, \]  
(7)

In our approach, the winding number \((\mathcal{W} \in \mathbb{Z})\) can be evaluated through the sign of the function \(\text{Det}(A_k)\) at the particle-hole symmetric points, \(\kappa = 0\) and \(\pi/q\),

\[ \mathcal{W} = \frac{1}{2} \left[ \text{sgn}\{\text{Det}(A_{\pi/q})\} - \text{sgn}\{\text{Det}(A_0)\} \right]. \]  
(8)

This expression is easy to understand, since for a model of nearest-neighbors interactions the winding vector \(z_k\) develops a single one-loop in \(C\) as a function of \(k\), which is symmetric with respect to the real axis. We note from its definition that \((A_k)^* = A_{-k}\) so the function \(\text{Det}(A_k)\) is real at the extreme points, \(\kappa = 0\) and \(\pi/q\). When the loop encloses the origin of \(C\), the real function \(\text{Det}(A_0)\) has opposite signs at these points. In that case, we have from equation (8): \(\mathcal{W} = \pm 1\), i.e. a topological \((T)\) phase. Meanwhile, if the loop does not include the origin of \(C\), we have a non-topological \((NT)\) phase, with \(\mathcal{W} = 0\).

The closure of the bulk gap, which occurs only for \(\kappa = 0\) and \(\pi/q\), is given by \(\text{Det}(A_0) = 0\). The latter can be inferred from equation (6), which implies \(\text{Det}(H_0) = \text{Det}(A_0)\text{Det}(A_{\pi/q})\), therefore, \(\text{Det}(A_0)\) can only vanish if \(H_0\) has a vanishing determinant or equivalently a zero eigenvalue. The gap-closing specifies the locations where the topological quantum phase transitions take place.

We have chosen some particular values of the parameters to show the variations induced by modulations on the phase diagrams. Examples for the spatial distributions (S,C,I), applied separately to the chemical potential and to the hopping amplitude, can be viewed in figure 1. Due to the particle-hole symmetry, the phase diagrams of figure 1 are symmetric with respect to \(\Delta/t\) and \(\mu/t\), thus we plot them for \(\mu > 0\) only. Apart from the variations of the Ising transition lines at the well-known values \(\mu = \pm 2t\) of the homogeneous case, especially those in figures 1(b) and (e), we observe in all cases the emergence of non-topological compact domains (‘bubbles’) around \(\Delta/t = 0\). The number and shape of these isolated bubbles depend on the cell size \(q\), on the inhomogeneity strength \(\lambda\), as well as on the spatial distribution. They look rather different when spatial modulations are applied either to the chemical potential or to the hopping amplitude, as can be seen from the top and bottom panels in figure 1, respectively.

### 3. Polynomial description

For the origin of the emerging bubbles in the topological regions of the phase diagram in the inhomogeneous cases, we consider some analytical aspects of the topological invariant. First, we rewrite the (real) function \(\text{Det}(A_k)\), for \(\kappa = 0\) and \(\pi/q\), as

\[ \text{Det}(A_k) = U(\mu, \Delta, q, \lambda) - \Lambda_k(\Delta, q, \lambda), \]  
(9)

where \(U\) is a \(\kappa\)-independent polynomial function that carries all the dependence on \(\mu\), and \(\Lambda_k\) is the difference, in our \((q, \lambda)\) scheme. According to equation (8), and the discussion following it, we observe that the system is topological \((\mathcal{W} \neq 0)\) when \(U\) is within the region delimited by both \(\Lambda_k\) (viz: \(\Lambda_0 < U < \Lambda_{\pi/q}\)) and non-topological \((\mathcal{W} = 0)\) otherwise. For the singular cases where \(\text{Det}(A_k) = 0\), namely \(U = \Lambda_k\), equation (8) is undefined, though these points demarcate the loci of the \(T\)-\(NT\) transitions in the phase diagram, namely, the closure of the bulk gap. For the purpose of analysis, we shifted our functions \(U\) and \(\Lambda_k\) according to the sum rule expression (12) below and refer, from now on, to the shifted functions. The shift is defined as to obtain \(\Lambda_0 = -\Lambda_{\pi/q}\).

To understand the role played by the functions \(U\) and \(\Lambda_k\), we have plotted in figure 2 the homogeneous case (left panels) and the inhomogeneous single-defect model applied to the chemical potential (right panels), respectively. The phase diagrams, (a) and (b), are given together with the related behavior of the functions \(U\) and \(\Lambda_k\), in (c) and (d).

In the homogeneous case, we see from figure 2(c) that the function \(U\) oscillates between the two \(\Lambda_k\) functions, for \(|\mu| \leq 2t\), defining thus a topological phase in that region. Whereas in the single-defect case of figure 2(d), the function \(U\) leaves these two limits because its oscillations are now enhanced by the presence of modulations. These extrapolations of the function \(U\) produce the bubbles seen in figure 2(b). These bubbles have alternating sign, as seen from the figure. The borders of these bubbles, as described above, are the points of gap-closings, origin of the topological quantum phase transitions. We observed that at the places where \(U = \Lambda_{\pi/q}\) the gap closes at \(k = 0\), while at the places where \(U = \Lambda_0\) the gap closes at \(\pi/q\). Beyond the topological phase, in the \(\mu/t\) axis, the oscillating function \(U\) changes character and becomes unbounded in all cases. These are the trends caused by the modulations and they can be explained analytically as given below.

### 4. Analytical properties of the topological invariant

#### 4.1. The homogeneous case

After detailed algebraic and numerical manipulations we found, in the homogeneous case \((\lambda = 0)\), that the function \(U\) can be written as

\[ U(\mu, \Delta, q, 0) = \left(\sqrt{1 - (\Delta/t)^2} \right)^q \bar{U}_H(\bar{\mu}, q), \]  
(10)

where \(\bar{\mu} = \mu/\sqrt{1 - (\Delta/t)^2}\) is a scaled chemical potential, identical to the one found in DeGottardi et al [12, 13], while \(\bar{U}_H(\bar{\mu}, q)\) is described by a polynomial in \(\bar{\mu}\) of degree \(q\), restricted to integers \(q \geq 2\)

\[ \bar{U}_H(\bar{\mu}, q) = \sum_{n=1}^{q} a_q^n \bar{\mu}^n, \]  
(11)

whose coefficients \(\bar{a}_q^n \in \mathbb{Z}\) can be obtained through the following recurrence formula: \(a_q^0 = 1\) for all \(q\), \(a_q^q = \mp q\) (alternating) for \(q\) odd and \(a_q^n = 0\) for \(q\) even, while for \(1 < n < q\) we have \(a_q^n = a_{q-1}^{n-1} - a_{q-2}^n\) for \(q - n\) even and \(a_q^n = 0\) for \(q - n\) odd. Some of these \(a_q^n\) coefficients are given in table A1, of the appendix. We notice that the nonzero coefficients of this polynomial expansion have alternating signs for each \(q\). The oscillatory behavior of the function \(U\) is due to this fact. It is easily seen that \(U\), as a function of \(\mu\) is symmetric for \(q\) even.
and antisymmetric for \( q \) odd, while it is always symmetric with respect to \( \Delta \).

As for the delimiting functions \( \Lambda_n \) in equation (9), we found a useful relation in the form of a sum rule

\[
\Lambda_{n/q} + \Lambda_0 = \left( \frac{1}{\sqrt{1 - (\Delta/t)^2}} \right)^q s^{1/2} (1 + s)^2, \tag{12}
\]

where \( s = (-1)^q \) and the factor \((1 + s)^2\) dictates that this sum is zero for \( q \) odd, while for even \( q \) the sum rule can be shifted to zero using this expression. All three functions \( U, \Lambda_{n/q} \) and \( \Lambda_0 \) will be shifted in the same way, keeping equation (9) unaltered. This is an important point in our approach to get the fermion parity switches locations for homogeneous finite wires.

Using (12), we thus need to deal with only one of these polynomials. In this work we study \( \Lambda_0 = \Lambda_0(\Delta, q) \), which is given by an even polynomial in \( \Delta \) \((b_q^0 = 0 \text{ for } n \text{ odd})\)

\[
\Lambda_0(\Delta, q) = \sum_{n=0}^{q} b_n^0 \Delta^n. \tag{13}
\]

Some of these \( b_n^0 \) coefficients are given in table A2, of the appendix. They do not have a simple constructing rule, although we observe the cyclic pattern ‘4202’ for \( b_0^0 \), we also have \( b_q^0 = 0 \) for all \( q \), while \( b_{q-1}^0 = 2q \) for \( q \) odd, also \( b_{q-2}^0 = q^2 \) for \( q \) even, etc. Such description is not complete however.

An interesting point is that the alternating integer polynomial \( \overline{U}_H(\mu, q) \) in (11) has more than one root (in fact, \( q \) real roots), that yield an oscillatory behavior for \( U \) within the dome \( \bar{\mu} = 2t \), that is, inside the ellipse \((\mu/2t)^2 + (\Delta/t)^2 = 1 \) (see figure 2(a)). Outside from this elliptical dome \( U \) has no more oscillations, as \( \overline{U}_H \) turns from an alternating to a positive polynomial in \( \mu \) in that case. Such analytical behavior is a critical combination of the prefactor \( \left( \frac{1}{\sqrt{1 - (\Delta/t)^2}} \right)^q \) and the scaled \( \bar{\mu} = \mu/\sqrt{1 - (\Delta/t)^2} \) that appear in equation (10).

This result is quite consistent with those seen in Hegde et al [15, 16], about the positions of fermion parity switches for homogeneous finite wires.

4.2. Modulated chemical potential

When site modulations are applied to the chemical potential the sum rule (12) still applies, the polynomial expansion of \( \Lambda_0(\Delta, q) \) is thus the same as in (13), viz table A2, while the function \( U \) can be written now as

\[
U(\mu, \Delta, q, \lambda) = \left( \frac{1}{\sqrt{1 - (\Delta/t)^2}} \right)^q (\overline{U}_H + \overline{U}_\lambda). \tag{14}
\]
For the (S) single-defect case, apart from the polynomial $U_H$ we have an additional inhomogeneous contribution which is linear on $\lambda$, that is

$$U(\bar{\mu},q,\lambda) = \lambda U_S(\bar{\mu},q)$$

(14), with the same recurrence formula for the coefficients $a^q_n$, except that $a^q_1 = \pm 1$ (alternating) for $q$ odd and $a^q_1 = 0$ for $q$ even. Some of these $a^q_n$ coefficients are given in table A3, of the appendix.

On the other hand, for the commensurate (C) and the incommensurate (I) potentials applied to $\mu_s$, the extra contributions in (14) do not depend on $\Delta$ but are nonlinear on $\lambda$. That is, we have integer polynomials $U^c_\lambda$ written as $U^c_\lambda(\bar{\mu},q,\lambda)$ and $U^I_\lambda(\bar{\mu},q,\lambda)$, respectively. We have not yet found a simple recurrence formula for them, but we can give some examples. For the (C) commensurate case, for $q = 3$, we have

$$U^c_\lambda(\bar{\mu},q = 3,\lambda) = \frac{1}{4} \lambda^3(\lambda - 3) \bar{\mu}^3,$$

(15)

whilst for the (I) incommensurate case, also for $q = 3$, we have

$$U^I_\lambda(\bar{\mu},q = 3,\lambda) = -[\cos(2\pi\beta) + \cos(4\pi\beta) + \cos(6\pi\beta)] \lambda(\bar{\mu} - \bar{\mu}^3) + [\cos(2\pi\beta) \cos(4\pi\beta) + \cos(2\pi\beta) \cos(6\pi\beta)] \lambda^2 \bar{\mu}^3$$

(16)

$$+ [\cos(4\pi\beta) \cos(6\pi\beta)] \lambda^3 \bar{\mu}^3.$$

4.3. Modulated hopping amplitude

Significant differences already begin when spatial modulations are applied to the hopping amplitude $t_s$. For the (S) single-defect case, for example, we found a function $U$ described as

$$U(\mu,\Delta,\lambda) = \left(1 - \frac{(\Delta/t)^2}{(1 - (\Delta/t)^2)^2}\right)^q \times \left[U^c_H(\bar{\mu},q) + \frac{\lambda^2(\lambda + 2)}{(1 - (\Delta/t)^2)^2} U^H_S(\bar{\mu},q)\right].$$

(17)
Likewise, the sum rule for the $\Lambda_\kappa$ functions is now
\[
\Lambda_{\pi/q} + \Lambda_0 = \left(\sqrt{1 - (\Delta/t)^2}\right)^q s^{1/2} (1 + s)^2 \\
\times \left(1 + \frac{\lambda(\lambda + 2)}{1 - (\Delta/t)^2(1 + s)}\right).
\]

In (17) we have $\tilde{U}_S = \tilde{U}_S(\mu, q)$, which is a polynomial in $\mu$ of degree $q \geq 3$, given by the same recurrence formula as in (11), except that the largest-power non-zero coefficients are now given by $a_q^q = -1$ (viz.: $a_q^q = a_q^{q+1} = 0$ for all $q$). Some of these coefficients are given in table A4, of the appendix. Interestingly enough, we see that by eliminating the first column in table A3 and inverting signs we find an equivalence with table A4. We have not yet understood the origin of this similarity.

We notice in equations (17) and (18) the extra terms in $\lambda(\lambda + 2)$, which depend also on $\Delta$. This contribution expands the dome of the oscillations of the function $U$ beyond the limits $\Delta/t = \pm 1$, as is indeed observed in figure 1(d).

The sum rule (18) of the $\Lambda_\kappa$ functions, gives us a selected polynomial $\Lambda_0(\Delta, q, \lambda) = \sum_{\alpha=0}^{q} b_{\alpha}^q \Delta^\alpha$ which is an even polynomial in $\Delta$ whose coefficients are nonlinear in $\lambda$. Some of these coefficients can be seen from table A5, of the appendix. We notice that when $\lambda = 0$ they match those in table A2, as it should be.

Lastly, for the commensurate (C) and the incommensurate (I) potentials applied to the hopping, a general expression for the function $U$ is
\[
U(\mu, \Delta, q, \lambda) = \left(\sqrt{1 - (\Delta/t)^2}\right)^q \frac{U_H + \tilde{U}_\lambda}{\mu}.
\]

Namely, the corresponding inhomogeneous $\tilde{U}_\lambda$ terms, $U_C = \tilde{U}_C(\mu, \Delta, q, \lambda)$ or $U_I = \tilde{U}_I(\mu, \Delta, q, \lambda)$, respectively, are now polynomials of degree $q$ in $\mu$ and $\Delta$, which cannot be simply factorized as in (14) or in (17). The latter two cases in (19) are examples where the above elliptical description does not apply anymore, as can be inferred from the dashed lines in figures 1(e) and (f). The farthest case from an elliptical description is the latter one in figure 1(f), for which the incommensurate (I) distribution provides a rather complex $U$ function. In these cases, we do not have integer polynomials anymore, and a new approach should be devised.

Neither recurrence formulas for $\tilde{U}_C$, $\tilde{U}_I$ nor sum rules for $\tilde{\Lambda}_\kappa$ in the modulated $t_i$ case were yet found, but we can give some examples. The function $\tilde{U}_C$ in the (C) commensurate case applied to the hopping, when $q = 5$, for instance, is given by
\[
\tilde{U}_C(\mu, \Delta, q = 5, \lambda) = -5\Delta^2 \lambda^2 \mu + 5\sqrt{3} + 7 - \lambda^4 \mu - \frac{5}{2} \lambda^2 \mu^3 - 5\sqrt{3} + 1 - \lambda^2 \mu,
\]
while the new delimiting function $\tilde{\Lambda}^C_q$, for $q = 5$, is

$$
\tilde{\Lambda}^C_5(\Delta, q = 5, \lambda) = 2 + \frac{1}{8}\lambda^2\left(140 + 75\lambda^2 + \lambda^3 - 60\Delta^2\right).
$$

Similarly, the function $\tilde{U}_1$ in the (I) incommensurate case applied to the hopping, for $q = 3$, is given by

$$
\tilde{U}_1(\mu, \Delta, q = 3, \lambda) = -\mu\left[2\lambda(\cos(2\pi\beta) + \cos(4\pi\beta)) + \lambda^2(\cos^2(2\pi\beta) + \cos^2(4\pi\beta)) + \cos(4\pi\beta)(6\pi\beta)\right],
$$

while for the new delimiting function $\tilde{\Lambda}^I_3$, for $q = 3$, we have

$$
\tilde{\Lambda}^I_3(\Delta, q = 3, \lambda) = 2(1 + 3\Delta^2)
$$

$$
+ 2\lambda(1 + \Delta^2)\left[\cos(2\pi\beta) + \cos(4\pi\beta) + \cos(6\pi\beta)\right]
+ 2\lambda^2\left[\cos(2\pi\beta)\cos(4\pi\beta)\cos(6\pi\beta) + \cos(2\pi\beta)\cos(6\pi\beta)\right]
+ \cos(4\pi\beta)(6\pi\beta)
+ 2\lambda^3\left[\cos(2\pi\beta)\cos(4\pi\beta)\cos(6\pi\beta)\right].
$$

5. Concluding remarks

In order to have some insight into the new phases found in this work, we have studied the eigenstates of $H_k$ to see the characteristics of the band structure at both sides of a bubble. We will use a strategy which is successfully employed nowadays in topological band theory [38]. We took as an example the (S) single-defect case applied to the chemical potential, which is given in figure 2(b), but this analysis is equally valid for other distributions. We see the comparison of the low-lying bands in figure 3 at two points that are close in the phase diagram, 3(a) outside and 3(b) inside a bubble, whose gap closes at $\pi/q$, as explained in section 3. The way our BdG Hamiltonian (5) was built in, we can distinguish the particle-part from the hole-part of these eigenstates. We used a particle-projection operator applied to the eigenstates to plot them blue for particle-like (projection above 50%) and red for hole-like (projection below 50%). What is interesting is that there is a band inversion in the states from $k = 0$ to $\pm\pi/q$ close to the gap at $E = 0$, when comparing the topological bands in 3(a) with the non-topological bands in 3(b), which is an indication of a change in the fermion parity. The parity inversion between (a) and (b) indicates a change of occupancy of one fermion state, which is another way of detecting the presence of Majorana edge modes in the topological phase. This is a confirmation example of the utility of our method for detecting the fermion parity switches in the general inhomogeneous cases, as proposed in the Introduction.

In summary, we have studied the effects of spatial inhomogeneities in the 1D $p$-wave Kitaev model, for which we constructed a polynomial description for the topological invariant using an enlarged-unit cell approach. We applied the method to three different classes of spatial distributions, (S,C,I), although it can be easily expanded to more general cases, like those including longer-range hoppings and pairings [39-41].

A comparative study was made for modulated chemical potentials and modulated hopping amplitudes, using the same site distributions, finding very clear differentiations, as the examples from figure 1 have demonstrated. The modulations applied to the chemical potential, for example, preserve the elliptical region of the oscillations in $(\mu/2\Delta)^2 + (\Delta/\mu)^2 = 1$, as mentioned above, while those applied to the hopping amplitude do not. This marked difference will establish a strong dichotomy for diagonal versus off-diagonal disordered systems. These differentiations would not have been seen if we had applied the modulation in both parameters. Additionally, our results are fully consistent with previous works [11-19].

The oscillatory behavior of the polynomial function $U$ and its delimiting functions $\Lambda_e$ take account of most of the topological features of the model, not only on the origin of emerging non-topological bubbles around the anisotropy line $(\Delta = 0)$ in the topological region of the phase diagram, but also about the exact positions of the ground-state fermion parity switches for homogeneous finite wires which, according to Hegde et al [15, 16], are given by the elliptical curves

$$
\mu = 2t\cos\left(\frac{\pi p}{q + 1}\right)
$$

where $p = 1, 2, \ldots, [q/2]$, with $[q/2]$ the integer part of $q/2$.

The fact that our periodic boundary bulk results are consistent with those for open boundary systems, with edge Majorana fermions, obtained otherwise through the large size limit of the transfer matrix approach [15, 16], is a consequence of the bulk-edge correspondence. Therefore, with this validity test we propose to use these results also for the inhomogeneous cases. The new zeros of the shifted function $U$, like those seen in the examples of figures 1 and 2, should be the positions of the new fermion parity switches in those cases. This proposal was confirmed using a single test, shown in figure 3, where a fermion parity inversion was obtained.

Moreover, as a by-product, since the Kitaev chain is exactly mapped onto the XY model through a Jordan-Wigner transformation [27, 28], we hope that other authors would be willing to observe paramagnetic bubbles in the ferromagnetic region of the inhomogeneous dual XY model, as well.

What would remain to verify is whether the oscillations of the spin correlation function for the XY model will be at the same oscillatory region of the shifted function $U$, as it is in the homogeneous case.

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Appendix. Polynomial coefficients

In the following, we write some tables for the coefficients of the polynomials introduced in the main text.

Table A1. Some coefficients \( a_n \) with \( 1 \leq n \leq q \), of the polynomial \( \mathcal{U}_3 \) in the homogeneous case. It is easy to observe the constructing rule \( a_n = a_{n-1}^2 - a_{n-2}^2 \).

| \( n \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| \( q \) | 2 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | 3 | −3 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| | 4 | 0 | −4 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| | 5 | 5 | 0 | −5 | 0 | 1 | 0 | 0 | 0 | 0 |
| | 6 | 0 | 9 | 0 | −6 | 0 | 1 | 0 | 0 | 0 |
| | 7 | −7 | 0 | 14 | 0 | −7 | 0 | 1 | 0 | 0 |
| | 8 | 0 | −16 | 0 | 20 | 0 | −8 | 0 | 1 | 0 |
| | 9 | 9 | 0 | −30 | 0 | 27 | 0 | −9 | 0 | 1 |
| | 10 | 0 | 25 | 0 | −50 | 0 | 35 | 0 | −10 | 0 | 1 |

Table A2. Some coefficients \( b_q \) of the delimiting function \( \Lambda_0(\Delta, q) \) in the homogeneous and the modulated \( \mu_i \), cases.

| \( n \) | \( q \) | 0 | 2 | 4 | 6 | 8 |
|---|---|---|---|---|---|---|
| 2 | 4 | 0 | 0 | 0 | 0 |
| 3 | 2 | 6 | 0 | 0 | 0 |
| 4 | 0 | 16 | 0 | 0 | 0 |
| 5 | 2 | 20 | 10 | 0 | 0 |
| 6 | 4 | 24 | 36 | 0 | 0 |
| 7 | 2 | 42 | 70 | 14 | 0 |
| 8 | 0 | 64 | 128 | 64 | 0 |
| 9 | 2 | 72 | 252 | 168 | 18 |
| 10 | 4 | 80 | 440 | 400 | 100 |

Table A3. Some coefficients \( c_q \) of the polynomial \( \mathcal{U}_3(\bar{\mu}, q) \) for the (S) single-defect model in the modulated \( \mu_i \), case.

| \( n \) | \( q \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | −1 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 0 | −2 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| 5 | 1 | 0 | −3 | 0 | 1 | 0 | 0 | 0 | 0 |
| 6 | 0 | 3 | 0 | −4 | 0 | 1 | 0 | 0 | 0 |
| 7 | −1 | 0 | 6 | 0 | −5 | 0 | 1 | 0 | 0 |
| 8 | 0 | −4 | 0 | 10 | 0 | −6 | 0 | 1 | 0 |
| 9 | 1 | 0 | −10 | 0 | 15 | 0 | −7 | 0 | 1 |
| 10 | 0 | 5 | 0 | −20 | 0 | 21 | 0 | −8 | 0 | 1 |

Table A4. Some coefficients \( \sigma_q \) of the polynomial \( \mathcal{U}_3(\bar{\mu}, q) \) for the (S) single-defect model in the modulated \( \mu_i \), case.

| \( n \) | \( q \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | −1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 0 | −1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 2 | 0 | −1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | 3 | 0 | −1 | 0 | 0 | 0 | 0 | 0 |
| 7 | −3 | 0 | 4 | 0 | −1 | 0 | 0 | 0 | 0 |
| 8 | 0 | −6 | 0 | 5 | 0 | −1 | 0 | 0 | 0 |
| 9 | 4 | 0 | −10 | 0 | 6 | 0 | −1 | 0 | 0 |
| 10 | 0 | 10 | 0 | −15 | 0 | 7 | 0 | −1 | 0 |
| 11 | −5 | 0 | 20 | 0 | −21 | 0 | 8 | 0 | −1 |

Table A5. Some coefficients \( b_q \) of the function \( \Lambda_0(\Delta, q, \lambda) \) for the (S) single-defect model in the modulated \( \mu_i \), case.

| \( n \) | \( q \) | 0 | 2 | 4 | 6 |
|---|---|---|---|---|---|
| 2 | (2 + \lambda)^2 | 0 | 0 | 0 |
| 3 | (2 + \lambda)^2 | (2 + \lambda)^2 | 0 | 0 |
| 4 | −\lambda^2 | (4 + \lambda)^2 | 0 | 0 |
| 5 | (2 + \lambda)^2 | (4 + \lambda)^2 | (2 + \lambda)^2 | 0 |
| 6 | (2 + \lambda)^2 | (2 + \lambda)^2 | (2 + \lambda)^2 | (6 + \lambda)^2 | 0 |
| 7 | 2(1 + \lambda)^2 | 2(1 + \lambda)^2 | (7 + 3\lambda)^2 | 10(7 + 3\lambda)^2 | 2(7 + \lambda)^2 |
| 8 | −\lambda^2 | (64 + 48\lambda + 3\lambda^2) | (128 + 64\lambda - 3\lambda^2) | (8 + \lambda)^2 |

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