In quantum mechanics, the spaces of momentum and its conjugate, the position, are related via Fourier transforms and thus the properties are interwoven with their structure. In particular, for lattice systems possessing an underlying discrete position space, the momentum becomes finite. Moreover, if the lattice length is finite, \( L < \infty \), the momentum space also becomes both finite and discrete breaking altogether the continuity of the dispersion relation. This aspect is relevant in new systems such as the topological materials. We address this point paving the path for new ways to the observation of Majorana quasi-particles. Furthermore, the Kitaev model, which is the simplest Hamiltonian supporting Majorana fermions, is therefore taken as a starting point for the theoretical description of the work. Our study focuses on finding the zero-energy modes in an artificial arrangement of a non-interacting superconducting finite nanowire by using a discrete-sine transform with the purpose of going from position to momentum space considering hard-wall boundary conditions in the process. Here, a new \( L \)-dimensional Nambu operator to diagonalize the system in the Bogoliubov-de Gennes formalism is proposed and, further, we arrive to a new space with a considerable reduced dimension allowing the treatment of larger system sizes. We also present a comparison between the numerical and third order perturbation theory for the weak coupling regime results presenting an excellent agreement. Finally, we analyze the wavefunctions of the retrieved zero-energy modes showing that they are indeed edge states and thus they have an exponential decay.

I. INTRODUCTION

Nature always surprises us with novel wonders. Nowadays, the condensed matter community focuses efforts on rare materials such as topological insulators that behave as insulators in the inside keeping conducting states on its surface [1]. Although band insulators may present surface states with conducting properties, the main feature of the topological version is that they present a non-trivial symmetry-protected topological order [2–7]. This fact can be used to achieve nanometric scale holograms using nanometric topological insulator thin films as an optical resonant cavity [4], to name but an instance.

On the other hand, one of the most attractive phenomena expected to appear in high-energy physics is unveiling itself as low energy excitations in condensed matter systems. This is the particular case of both Weyl and Majorana fermions [5–7]. The former appear as solution of the Dirac equation for massless spin-1/2 particles [8] and were discovered as collective excitations in TaSa since its linearly dispersing valence and conduction bands cross at discrete points enabling the material to host them [9]. More recently, new effects have come to light as the Kondo effect on such materials rendering them as Weyl-Kondo semimetals [10], widening the possibilities of innovation and technology out of this field. The later rise from superconducting topological materials where the surface states may host non-fundamental excitations known as Bogoliubov quasiparticles that are their own antiparticles thus bringing them the nickname of Majorana zero modes.

The Majorana fermions idea permeates several fields going from high energy physics theories [11, 12], to condensed matter experimental realizations [13–16] including quantum computing and spintronics applications. In the later, the Majoranas are presented in form of non-trivial emergent excitations rather than fundamental particles.

The immense development of experimental techniques in ultracold atomic Fermi gases in the last years has opened new avenues for the research of strongly correlated systems in condensed matter physics and beyond. The ability to control the interactions via Feshbach resonances [17] sets new perspectives for experimental realization and study of several different exotic systems such as spin-polarized superfluidity (with population imbalance), superconductivity with nontrivial Cooper pairing and Bose-Fermi mixtures or mixtures of fermions with unequal masses, among others [18–20]. Currently, the unconventional superconductivity with a non-trivial Cooper pairing lays down one of the most important directions of studies in the theory of condensed matter [21] and ultracold quantum gases [22, 23].

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(Dated: August 8, 2018)

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Retrieval of free-Majorana wavefunctions for the finite Kitaev chain using an appropriate momentum representation
A remarkable simple model holding unpaired Majorana fermions has been presented by Kitaev [24], which is a model of topological superconductor comprised of spinless fermions and thus is the model we consider. It can be experimentally realized by a semiconducting finite nanowire device able to accommodate Cooper pairs through an artificial arrangement holding a strong spin-orbit interaction in proximity to an s-wave superconductor under the action of a external magnetic field [13–16]. Moreover, the Kitaev chain is equivalent to the Su-Schrieffer-Heeger (SSH) model [25] that has several experimental realizations where the topological features are observed [26, 27].

Keeping all that in mind, this paper is organized as follows. In Sec. II we briefly introduce the Kitaev model and use the Bogoliubov-de Gennes formalism in momentum space to retrieve its energy spectrum however missing the unpaired Majoranas due to the unbroken translational symmetry. Then, we employ a revised version of the Fourier transform that imposes hard-wall boundary conditions allowing the rise of edge states. Later, in Sec. III, we consider a weak coupling regime where the pairing is treated as a small perturbation up to 3rd order on a tight-binding model to retrieve the system spectrum. Then, Sec. IV focuses on the edge states retrieving the wave function in both momentum and position spaces and thus is devoted to conclusions and exponential decay. And finally, Sec. V is devoted to conclusions and remarks.

II. MODEL AND METHOD

We consider the Kitaev model described by the Hamiltonian [24]

$$\hat{H} = \sum_l \left[ \left( -t a_l^{\dagger} a_{l+1}^{} - \Delta a_l^{\dagger} a_{l+1}^{} + \text{h.c.} \right) - \mu \left( a_l^{\dagger} a_l^{} - \frac{1}{2} \right) \right],$$

(1)

where $a_l^{\dagger}$ ($a_l^{}$) is the operator that creates (annihilates) a fermion at the $l$-th site, the hopping rate is given by $t$, $\mu$ is the chemical potential and $\Delta$ is the pairing parameter or superconducting gap.

- **Translational invariant momentum representation:** The customary Fourier transform relating momentum and position spaces, $a_l = (1/\sqrt{L}) \sum_k \exp(-ikl) a_k^{}$, with $l$ the lattice site index and $k$ the momentum index, holds only for periodic boundary conditions with a periodicity of $L$ and thus it may even represent infinite chains in the uniform case. It is worth to mention that there exist two particular points, $k = \{0, \pi\}$, where destructive interference breaks the translational invariance as shown in Fig. 1. Hence, only in that case the system behaves as a finite chain.

The Hamiltonian (1) represented in momentum space is written in a matrix form by using the Nambu operators $\hat{C}_k = (\hat{a}_k^{}, \hat{a}_{-k}^{\dagger})^T$ and $\hat{C}_k^\dagger = (\hat{a}_k^{\dagger}, \hat{a}_{-k})^T$. Following the Bogoliubov and de Gennes (BdG) formalism [28], it takes the form $\hat{H} = \sum_k \hat{C}_k^\dagger \mathbb{H}_{\text{BdG}} \hat{C}_k + \sum_k \epsilon_k$ where the coupling matrix is given by

$$\mathbb{H}_{\text{BdG}} = \begin{pmatrix} \epsilon_k & -\Delta_k \\ -\Delta_k^* & -\epsilon_k \end{pmatrix}$$

and $\epsilon_k = -t - 2t \cos(k)$. The eigenvalues of $\mathbb{H}_{\text{BdG}}$ are: $\lambda_\pm = \mp \sqrt{\epsilon_k^2 + |\Delta_k|^2}$. In Fig. 2, we plot the difference $\Delta E = |\lambda_+ - \lambda_-|$ for a set of $\Delta \in \{0.2, 0.4, 0.6, 0.8\}$, being $t$ the energy unit, i.e. $t \equiv 1$. For $\Delta > 0$, when the gap is finite the phase is trivial, otherwise the system has a topological phase supporting free Majorana states [29]. As it is observed, the gap closes only at $|\mu| = 2$ and $\Delta \ll 1$, the number of visible wrinkles is the exactly $L$ (see curve $\Delta = 0.2$ in Fig. 2). Hence, the formalism is not suitable to describe the system with unpaired Majoranas since the expected results are not obtained.

- **Sine discrete Fourier transform type I:** In order to seek the unpaired Majoranas, we should express the Kitaev model in the so-called Majorana representation in position space. The usual relations are
presents the usual Kitaev’s phase
4
54x-373|
54x502|
t
54x513|
taev chain, the topological phase is located in the color region
FIG. 3. (Color online.) Usual phase diagram for the Ki-
3
opposite momenta
the required boundary conditions. To achieve this, we
therefore, we use an specific transform that complies with
form leaves out the possibility of having edge states,
α ∈ {A, B} kind at the l-th site. These operators hold
the Hamiltonian takes the form
\[ H \equiv \gamma \left[ \sum_\alpha \rho^{\alpha \beta} \right] \]
After applying this appropriate transform to equation
the states
\[ \langle \eta | \hat{\rho}^A | \eta' \rangle = \delta_{\eta \eta'} \]
FIG. 4. The coupling matrix spectrum goes from real (η = 0)
to pure imaginary (η = 1) values, showing the transition
regime from the weak coupling (free-electrons with reduced
mobility) to strong coupling where the pairing gives rise to
Majorana quasiparticles.
with
\[ E_\zeta(\mu) = -\mu - 2t \cos \left( \frac{\pi \zeta}{L + 1} \right), \]
\[ F_{\zeta\zeta'} = \frac{2}{L + 1} \left( \frac{S_\zeta S_{\zeta'}}{C_{\zeta} - C_{\zeta'}} \right), \zeta + \zeta' \text{ odd}, \]
where \( S_\zeta = \sin \left( \frac{\pi \zeta}{L + 1} \right) \) and \( C_\zeta = \cos \left( \frac{\pi \zeta}{L + 1} \right) \). Accordingly,
the numerical problem has been reduced from an
exponentially large matrix dimension of \( (2^L \times 2^L) \) to
\( (L \times L) \), allowing us to study much larger system sizes
without losing any information during the process since
no approximation has been done.

The notation is significantly simplified by
the use of the following Nambu-like operators:
\[ \Gamma^\alpha = (\tilde{\gamma}_0^\alpha, \ldots, \tilde{\gamma}_0^\alpha, \ldots, \tilde{\gamma}_L^\alpha)^T, \text{ where } \alpha \in \{A, B\}. \]
In this way, the Hamiltonian \( (5) \) becomes,
\[ \hat{H} = i \Gamma^A \cdot [\mathbb{H}_D + \mathbb{H_S}] \Gamma^B, \]
with \( \mathbb{H}_D \) being a diagonal matrix displaying the dispersion
relation of free fermions in the chain and \( \mathbb{H}_S \) is a
skew-symmetric matrix containing the pairing term that
switches on the topological phase along with the free
Majoranas. Figure 3 presents the usual Kitaev’s phase
diagram for which the color region holds the topologi-
ical phase whereas in the white region the phase remains
trivial. The figure is obtained by calculating the singular
value decomposition (SVD) of the Bogoliubov-de Gennes
coupling matrix, \( [\mathbb{H}_D + \mathbb{H}_S] \) of equation \( (7) \) for a given
pairing value \( \Delta = 0.3 \), depicting in color only where the
lowest singular value vanishes, \( d_0 = 0 \).

The parameter space of the Hamiltonian can be reduced
by introducing the following parameterization \( t = E_0 \cos^2(\pi \eta/2), \Delta = E_0 \sin^2(\pi \eta/2) \) with
\( \hat{H} = \hat{H}/E_0 \) and
\( \hat{\mu} = \mu/E_0 \) with \( E_0 = \mu + \Delta \) as an energy scaling where
\( \eta \in [0, 1] \). This parameterization determines four inter-
esting regions which are shown in Fig. 4: \( \eta = 0 \) for free
electrons and real eigenvalues, \( 0 < \eta \ll 1 \) or weak
coupling where perturbation theory holds keeping the eigen-
values real, \( \eta = 1 \) where the physics is dominated only
by the pairing with purely imaginary eigenvalues, and fi-
nally, the remaining values of \( \eta \) form the fully dimerized
region with complex eigenvalues and presenting unpaired

\[ \hat{a}_l = \frac{i}{2} (\tilde{\gamma}_l^A + i \tilde{\gamma}_l^B), \] and \( \hat{a}_l^\dagger = \frac{i}{2} (\tilde{\gamma}_l^A - i \tilde{\gamma}_l^B), \)
where \( \tilde{\gamma}_l^\alpha \) creates/annihilates a Majorana quasi-particle of the
\( \alpha \in \{A, B\} \) at the edges (\( \zeta, \zeta' \)) and \( \alpha \in \{A, B\} \) which leaves the quasi-particles to be their
own antiparticles or, in other words, \( \tilde{\gamma}_l^A = (\tilde{\gamma}_l^A)^\dagger \). In this way,
the Hamiltonian \( (1) \) in the Majoranas representation
reads
\[ \hat{H} = -i \sum_j \left[ (t + \Delta) \tilde{\gamma}_j^A \tilde{\gamma}_{j+1}^B + (t - \Delta) \tilde{\gamma}_j^A \tilde{\gamma}_{j+1}^B \right] \]
\[ - i \mu \sum_j \tilde{\gamma}_j^A \tilde{\gamma}_{j+1}^B. \]
As we have seen previously, the typical Fourier trans-
form leaves out the possibility of having edge states,
therefore, we use an specific transform that complies with
the required boundary conditions. To achieve this, we
consider the kinetic eigenfunctions given by plane waves,
where due to the degeneracy, every pair of states with
opposite momenta \( \{ | \pm k \rangle \} \) form a subspace, and on
that account, one can use a convenient basis given by \( | \zeta \rangle = \frac{1}{\sqrt{2}} \left( | k \rangle + \beta | -k \rangle \right) \) with \( \beta = \pm 1 \). In order to be
consistent with the hard-wall boundary conditions the
edge states require, we impose the eigenfunctions to van-
ish at the edges \( (l = 0 \text{ and } l = L + 1) \) leaving us only with
the states \( | \zeta^- \rangle \) and an effective system size of \( L \). The ba-
sis orthonormality is granted since \( \langle \zeta^- | \zeta'^- \rangle = \delta_{\zeta \zeta'} \) (see appendix A).
The corresponding sine discrete Fourier transform type I
on the ladder operators is finally given by
\[ \hat{a}_l = \sqrt{\frac{2}{L + 1}} \sum_{\zeta=1}^L \sin \left( \frac{\pi \zeta}{L + 1} \right) \hat{a}_\zeta. \]

After applying this appropriate transform to equation
\( (3) \) we are led into the momentum representation where
the Hamiltonian takes the form
\[ \hat{H} = i \sum_{\zeta=1}^L \hat{\zeta}_\zeta^A \left[ E_\zeta - 2\Delta \sum_{\zeta'} F_{\zeta\zeta'} \right] \hat{\zeta}_\zeta^B, \]
Majoranas. Henceforth, we concentrate in the parameter region displaying Majoranas, they are the weak coupling and the fully dimerized regimes.

III. WEAK COUPLING REGIMEN: $0 \leq \eta < 1$

In the Hamiltonian (7) the $\mathbb{H}_S$ term can be treated as a small perturbation compared to the $\mathbb{H}_D$ term when $\eta$ is small enough. The correction to the energy for a given $\zeta$ up to third order is given by,

$$E^{(3)}_\zeta = E_\zeta - \frac{8\zeta^2}{t(L+1)^2} \sum_{\zeta' \text{ odd}} S^z_\zeta S^z_{\zeta'} |C_\zeta - C_{\zeta'}|^2.$$  

By analyzing this expression one can observe that, for $L \gg 1$, the perturbation only modify the band-width of the dispersion relation through an effective hopping parameter, $t_{\text{eff}} = t - \frac{2\Delta^2}{L}$, and thus

$$E^{(3)}_\zeta \approx -\mu - 2t_{\text{eff}} \cos \left( \frac{\pi \zeta}{L+1} \right).$$

Figure 5 presents the Kitaev spectrum for a given parameter set and a system size $L = 51$. It shows the comparison between the full diagonalization of the Bogoliubov-de Gennes coupling matrix, the perturbation theory and the effective dispersion relation of Eq. (9). We can see there the perfect agreement among all three curves. The free-particles spectrum ($\Delta = 0$) is shown as a guide to the eyes making evident that the functional form of the spectrum does not change where the perturbation theory is still valid.

IV. FULLY DIMERIZED LIMIT: $0 < \eta < 1$

Let us consider the fully dimerized limit where zero energy modes (unpaired Majorana fermions) can be hosted embedded in a fermionic environment. For odd system sizes there is always a real eigenvalue and under the adequate parameter set it can be tuned to zero. In order to generate a $-\eta\tilde{\mu}$ phase diagram, we plot solely the minimum singular value, $d_0$, from equation (7). In this fashion, we retrieve Fig. 6 which, for $L = 51$ sites, displays two distinct regions: the outside region in white where $d_0 > 0$, representing a trivial phase and the color region where the minimum singular value strictly annihilates, $d_0 = 0$, and thus there should be a zero eigenvalue of the system. Moreover, for the regime $\eta \ll 1$, the system energy vanishes ($E^{(3)}_\zeta = 0$) when the transcendental equation $\cos (\zeta \pi / (L+1)) = \tilde{\mu} / (-2t_{\text{eff}})$ holds. Only for certain values of $\tilde{\mu}$ there are zero-energy modes, hence Fig. 6 presents wrinkles in the weak coupling regime. Nevertheless, this region smooths as the system size grows and the whole region homogenizes.

In order to retrieve the zero-energy eigenstates, we consider the fact that wherever the coupling matrix $\mathbb{H}_D + \mathbb{H}_S$ has a zero eigenvalue, it also has a null determinant. In other words, its columns (rows) are linearly dependent vectors and thus it is possible to find at least one vector with dimension $L$ linearly independent to them. In this way, we take a random vector and diminish it by the projections upon each of the the columns (rows) of the interaction matrix. The result is a vector such that it is a right (left) eigenvector with an eigenvalue equals to zero. Figure 7 shows the eigenfunctions of the zero-energy modes, Fig. 7(a) presents it in momentum space, $\phi_\zeta$, for both Majoranas species A and B. One can observed a delocalization for both wavefunctions being an oscillatory type for B-kind and its envelope given by A-kind. On the other hand, Fig. 7(b) displays both eigen-
functions in position space, \( \phi_i \), a strong localization at the edges is clearly seen with exponential decays, distinct signatures of unbound Majorana states.

V. SUMMARY AND REMARKS

We focus on the study of zero-energy modes of the Kitaev model putting special attention on a suitable transformation to bring the system from the position to the momentum representation considering the proper boundary conditions. The necessity lies in the fundamental fact that these are edge modes meaning the precondition of a finite chain. Hence, the customary Fourier transform, which holds solely for periodic boundary conditions, precludes the support of such unbound Majorana states. The parameters considered are \( L = 51, \eta = 0.3 \) and \( \mu = 0.1 \).

The authors acknowledge the support from CIBioFi and the Colombian Science, Technology and Innovation Fundation–COLCIENCIAS “Francisco José de Caldas” under project 1106-712-49884 (contract No.264-2016) and –General Royalties System (Fondo CTI-SGR) under contract No. BPIN 2013000100007.

Appendix A: Orthonormalized sine discrete Fourier transform type I

The basis orthonormality is given by

\[
\langle k^-_\zeta | k^-_{\zeta'} \rangle = \frac{2}{L+1} \sum_{l=1}^{L} \sum_{l'=1}^{L} \sin \left( \frac{\pi}{L+1} \zeta l \right) \sin \left( \frac{\pi}{L+1} \zeta' l' \right) \langle \varnothing | \hat{a}_l \hat{a}_{l'}^\dagger | \varnothing \rangle,
\]

\[
= \frac{1}{L+1} \sum_{l=1}^{L} \left[ \frac{1}{2} \{ 1 + (-1)^\zeta - \zeta' \} - 1 - \left( \frac{1}{2} \{ 1 + (-1)^{\zeta + \zeta'} \} - 1 \right) \right]
\]

\[
= \frac{1}{L+1} \sum_{l=1}^{L} \frac{1}{2} \left[ (-1)^{\zeta - \zeta'} - (-1)^{\zeta + \zeta'} \right] = 0, \text{ if } \zeta \neq \zeta',
\]

where we have used the summation

\[
\sum_{p=1}^{q} \cos px = \frac{1}{2} \left( 1 + \frac{\sin \left( \frac{q + \frac{1}{2}}{2} \right)}{\sin \left( \frac{1}{2} \right)} \right) - 1.
\]

In the remaining case, \( \zeta = \zeta' \), we have

\[
\langle k^-_\zeta | k^-_\zeta \rangle = \frac{2}{L+1} \sum_{l=1}^{L} \sin^2 \left( \frac{\pi}{L+1} \zeta l \right) = 1.
\]
here we have used the sum
\[ \sum_{p=1}^{q} \sin^2(p \pi x) = \frac{q}{2} - \frac{\cos((q + 1) \pi x) \sin(q \pi x)}{2 \sin(x)}. \]  
\[ \text{(A4)} \]

Hence the orthonormalization, \( \langle k^-_\zeta | k^-_{\zeta'} \rangle = \delta_{\zeta, \zeta'} \), is granted for all basis states. Finally, the completeness relation is given by,
\[ \sum_{l=1}^{L} \sin\left(\frac{\pi l}{L+1} \zeta \right) \sin\left(\frac{\pi l}{L+1} \zeta' \right) = \frac{L+1}{2} \delta_{\zeta, \zeta'}. \]  
\[ \text{(A5)} \]

Having the sine transform, we can now determine how to relate the position and momentum space operators using it as shown above in equation (4).

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