

INTRODUCTION TO TOPOLOGICAL BOUND STATES

Research Project

Laboratoire de Physique des Solides, Orsay

Mateo ULDEMOLINS NIVELA*

17 January 2019

Abstract

This report starts with a brief revision of the second quantization formalism, emphasizing its application rather than rigorous derivations. Subsequently, several models of spinless fermionic one-dimensional chains are presented and a discussion on some numerical results follows. Finally, the existence of Majorana modes in one-dimensional quantum wires is examined.

1 Motivation

In 1961, G. Gamow wrote “Only the number theory and topology (*analysis situs*) still remain purely mathematical disciplines without any application to physics. Could it be that they will be called to help in our further understanding of the riddles of nature?” Less than sixty years later, the term “topology” seems to be ubiquitous in today’s condensed matter area of focus. Topological phase transitions, topological insulators, topological superconductors are just a few examples of a large plethora of the so-called topological states of matter [1].

Topological quantum computation is perhaps one of the most promising topic in this emerging field. The approach aims at storing and manipulating quantum information in exotic quasiparticles which generalise bosonic and fermionic statistics, hence referred to as anyons. Their unusual behaviour allows to abstract them from local geometrical details and realise a “topological description” which provides a much desired resilience against control errors and perturbations [2]. The ultimate goal of this report will be to introduce the Majorana zero-modes, a recent proposal to implement decoherence-protected degrees of freedom in one-dimensional systems [3].

Nonetheless, in order to prepare the ground for these enticing advancements, we shall begin by the much more humble task of studying the second quantization formalism, since as one can imagine, most of the aforementioned phenomena are rooted in the many-body quantum physics.

2 Second quantization preliminaries

In order to motivate the need of a new formalism to deal with many-body quantum mechanics, we shall briefly review the many-particle Hilbert space [4]. Let us consider the set of normalized eigenfunctions $|\lambda\rangle$ of some single-particle Hamiltonian such that $\hat{H}|\lambda\rangle = \epsilon_\lambda|\lambda\rangle$. If we consider now the wavefunction corresponding to N particles populating the spectrum of the Hamiltonian, we must take into account the quantum mechanics principle of indistinguishability, i.e. the total wavefunction has to be symmetric or anti-symmetric if the particles are identical bosons or fermions, respectively. Such wavefunction reads

$$|\lambda_1, \lambda_2, \dots, \lambda_N\rangle = \frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} (n_\lambda!)}} \sum_{\mathcal{P} \in S_N} \zeta^{\mathcal{P}} |\lambda_{\mathcal{P}_1}\rangle \otimes |\lambda_{\mathcal{P}_2}\rangle \otimes \dots \otimes |\lambda_{\mathcal{P}_N}\rangle, \quad (1)$$

*mateo.uldemolins-nivela@u-psud.fr

where the summation runs over all the permutations of $\{1, \dots, N\}$. The term n_λ in the normalizing pre-factor is the number of particles in the $|\lambda\rangle$ eigenstate (restricted to 0 or 1 in the case of fermions), ζ is 1 for bosons and -1 for fermions, and its exponent is 0 or 1 depending on whether the permutation is even or odd. In the case of fermions, Eq. (1) is the well-known Slater determinant.

A quick glance at the previous expression is enough to realize how inconvenient this formulation would be when trying to compute the overlap of two wavefunctions, since the number of products quickly scales with N . Furthermore, one can see that this approach will also pose some issues in a system where the number of particles is not a fixed number N , but rather, a fluctuating variable.

The second quantization formalism [5] is a mathematical apparatus which aims at overcoming the aforementioned burdens. It is built upon the notion of the occupation number representation. Now, instead of characterizing a many-body state (anti)symmetrizing a product of single-particle states, we shall consider the set of single-particle states, together with the number of particles occupying each of them. It is written as follows

$$|\{n_\lambda\}\rangle = |n_{\lambda_1} n_{\lambda_2} \dots n_{\lambda_N}\rangle, \quad (2)$$

where n_{λ_i} is the number of particles occupying the λ_i state, which is of course restricted to 0 or 1 in the case of fermions due to Pauli Exclusion Principle. Indeed, $N = \sum_\lambda n_\lambda$. However, this constraint is usually relaxed extending the usual Hilbert space to the Fock space, defined in Eq. (3).

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N, \quad (3)$$

where $\mathcal{H}_N = \mathcal{H}_1^{\otimes N}$ is the Hilbert space of N particles. Please note that one might have to restrict \mathcal{H}_N to its (anti)symmetrized subspace when dealing with identical (fermions) bosons. \mathcal{H}_0 stands for the vector space containing one single state, namely, the vacuum.

In Fock space, we define the creation and annihilation operators which respectively raise and lower the number of particles in a given single-particle state by 1. The annihilation operator c_λ and the creation operator c_λ^\dagger are hermitian conjugates. The latter allows to define the full basis of the Fock space \mathcal{F} , applying it consecutively to the vacuum: $|n_{\lambda_1} = 1 \dots n_{\lambda_N} = 1\rangle = c_{\lambda_1}^\dagger \dots c_{\lambda_N}^\dagger |\text{vac}\rangle$. Let us see an example of how we would define a 2-electron state:

$$c_\uparrow^\dagger c_\downarrow^\dagger |\text{vac}\rangle = c_\uparrow^\dagger |\downarrow\rangle = |\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle). \quad (4)$$

The last equality relates the state in the second quantization formalism to its representation as a fixed-number-of-particles Hilbert state. We adopt the convention that the first quantum state in the occupation representation appears with a positive sign in the corresponding anti-symmetrized wavefunction, in the fermionic case. In other words, that $|\uparrow\downarrow\rangle = -|\downarrow\uparrow\rangle$. The (anti)symmetric properties of the wavefunctions will naturally arise as some (anti)commutation relationships between the operators that we will define next.

Moreover, we shall note that a fermionic operator acting on an occupied quantum state yields 0 by virtue of the Pauli Principle, and similarly any annihilation operator also returns 0 when acting on an empty state.

The anti-commutation relations for fermions read

$$\{c_\alpha^\dagger, c_\beta^\dagger\} = \{c_\alpha, c_\beta\} = 0, \quad (5)$$

$$\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha\beta}. \quad (6)$$

Although in this report we will be mainly interested in characterizing electrons, we shall add the bosonic commutation relations for the sake of completeness:

$$[b_\alpha^\dagger, b_\beta^\dagger] = [b_\alpha, b_\beta] = 0, \quad (7)$$

$$[b_\alpha, b_\beta^\dagger] = \delta_{\alpha\beta}. \quad (8)$$

In addition, it will be useful to define the number operator, whose eigenvalues are the number of particles occupying the corresponding state $|\lambda\rangle$:

$$c_\lambda^\dagger c_\lambda |\{n_\lambda\}\rangle = n_\lambda |\{n_\lambda\}\rangle. \quad (9)$$

Change of basis is defined naturally for these operators. As an example, let us consider the Fourier transformation to momentum space in a 1D lattice, which will prove useful in Section 3:

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikr_j} c_k. \quad (10)$$

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikr_j} c_k^\dagger. \quad (11)$$

Indeed, the creation operator in real space is related to creation operators in momentum space, and as one would expect, anti-commutation relations also hold for c_k^\dagger and c_k .

To conclude this brief revision, we shall include how one-body operators look like in the formalism:

$$\hat{O} = \sum_{\alpha\beta} O_{\alpha\beta} c_\alpha^\dagger c_\beta \quad (12)$$

where $O_{\alpha\beta}$ are the matrix elements of the operator in the chosen basis. Certainly, a one-body operator engages particles one by one. Let us consider for example the z-component of the spin operator, where the matrix elements are those of the σ_z Pauli matrix. Following Eq. (12) we obtain

$$\hat{S}_z = \frac{\hbar}{2} (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow).$$

Physically, it seems logical: if one recalls the number operator defined in Eq. (9), it is immediate to notice that we are indeed “counting” the number of spin-up electrons and then “subtracting” its spin-down counterpart. Furthermore, it is interesting to notice that we have one single operator acting on the Fock space of none, one or two particles, which we do not need to extend as it happens when working in first quantization Hilbert spaces.

In the following subsection we will perform some calculations on a 2-level system, in order to illustrate a basic usage of the formalism.

2.1 Singlet and triplet states in a 2-level system

Let us consider a system of 2 electrons characterized by the spin and another quantum number that we shall designate orbital. In the first quantization formalism, a state would be represented by the anti-symmetrized product of each electron’s wavefunction. However, commutativity of the tensor product allows us to (anti)symmetrize orbital and spin functions separately, so that the total state is defined by a product of a symmetric orbital function and an anti-symmetric spin function or vice-versa. Possible options are gathered in Table 1. The anti-symmetrization constraint reduces the 16 possible combinations to only 6 valid states: $|aa\rangle \otimes \frac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{\sqrt{2}}$, $|bb\rangle \otimes \frac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{\sqrt{2}}$, $\frac{(|ab\rangle + |ba\rangle) \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{2}$, $\frac{(|ab\rangle - |ba\rangle)}{\sqrt{2}} \otimes |\uparrow\uparrow\rangle$, $\frac{(|ab\rangle - |ba\rangle)}{\sqrt{2}} \otimes |\downarrow\downarrow\rangle$, and $\frac{(|ab\rangle - |ba\rangle) \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)}{2}$.

	Orbital	Spin
Symmetric	$ aa\rangle$	$ \uparrow\uparrow\rangle$
	$ bb\rangle$	$ \downarrow\downarrow\rangle$
	$ ab\rangle + ba\rangle$	$ \uparrow\downarrow\rangle + \downarrow\uparrow\rangle$
Antisymmetric	$ ab\rangle - ba\rangle$	$ \uparrow\downarrow\rangle - \downarrow\uparrow\rangle$

Table 1: Possible orbital and spin functions for 2 electrons in the 2-level system. Normalization constants have been omitted for readability.

Now, let us tackle the problem within the second quantization formalism. The most generic 2-fermion creation operator in our 2-level system reads

$$\hat{C}(\nu) = \sum_{\substack{\alpha,\beta=\{a,b\} \\ \sigma,\rho=\{\uparrow,\downarrow\}}} \nu_{\alpha\beta}^{\sigma\rho} c_{\alpha\sigma}^\dagger c_{\beta\rho}^\dagger = \sum_{\substack{\alpha,\beta=\{a,b\} \\ \sigma,\rho=\{\uparrow,\downarrow\}}} \nu_{\alpha\beta}^{\sigma\rho} (-c_{\beta\rho}^\dagger c_{\alpha\sigma}^\dagger), \quad (13)$$

where the second equality is a direct consequence of the anti-commutation relationship (5). After having rearranged indices, it is straightforward to notice that $\nu_{\alpha\beta}^{\sigma\rho} = -\nu_{\beta\alpha}^{\rho\sigma}$. Once again, we find that from the 16 possible coefficients only 6 of them are truly independent. This means that we have 6 different creation operators and that we can write any possible state of our system as a linear combination of them. To relate these operators to their corresponding “first-quantized” state, one just has to act them on the vacuum state, as we did in the example of Eq. (4). These relationships are shown in Table 2.

Hilbert state	Operator	Total spin	Spin z-component
$ aa\rangle (\uparrow\downarrow\rangle - \downarrow\uparrow\rangle)$	$c_{a\uparrow}^\dagger c_{a\downarrow}^\dagger$	$S = 0$	$S_z = 0$
$ bb\rangle (\uparrow\downarrow\rangle - \downarrow\uparrow\rangle)$	$c_{b\uparrow}^\dagger c_{b\downarrow}^\dagger$		
$(ab\rangle + ba\rangle) (\uparrow\downarrow\rangle - \downarrow\uparrow\rangle)$	$c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger - c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger$	$S = 1$	$S_z = +1$
$(ab\rangle - ba\rangle) \uparrow\uparrow\rangle$	$c_{a\uparrow}^\dagger c_{b\uparrow}^\dagger$		
$(ab\rangle - ba\rangle) \downarrow\downarrow\rangle$	$c_{a\downarrow}^\dagger c_{b\downarrow}^\dagger$		
$(ab\rangle - ba\rangle) (\uparrow\downarrow\rangle + \downarrow\uparrow\rangle)$	$c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger + c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger$		

Table 2: Possible independent states and their corresponding operators for 2 electrons in a 2-level system. Normalization constants have been omitted for readability.

In order to calculate the total spin and the z-component we compute the second-quantized operators using Eq. (12). In order to apply them to a state we will adopt the following prescription: first express the state as a succession of operators acting on the vacuum and then apply the anti-commutation relations to shift the annihilation operators to the right, which will vanish when acting on the vacuum. The remaining terms will be the resulting state. Although this procedure is straightforward, algebraic manipulations can become a bit cumbersome, therefore a *Mathematica* package [6] was employed to verify results in Table 2.

3 Hopping model

We shall start this section analysing a very simple model of spinless fermions in a 1D chain to become acquainted with the notion of diagonalizing a Hamiltonian within the second quantization formalism. Then, we will progressively increase the complexity of the model to obtain a system which exhibits some topological bound states, paving the way towards the Kitaev chain.

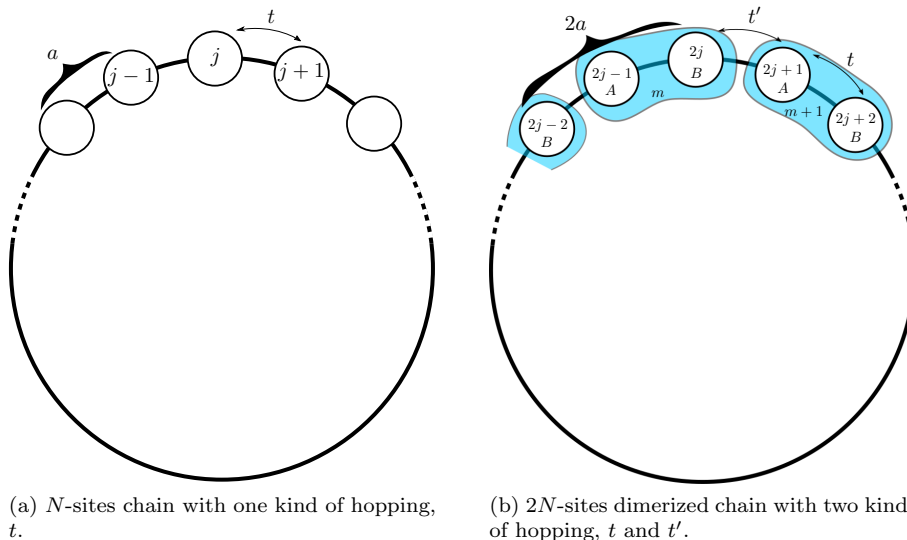


Figure 1: Spinless fermionic 1D hopping model with periodic boundary conditions.

To start with, let us consider a simple N -sites one-dimensional chain with only one type of hop-

ping allowed between nearest neighbours, where $r_j = aj$, being a some constant which determines the periodicity of the model (Fig. 1a). The Hamiltonian of the system is expressed as follows

$$\hat{H} = -t \sum_{j=1}^N (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}), \quad (14)$$

where t is a real and positive constant, the hopping amplitude. The operator formalism provides a good intuition of the physics in the model: indeed, the hopping is represented by the annihilation of an electron at site j (operator c_j) followed by the creation of a new electron at the neighbouring site $j+1$ (operator c_{j+1}^\dagger) and vice-versa.

Roughly speaking, we could say that the main idea behind the diagonalization scheme will be to rewrite the Hamiltonian in some other basis such that $\hat{H} = \sum_\lambda \epsilon_\lambda c_\lambda^\dagger c_\lambda$. By doing so and identifying $c_\lambda^\dagger c_\lambda$ with the number operator, the physical meaning is clear: the Hamiltonian can be understood as the sum of all its eigenvalues (ϵ_λ) times the number of particles in each of the corresponding eigenstates.

In the present case, the chain periodicity suggests the problem could be greatly simplified by Fourier transforming, so we will make use of the expressions proposed early, (10) and (11). Firstly, we shall notice that the periodic boundary conditions impose some restrictions on the possible values of the momentum k :

$$c_j^\dagger = c_{j+N}^\dagger \Rightarrow \frac{1}{\sqrt{N}} \sum_k e^{ikaj} c_k = \frac{1}{\sqrt{N}} \sum_k e^{ika(j+N)} c_k \Rightarrow e^{ikNa} = 1 \Rightarrow k = \frac{2\pi m}{Na}, \quad (15)$$

where we adopt the convention $m = (-\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1)$. As expected, we also have N independent operators in momentum space and for $N \rightarrow \infty$ we recover the usual first Brioullin zone. Proceeding as announced, the Hamiltonian writes

$$\begin{aligned} \hat{H} &= \frac{-t}{N} \sum_{j=1}^N \sum_{kk'} \left(e^{-ika(j+1)} c_k^\dagger e^{ik'aj} c_{k'} + e^{-ik'aj} c_{k'}^\dagger e^{ika(j+1)} c_k \right) \\ &= -t \sum_{kk'} \left(e^{-ika} c_k^\dagger c_{k'} + e^{ika} c_{k'}^\dagger c_k \right) \delta_{kk'} \\ &= \sum_k (-2t \cos(ka)) c_k^\dagger c_k = \sum_k \epsilon_k \hat{N}_k, \end{aligned} \quad (16)$$

where the second equality results from the fact that $\sum_{j=1}^N e^{-i(k-k')ja} = N\delta_{kk'}$ due to the restrictions PBC impose on k . As we suggested before, the Hamiltonian appears to be an operator counting the number of electrons with momentum k , multiplying the count by the energy of such electron and returning the sum. The eigenvalues $\epsilon_k = -2t \cos(ka)$; $k = (-\frac{\pi}{a}, -\frac{\pi}{a} + 1, \dots, \frac{\pi}{a} - 1)$ are actually a discrete version of the energy dispersion relation that one finds in the simplest version of the tight-binding model, but we shall not dwell further on the physics of this model, since it is not the purpose of the example. Instead, we will add some complexity to it.

Now, we will allow two different types of hopping, t and t' . Therefore, the periodicity of the model is given by $2a$, as showed in Figure 1b. (For convenience we will consider a chain with $2N$ sites in this case). The Hamiltonian of the system reads

$$\hat{H} = \sum_{j=1}^N \left[-t \left(c_{2j-1}^\dagger c_{2j} + c_{2j}^\dagger c_{2j-1} \right) - t' \left(c_{2j+1}^\dagger c_{2j} + c_{2j}^\dagger c_{2j+1} \right) \right]. \quad (17)$$

Once again, the second quantization operators provide a clear picture of the hopping, but unfortunately this notation somehow conceals the periodicity of the model. Thus, we shall reinterpret the system as a chain of N dimers as depicted in Figure 1b. We will assign the operator c_A^\dagger to the odd sites (first site of each dimer) and c_B^\dagger to its even counterpart. In other words, $c_{Am}^\dagger = c_{2j-1}^\dagger$ and $c_{Bm}^\dagger = c_{2j}^\dagger$. The Hamiltonian of Eq. (17) can now be rewritten as:

$$\begin{aligned}
\hat{H} &= \sum_{m=1}^N \left[-t \left(c_{Am}^\dagger c_{Bm} + c_{Bm}^\dagger c_{Am} \right) - t' \left(c_{Am+1}^\dagger c_{Bm} + c_{Bm}^\dagger c_{Am+1} \right) \right] \\
&= \sum_{m=1}^N \left[-t \tilde{c}_m^\dagger \sigma_x \tilde{c}_m - t' \left(\tilde{c}_{m+1}^\dagger \sigma_+ \tilde{c}_m + \tilde{c}_m^\dagger \sigma_- \tilde{c}_{m+1} \right) \right],
\end{aligned} \tag{18}$$

where in the second equation we introduced matrix notation to make the expression more compact. We set $\tilde{c}_m^\dagger = (c_{Am}^\dagger \ c_{Bm}^\dagger)$ and $\tilde{c}_m = \begin{pmatrix} c_{Am} \\ c_{Bm} \end{pmatrix}$. On the other hand, σ_x is the usual Pauli matrix and $\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$. Once the Hamiltonian is expressed in terms of these “new” operators, we can continue going to Fourier space to diagonalize it. The procedure is analogous to that of the previous example, with the exception that periodicity is now $2a$, therefore periodic boundary conditions $\tilde{c}_{N+1}^\dagger = \tilde{c}_1^\dagger$ imply that $k = \frac{\pi}{Na}n$ with $n = (-\frac{N}{2}, \dots, \frac{N}{2} - 1)$. Hence Eq. (18) reads

$$\begin{aligned}
\hat{H} &= \sum_k \tilde{c}_k^\dagger \begin{pmatrix} 0 & -t - t' e^{-ik2a} \\ -t - t' e^{ik2a} & 0 \end{pmatrix} \tilde{c}_k \\
&= \sum_k \epsilon_+(k) \tilde{D}_{+,k}^\dagger \tilde{D}_{+,k} + \epsilon_-(k) \tilde{D}_{-,k}^\dagger \tilde{D}_{-,k}.
\end{aligned} \tag{19}$$

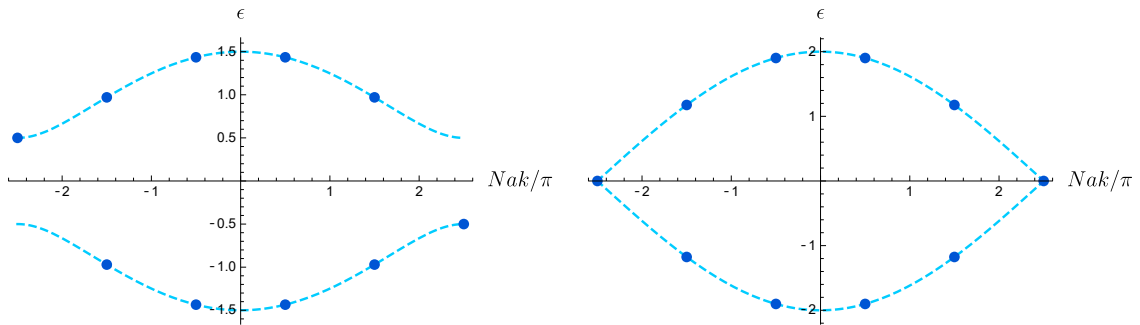
As we can observe, we rephrased the Hamiltonian in terms of some abstract “number operators” which count the number of excitations present in the system. Renaming $\gamma = -t - t' e^{ik2a}$ to lighten notation one easily finds that

$$\epsilon_\pm = \pm |\gamma| = \pm \sqrt{t^2 + t'^2 + 2tt' \cos(2ka)}. \tag{20}$$

$$\tilde{D}_k^\dagger = \left(\tilde{D}_{+,k}^\dagger \ \tilde{D}_{-,k}^\dagger \right) = \tilde{c}_k^\dagger U^\dagger. \tag{21}$$

$$\tilde{D}_k = \begin{pmatrix} \tilde{D}_{+,k} \\ \tilde{D}_{-,k} \end{pmatrix} = U \tilde{c}_k, \tag{22}$$

with $U = \begin{pmatrix} \gamma_+^* & \gamma_-^* \\ \epsilon_+ & \epsilon_- \end{pmatrix}$ being the matrix for the change of basis. A quick glance at Equation (20) already provides an interesting insight: the energy spectrum of the system is symmetric under the exchange $t \leftrightarrow t'$, which is in agreement with the periodic structure of the model. When plotting the spectrum in k -space (Fig. 2) we find that a gap opens at $\epsilon = 0$ for $t \neq t'$. In fact, this corresponds to the well-known picture of an insulator. At $t = t'$ this gap closes and the system is equivalent to the simple chain studied initially, which describes a conductor. In this case, the plot is nothing more than $\epsilon_k = -2t \cos(ka)$ but folded onto itself, as we imposed a periodicity of $2a$. On the other hand, setting one amplitude to 0 would trivially result in a flat band.



(a) Solution corresponding to $N = 10$, $t = 0.5$ and $t' = 1$. Exchanging t and t' yields the same result. (b) Solution corresponding to $N = 10$, $t = 1$ and $t' = 1$.

Figure 2: Energy spectrum in momentum space for the dimerized hopping model with periodic boundary conditions. The dotted line represents the continuum solution and the dots are the actual eigenvalues for a 10-sites chain.

Even though this brief analysis might suggest that our model is totally symmetric under the exchange of the hopping amplitudes, this is not totally accurate. Indeed, the eigenfunctions exhibit some non-trivial dependence of t and t' through $\gamma = -t - t'e^{ik2a}$ which can be characterized by the *bulk winding number* [7]. However, this matter is outside the scope of this report.

We shall finish this section analysing again this model, but this time we will impose open boundary conditions. As a matter of fact, this is the Su-Schrieffer-Heeger (SSH) model which after some adjustments can be used to describe some physical systems, such as poly-acetylene [7].

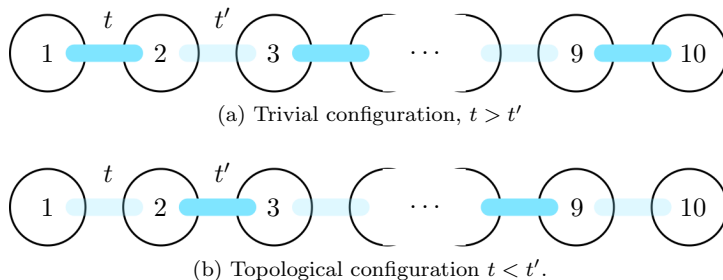


Figure 3: Fermionic 1D chain of $N = 10$ sites. Two hopping amplitudes are allowed, t and t' .

For an even number of the sites, the Hamiltonian of the system can be expressed in a real space basis as follows

$$\hat{H} = \begin{pmatrix} 0 & -t & 0 & \dots & 0 \\ -t & 0 & -t' & \dots & 0 \\ 0 & -t' & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -t & 0 \end{pmatrix}. \quad (23)$$

We shall particularize the model for the case of $N = 10$ and approach the problem numerically, diagonalizing the previous Hamiltonian with the software *Mathematica*. We present the obtained results below.

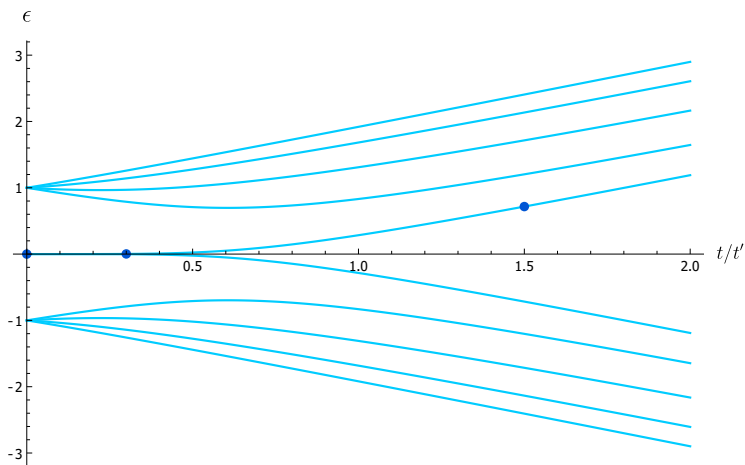


Figure 4: Energy spectrum as a function of the hopping parameter quotient t/t' for $N = 10$ sites.

In Figure 4 we study the evolution of the spectrum as a function of the hopping parameter quotient t/t' . We can observe that for large values of such ratio, the system behaves essentially as if it had periodic boundaries: the spectrum is symmetric around an energy gap at $\epsilon = 0$. Physically this corresponds to the depiction in Figure 3a: since t is much greater than t' the system is trivially dimerized. However, as we decrease the value of t/t' some interesting effect emerges. We observe that instead of having the gap closed at $t = t'$ and intermediately reopened as happened in the previous case, two states decay towards zero energy. Here again, a schematic figure sheds a lot of light on the physics of the model: the difference between the hopping parameters also leads the

sites to dimerize but now it happens in a different fashion (called topological [7]), so that the sites in the boundaries are somehow disconnected. In fact, at the limit $t = 0$ no hopping is allowed to such sites and since there is not any on-site potential, the so-called zero-energy bound states arise. On the other hand, the bulk of the chain is flat and fully degenerated. From the diagrams in Figure 3 it is clear that this situation would not arise if we set $t' = 0$ instead, and interestingly, we would always have a zero-energy state if the chain had an odd number of sites.

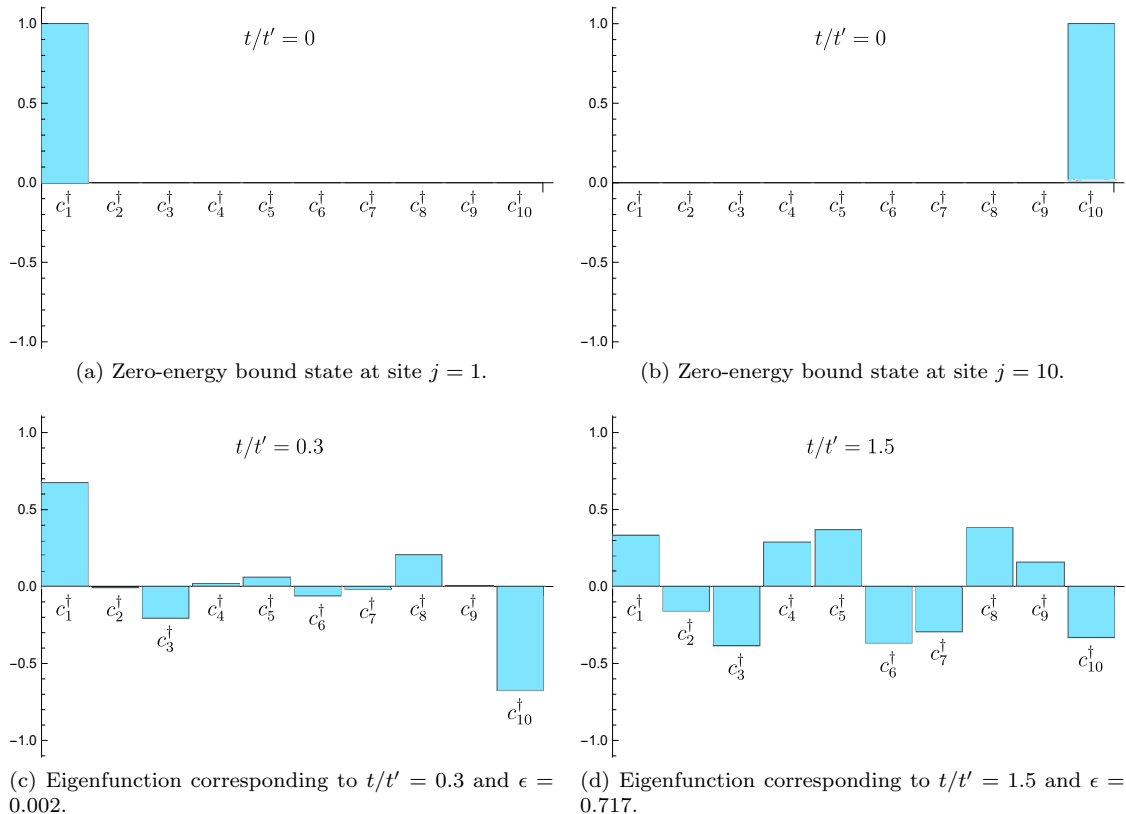


Figure 5: Eigenfunctions of the Hamiltonian for open boundary conditions and $N = 10$. The functions correspond to the dots in the energy spectrum plot (Fig. 4). The vertical axis represents the probability amplitude.

A careful analysis of some of the eigenfunctions corroborates the previous comments. Indeed, we can observe how for $t/t' = 0$ we obtain two definite modes at the extremes of the chain (Fig. 5a and 5b). This situation would remain unchanged for any even number of sites. As we increase the ratio between the hopping parameters those bound states delocalize progressively, becoming a superposition of the electron in every site (Fig. 5d). We shall remark that the probability of occupation associated to each site exhibits some symmetry (notice that in Fig. 5 only amplitudes of probability are represented). This is due to the fact that the chain is symmetric itself [8].

4 Kitaev chain

As we have seen in the previous models, fermionic sites in the chain are described by a pair of creation and annihilation operators, c_j^\dagger, c_j which satisfied the anti-commutation relations mentioned in Eq. (5) and (6). We can formally rewrite such operators in terms of the so-called *Majorana operators* [9]:

$$c_j^\dagger = \frac{1}{2} (\gamma_{A_j} + i\gamma_{B_j}), \quad c_j = \frac{1}{2} (\gamma_{A_j} - i\gamma_{B_j}), \quad (24)$$

which have the remarkable property of being hermitian, i.e., $\gamma_{A_j}^\dagger = \gamma_{A_j}$ and $\gamma_{B_j}^\dagger = \gamma_{B_j}$. This implies that we cannot think of a single Majorana mode as being “empty” or “filled”, as we have done with other fermionic modes. Nevertheless, these new operators also satisfy some similar

anticommutation relations, which can be condensed in the following expression:

$$\{\gamma_{\alpha j}, \gamma_{\beta k}\} = 2\delta_{\alpha\beta}\delta_{jk}. \quad (25)$$

The definitions in Eq. (24) can be somehow understood as rewriting a complex number as a pair of real numbers. Hence, Majorana operators will always come in an even number. Since condensed matter systems are underpinned by the physics of electrons, one might naively think that it is impossible to realise single isolated Majorana modes. However, it is not the case, and this was Kitaev's notable insight [3]: to engineer a toy model which allows such modes to arise. The proposed system is once again a spinless fermionic 1D-chain with the following Hamiltonian:

$$\hat{H} = \sum_j \left[-t \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) - \mu \left(c_j^\dagger c_j - \frac{1}{2} \right) + \Delta c_j c_{j+1} + \Delta^* c_{j+1}^\dagger c_j^\dagger \right]. \quad (26)$$

Here t characterizes the hopping amplitude as in the previous models. In addition we suppose that the chain is coupled to a superconducting reservoir which injects fermionic pairs in the adjacent sites. The coupling is characterized by the parameter Δ which represents the superconducting gap. As a side note we remark that since we are dealing with spinless fermions the antisymmetry of the Cooper pair wavefunction falls on the orbital part, hence it is a p -wave pairing [8]. Finally, the Hamiltonian must include the chemical potential μ , as the number of particles is not fixed. Following Kitaev's proposal, let us rewrite the Hamiltonian from Eq. (26) in terms of the Majorana operators:

$$\hat{H} = \frac{i}{2} \sum_j \left(-\mu \gamma_{Aj} \gamma_{Bj} + (t + |\Delta|) \gamma_{Bj} \gamma_{A_{j+1}} + (-t + |\Delta|) \gamma_{Aj} \gamma_{B_{j+1}} \right), \quad (27)$$

where we included a factor $e^{\pm\theta/2}$ in the expressions (24) respectively, in order to "hide" the phase dependence of the superconducting gap. In this report we will restrict ourselves to analysing two special cases [3]:

1. Case $|\Delta| = t = 0$, $\mu < 0$. This choice of parameters makes the system trivial, without any hopping or superconductivity. The Hamiltonian reads $\hat{H} = \frac{i}{2}(-\mu) \sum_j \gamma_{Aj} \gamma_{Bj}$, where only Majorana operators of the same site j are paired together. The ground state has certainly 0 occupation number.
2. Case $|\Delta| = t > 0$, $\mu = 0$. Now the Majorana operators from different sites are paired together. Indeed, $\hat{H} = it \sum_j \gamma_{Bj} \gamma_{A_{j+1}}$, and as we can see, the Majorana operators γ_{A1} and $\gamma_{B_{2N}}$ remain unpaired, i.e., they do not enter the Hamiltonian. In fact, they correspond to the zero-energy modes, as occurred similarly in the SSH model studied before.

We will finish this section pointing out that although it might seem that unpaired Majoranas appear as a result of the parameters fine-tuning, it is not the case. Actually, the Majoranas are protected until $\mu \simeq -2t$, that is, as long as the bulk energy gap is finite. This is a result of the particle-hole symmetry that exhibits the Hamiltonian. To move the energy levels from zero individually would break such symmetry, and moving them together requires them to be coupled, which only happens once the bulk energy gap is closed (namely, at $\mu = 2t$) [9].

5 Conclusion

Along the previous pages we have been able to appreciate the potential of the second quantization formalism. Indeed, if instead of assigning a position to each particle and (anti)symmetrizing all the possible permutations, one directly thinks in terms of occupation numbers, indistinguishability ensues naturally. Moreover, it has proven a very compact notation to write Hamiltonians.

The discussion on the hopping models has pointed out the similarities between the Su-Schrieffer-Heegerspectra model and a spinless p -wave superconducting wire (Kitaev's chain). Furthermore, we shall remark the important role that symmetries play in understanding the physics of the studied models, albeit mentioned just once and very briefly.

Finally, although the application of Majorana modes to quantum computation is far beyond the scope of this report, the analysis of the energy spectrum gives a slight hint on their interest. Indeed, Kitaev's chain allows for the existence of states of definite energy, which are situated far apart in space. Roughly speaking, it is this non-locality which suggests a promising future for decoherence-protected qubits.

References

- [1] M. Asorey, "Space, matter and topology," *Nature Physics*, vol. 12, no. 7, p. 616, 2016.
- [2] V. Lahtinen and J. Pachos, "A short introduction to topological quantum computation," *SciPost Physics*, vol. 3, no. 3, p. 021, 2017.
- [3] A. Y. Kitaev, "Unpaired Majorana fermions in quantum wires," *Physics-Uspekhi*, vol. 44, no. 10S, p. 131, 2001.
- [4] A. Altland and B. Simons, *Condensed Matter Field Theory*. Cambridge books online, Cambridge University Press, 2010.
- [5] C. Mora, "Lecture notes in second quantization."
- [6] R. Žitko, "Sneg – Mathematica package for symbolic calculations with second-quantization-operator expressions," *Computer Physics Communications*, vol. 182, no. 10, pp. 2259 – 2264, 2011.
- [7] J. K. Asbóth, L. Oroszlány, and A. Pályi, "A short course on topological insulators," *Lecture notes in physics*, vol. 919, 2016.
- [8] J. Dalibard, *La matière topologique et son exploration avec les gaz quantiques*. Collège de France.
- [9] A. Akhmerov, J. Sau, B. van Heck, S. Rubbert, and R. Skolasiński, *TU Delft TOPOCMx*. TU Delft Online Learning, 2014.