

# UNIVERSITÀ DEGLI STUDI DI PADOVA

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Topological order in fermionic superconductors and Kitaev chain generalizations

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**Abstract.** In this work, we provide a theoretical framework on the topological properties of a system of non-interacting spinless fermions in the presence of hopping between lattice sites and superconducting pairing. We mainly focus on two different approaches used to classify the topological phases of the system: the transfer matrix approach extracts information on the boundary properties of the system and is used to explicitly compute the wavefunctions of zero-energy states, while the bulk spectrum approach makes use of the energy-momentum dispersion to identify topological phase transitions with the closure of its gap. What characterizes topological phases is the presence of zero-energy Majorana modes localized at the boundary of the system. We give an overview on the application of these approaches on the Kitaev chain and its generalizations, focusing on the peculiarities of this system and the relations between the topological invariant used in the above-mentioned approaches.

# INDEX

1	INTRODUCTION			3
2	SETUP			4
	2.1	Diagor	nalization	5
	2.2	Bogoli	ubov equations	5
3	MAJORANA OPERATORS			6
	2.1	1 Diagonalization		
	2.2	2 Bogoliubov equations		8
	2.3	Major	ana zero modes	8
4	TOPOLOGICAL PHASES			9
	4.1	Boundary invariants		9
		4.1.1	Transfer matrix	9
		4.1.2	Edge modes	10
	4.2	Bulk in	11	
		4.2.1	Closed boundary conditions and diagonalization	12
		4.2.2	Winding number	14
		4.2.3	Broken time-reversal symmetry	14
5	APPLICATION: KITAEV CHAIN			15
	5.1	1 Transfer matrix approach		15
	5.2	Bulk s	pectrum approach	16
	5.3	Brokei	n time-reversal symmetry	17
	5.4	Finite	number of neighbours	18
6	CON	CONCLUSIONS		
APPENDIX: SYMMETRIES				20

# 1. INTRODUCTION

Topological orders in condensed matter systems have been a prolific field of research in recent years [1]. Boosted by Kitaev's pioneering work [2], a lot of attention has been focused on the study and realization of isolated Majorana fermions in 1-dimensional and 2-dimensional superconductors [3-4], both from a theoretical [5-14] and an experimental standpoint [15-18].

Kitaev's model, which will be referred to as *Kitaev chain*, describes a system of spinless fermions in a *p*-wave superconducting wire. The parameters of the system are the chemical potential  $\mu$  of the lattice sites, the tunnelling amplitude *w* that quantifies the probability of a fermion hopping from a lattice site to a nearest neighbour, and the superconducting gap  $\Delta$  that quantifies the *p*-wave pairing strength. Under certain conditions, the system is characterized by the appearance of zero-energy Majorana modes localized at the edges of the chain. This Majorana fermion is stable as long as the bulk spectrum of the system has an energy gap, which means it is robust under small parameter changes and as such it defines a *topological phase* of the system.

The main reason the Kitaev chain has been at the center of such rich literature, is perhaps its applications to quantum computing. As a matter of fact, the Majorana fermions that stem from this system are intrinsically immune to quantum decoherence, therefore they can be used as reliable qbits in the construction of quantum gates: let us see why.

Implementing quantum computation on a large scale has strong experimental limitations; fault tolerance is theoretically possible, but only if errors are kept under a threshold that is quite hard to achieve by current technology. This fragility comes from the fact that quantum states are sensitive to two kinds of error: a classical error that flips the qbit exchanging the empty state  $|0\rangle$  with the occupied state  $|1\rangle$ , and a phase error that changes the sign of the occupied state. In a fermionic system of qbits, the conservation of the electric charge (or the conservation of parity in superconductors) grants that single classical errors are physically impossible; two simultaneous classical errors are possible, but they require interaction between qbits, which can be made negligible by placing a suitable medium between them. Phase errors, though, are still possible. Now, a phase error acts through the operator  $1 - 2a^{\dagger}a$ , where  $a^{\dagger}$  and a are the creation and annihilation operators of the fermion; in terms of Majorana operators  $c_1 = a + a^{\dagger}$  and  $c_2 = -i(a - a^{\dagger})$ , the phase error becomes  $-ic_1c_2$ . This shows the phase error requires interaction between the two Majorana modes and it is negligible as long as these are mutually isolated, as in the case of the Kitaev chain.

Kitaev's toy-model has been extended in several directions, such as breaking time-reversal symmetry [19], increasing the range of site hopping and *p*-wave pairing [20-22], adding disorder in the chemical potential and interaction between particles [23]. The topological properties of the Kitaev chain are preserved and generalized under these looser conditions, which makes the system suitable for more realistic implementations.

Experimental realizations of the exotic *topological* superconductors that the Kitaev chain is based on, have been proposed in a variety of ways, for example by forming appropriate heterostructures with ordinary *s*-wave superconductors, based on diverse materials such as topological insulators [24], conventional semiconductors [25], ferromagnetic metals and others [26].

This work is structured as follows. In sections 2 we will develop the mathematical framework needed to study Kitaev's model and its generalizations, starting from a generic one-body Hamiltonian and focusing on the symmetries of the problem. In section 3 we will rework this framework using the formalism of

Majorana operators. In section 4 we will develop the tools to study the boundary properties of the system, as well as its bulk properties, and use this to detect topological phase transitions. In section 5, we will apply these tools to the Kitaev chain and its generalizations.

# 2 SETUP

We start from the Hamiltonian

$$H = \left(a_{1}^{\dagger} \dots a_{L}^{\dagger} a_{1} \dots a_{L}\right) \mathcal{H} \begin{pmatrix} a_{1} \\ \vdots \\ a_{L} \\ a_{1}^{\dagger} \\ \vdots \\ a_{L}^{\dagger} \end{pmatrix}, \qquad (1)$$

that describes a system of spinless fermions in a 1-dimensional lattice (*chain*) with a number of sites equal to *L*, subject to an external potential and with no interaction between particles.

 $a_i^\dagger$  and  $a_i$  are the creation and annihilation operators, thus

$$\{a_i, a_j\} = 0$$
,  $\{a_i^{\dagger}, a_j\} = \delta_{ij}$ , (2)

where indices *i* and *j* span from 1 to *L*.

The Hamiltonian H needs to be self-adjoint (i.e. observable), which means  $\mathcal H$  must be Hermitian:

$$\mathcal{H}^{\dagger} = \mathcal{H} \,. \tag{3}$$

The first property of the system we want to implement, is particle-hole symmetry (see Appendix):

$$\hat{\sigma}_{x}\mathcal{H}^{*}\hat{\sigma}_{x} = -\mathcal{H} ; \qquad (4)$$

here \* is the complex conjugation and  $\hat{\sigma}_x = \sigma_x \otimes \mathbb{1}_L$ , where  $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  is the first Pauli matrix.

This is equivalent to writing

$$\mathcal{H} = \begin{pmatrix} \mathcal{H}_0 & \mathcal{H}_p \\ -\mathcal{H}_p^* & -\mathcal{H}_0^* \end{pmatrix}, \tag{5}$$

where, due to  ${\mathcal H}$  being Hermitian, we must have

$$\mathcal{H}_0^{\dagger} = \mathcal{H}_0, \quad \mathcal{H}_p^{T} = -\mathcal{H}_p.$$
(6)

We can notice  $\mathcal{H}_0$  is coupled to the terms  $a_i^{\dagger}a_j$  and  $a_ia_j^{\dagger}$ , that stem from an ordinary external potential and kinetic term, while  $\mathcal{H}_p$  is coupled to the terms  $a_ia_j$  and  $a_i^{\dagger}a_j^{\dagger}$ , that stem from pairing mechanisms such as superconductivity.

Another property we may consider for the system is time-reversal symmetry:

$$\mathcal{H}^* = \mathcal{H} , \tag{7}$$

or, in terms of  $\mathcal{H}_0$  and  $\mathcal{H}_p$ :

$$\mathcal{H}_0^* = \mathcal{H}_0, \quad \mathcal{H}_p^* = \mathcal{H}_p.$$
(8)

#### 2.1 Diagonalization

By diagonalizing the matrix  $\mathcal{H}$ , we can define new creation and annihilation operators that represent a fermion with a given energy. Due to properties (3) and (4), we can find an operator  $\mathcal{U}$  such that

$$\mathcal{U}^{\dagger}\mathcal{U} = \mathbb{1}_{2L}, \quad \hat{\sigma}_{x}\mathcal{U}^{*}\hat{\sigma}_{x} = \mathcal{U}$$
(9)

or, equivalently,

$$\mathcal{U} = \begin{pmatrix} u^T & v^{\dagger} \\ v^T & u^{\dagger} \end{pmatrix},\tag{10}$$

$$u^*u^T + v^*v^T = \mathbb{1}_L, \quad uv^T + vu^T = \mathbb{O}_L,$$
(11)

which diagonalizes the Hamiltonian matrix:

$$\mathcal{U}^{\dagger}\mathcal{H}\mathcal{U} = \mathcal{D} = diag(\varepsilon_1, \dots, \varepsilon_L, -\varepsilon_1, \dots, -\varepsilon_L);$$
(12)

if we have time reversal symmetry, we can also choose  ${\mathcal U}$  such that

$$\mathcal{U}^* = \mathcal{U} \,. \tag{13}$$

Defining the new creation and annihilation operators as

$$\begin{pmatrix} \tilde{a}_1 \\ \vdots \\ \tilde{a}_L \\ \vdots \\ \tilde{a}_L^{\dagger} \\ \vdots \\ \tilde{a}_L^{\dagger} \end{pmatrix} = \mathcal{U}^{\dagger} \begin{pmatrix} a_1 \\ \vdots \\ a_L \\ a_1^{\dagger} \\ \vdots \\ a_L^{\dagger} \end{pmatrix},$$
(14)

the Hamiltonian takes the diagonalized form

$$H = \left(\tilde{a}_{1}^{\dagger} \dots \tilde{a}_{L}^{\dagger} \tilde{a}_{1} \dots \tilde{a}_{L}\right) diag(\varepsilon_{1}, \dots, \varepsilon_{L}, -\varepsilon_{1}, \dots, -\varepsilon_{L}) \begin{pmatrix} a_{1} \\ \vdots \\ \tilde{a}_{L} \\ \vdots \\ \vdots \\ \tilde{a}_{l}^{\dagger} \end{pmatrix} = \sum_{i=1}^{L} \varepsilon_{i} \left(2\tilde{a}_{i}^{\dagger} \tilde{a}_{i} - 1\right)$$
(15)

which shows  $\{\varepsilon_i\}_{i=1,\dots,L}$  are the excitation energies for particles and  $\{-\varepsilon_i\}_{i=1,\dots,L}$  can be interpreted as excitation energies for holes; due to properties (9) the transformation  $\{a_i\}_{i=1,\dots,L} \rightarrow \{\tilde{a}_i\}_{i=1,\dots,L}$  is consistent with  $\{a_i^{\dagger}\}_{i=1,\dots,L} \rightarrow \{\tilde{a}_i^{\dagger}\}_{i=1,\dots,L}$  and it is canonical, i.e.

$$\{\tilde{a}_i, \tilde{a}_j\} = 0, \quad \{\tilde{a}_i^{\dagger}, \tilde{a}_j\} = \delta_{ij}.$$
(16)

# 2.2 Bogoliubov equations

Moving to the index notation, the new creation and annihilation operators are defined as

$$\begin{cases} \tilde{a}_{i}^{\dagger} = \sum_{k=1}^{L} (u_{ik} \ a_{k}^{\dagger} + v_{ik} \ a_{k}) \\ \tilde{a}_{i} = \sum_{k=1}^{L} (u_{ik}^{*} \ a_{k} + v_{ik}^{*} \ a_{k}^{\dagger}) \end{cases};$$
(17)

eq. (12) gives us the general form of the Bogoliubov equations, which link u and v to  $\mathcal{H}_0$ ,  $\mathcal{H}_p$  and the excitation energies  $\varepsilon_1, ..., \varepsilon_L$ :

$$\begin{cases} \varepsilon_{i} u_{ij} = \sum_{k=1}^{L} (u_{ik} \mathcal{H}_{0 jk} + v_{ik} \mathcal{H}_{p jk}) \\ \varepsilon_{i} v_{ij} = -\sum_{k=1}^{L} (u_{ik} \mathcal{H}_{p jk}^{*} + v_{ik} \mathcal{H}_{0 jk}^{*}) \end{cases}$$
(18)

To have some insight on how to extract information on the system from equations (18), we must first introduce Majorana operators.

# **3 MAJORANA OPERATORS**

For any lattice site *i*, we define two Majorana operators:

$$c_{2i-1} = a_i + a_i^{\dagger}, \quad c_{2i} = -i(a_i - a_i^{\dagger}).$$
 (19)

In the vector-matrix notation this is written as

$$\begin{pmatrix} c_1 \\ \vdots \\ c_{2L} \end{pmatrix} = \sqrt{2} \Gamma^{\dagger} \begin{pmatrix} a_1 \\ \vdots \\ a_L \\ a_1^{\dagger} \\ \vdots \\ a_L^{\dagger} \end{pmatrix}, \qquad (20)$$

where

$$\Gamma = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & i & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & i \\ 1 & -i & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & -i & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & -i \end{pmatrix};$$
(21)

we take note of the following properties of  $\Gamma$ :

$$\Gamma^{\dagger}\Gamma = \mathbb{1}_{2L}, \quad \hat{\sigma}_{x}\Gamma^{*} = \Gamma, \quad \Gamma^{\dagger}\Gamma = diag(1, -1, \dots, 1, -1).$$
(22)

From (2) and (19), it is straightforward to see that Majorana operators have the following properties:

$$c_{\alpha}^{\dagger} = c_{\alpha} , \qquad (23)$$

$$\{c_{\alpha}, c_{\beta}\} = 2\delta_{\alpha\beta} , \qquad (24)$$

where the indices  $\alpha$  and  $\beta$  span from 1 to 2*L*.

We can write H in terms of Majorana operators:

$$H = \frac{1}{2} (c_1 \dots c_{2L}) \,\overline{\mathcal{H}} \begin{pmatrix} c_1 \\ \vdots \\ c_{2L} \end{pmatrix}, \tag{25}$$

where we have defined

$$\bar{\mathcal{H}} = \Gamma^{\dagger} \mathcal{H} \Gamma \,. \tag{26}$$

Due to (22), properties (3) (observability of  $\mathcal H$ ) and (4) (particle-hole symmetry) translate into

$$\overline{\mathcal{H}}^{\dagger} = \overline{\mathcal{H}}, \quad \overline{\mathcal{H}}^* = -\overline{\mathcal{H}},$$
 (27)

while property (7) (time-reversal symmetry) translates into

$$\bar{\mathcal{H}}_{\alpha\beta}^* = (-1)^{\alpha+\beta} \bar{\mathcal{H}}_{\alpha\beta} \,. \tag{28}$$

This means that  $\overline{\mathcal{H}}$ , i.e. the Hamiltonian matrix in the Majorana-operator representation, can be written as  $\overline{\mathcal{H}} = 2iA$ , where A is a real antisymmetric matrix whose even entries vanish if and only if the system is time-reversal symmetric.

#### 3.1 Diagonalization

Similarly to what we saw in the previous section for the creation and annihilation operators, we can diagonalize  $\overline{\mathcal{H}}$  in blocks of 2x2 antisymmetric sub-matrices

$$\bar{\mathcal{U}}^{\dagger}\bar{\mathcal{H}}\bar{\mathcal{U}} = \Gamma^{\dagger}D\Gamma = \bar{D} = i \, diag\left(\begin{pmatrix} 0 & \varepsilon_{1} \\ -\varepsilon_{1} & 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 & \varepsilon_{L} \\ -\varepsilon_{L} & 0 \end{pmatrix}\right)$$
(29)

and define a new set of Majorana operators

$$\begin{pmatrix} \tilde{c}_{1} \\ \vdots \\ \tilde{c}_{2L} \end{pmatrix} = \bar{\mathcal{U}}^{\dagger} \begin{pmatrix} c_{1} \\ \vdots \\ c_{2L} \end{pmatrix} = \sqrt{2} \Gamma^{\dagger} \begin{pmatrix} \tilde{a}_{1} \\ \vdots \\ \tilde{a}_{L} \\ \vdots \\ \tilde{a}_{L}^{\dagger} \end{pmatrix},$$
(30)

where we have defined

$$\bar{\mathcal{U}} = \Gamma^{\dagger} \mathcal{U} \Gamma ; \tag{31}$$

the second equivalence in (30) uses equations (14) and (20) and it shows that the definition of the new Majorana operators is consistent with the new creation and annihilation operators previously defined.

Due to (22), properties (9) (orthonormality of  $\mathcal{U}$  and particle-hole symmetry) translate into

$$\bar{\mathcal{U}}^{\dagger}\bar{\mathcal{U}} = \mathbb{1}_{2L} , \quad \bar{\mathcal{U}}^* = \bar{\mathcal{U}} , \tag{32}$$

while property (13) (time-reversal symmetry) translates into

$$\bar{\mathcal{U}}^*_{\alpha\beta} = (-1)^{\alpha+\beta} \bar{\mathcal{U}}_{\alpha\beta} ; \qquad (33)$$

this means that  $\overline{U}$ , which gives us the coefficients of the new Majorana operators  $\{\tilde{c}_{\alpha}\}_{\alpha=1,\dots,2L}$  as linear functions of the starting set  $\{c_{\alpha}\}_{\alpha=1,\dots,2L}$ , is a real orthonormal matrix whose odd entries vanish if and only if the system is time-reversal symmetric.

We can now write the Hamiltonian in its diagonalized Majorana form:

$$H = \frac{i}{2} (\tilde{c}_1 \dots \tilde{c}_{2L}) \operatorname{diag} \left( \begin{pmatrix} 0 & \varepsilon_1 \\ -\varepsilon_1 & 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 & \varepsilon_L \\ -\varepsilon_L & 0 \end{pmatrix} \right) \begin{pmatrix} c_1 \\ \vdots \\ \tilde{c}_{2L} \end{pmatrix} = i \sum_{i=1}^L \varepsilon_i \, \tilde{c}_{2i-1} \tilde{c}_{2i} \,. \tag{34}$$

# 3.2 Bogoliubov equations

Again, similarly to the previous section, we move now to the index notation. Equation (31) gives:

$$\begin{cases} \bar{u}_{2i-1,2j-1} = Re(u_{ji} + v_{ji}^{*}) \\ \bar{u}_{2i,2j-1} = Im(u_{ji} + v_{ji}^{*}) \\ \bar{u}_{2i-1,2j} = -Im(u_{ji} - v_{ji}^{*}) \\ \bar{u}_{2i,2j} = Re(u_{ji} - v_{ji}^{*}) \end{cases}$$
(35)

setting

$$u_{ij} + v_{ij}^* = \phi_{ij}, \quad u_{ij} - v_{ij}^* = \psi_{ij}$$
 (36)

and using the first equivalence in (30), we obtain

$$\begin{cases} \tilde{c}_{2i-1} = \sum_{k=1}^{L} (Re\phi_{ik} c_{2k-1} + Im\phi_{ik} c_{2k}) \\ \tilde{c}_{2i} = \sum_{k=1}^{L} (-Im\psi_{ik} c_{2k-1} + Re\psi_{ik} c_{2k}) \end{cases}.$$
(37)

Finally, plugging (36) into (18), we obtain the Bogoliubov equations

$$\begin{cases} \varepsilon_{i} \phi_{ij} = \sum_{k=1}^{L} (\psi_{ik} \mathcal{H}_{0 jk} - \psi_{ik}^{*} \mathcal{H}_{p jk}) \\ \varepsilon_{i} \psi_{ij} = \sum_{k=1}^{L} (\phi_{ik} \mathcal{H}_{0 jk} + \phi_{ik}^{*} \mathcal{H}_{p jk}) \end{cases}$$
(38)

which are in accordance with (29).

#### 3.3 Majorana zero modes

Equations (38) are particularly useful to examine Majorana zero modes. Let's say the system has a state with excitation energy equal to zero, i.e. there is an index n for which  $\varepsilon_n = 0$ :

$$\begin{cases} \sum_{k=1}^{L} (\psi_{nk} \mathcal{H}_{0 jk} - \psi_{nk}^{*} \mathcal{H}_{p jk}) = 0 \\ \sum_{k=1}^{L} (\phi_{nk} \mathcal{H}_{0 jk} + \phi_{nk}^{*} \mathcal{H}_{p jk}) = 0 \end{cases};$$
(39)

solving this system of equations means finding the coefficients of the Majorana zero modes  $\tilde{c}_{2n-1}$  and  $\tilde{c}_{2n}$ .

In general, the equations in (39) have complex values, but in the case of time-reversal symmetry all quantities must be real and the system simplifies:

$$\begin{cases} \sum_{k=1}^{L} \psi_{nk} (\mathcal{H}_0 - \mathcal{H}_p)_{jk} = 0\\ \sum_{k=1}^{L} \phi_{nk} (\mathcal{H}_0 + \mathcal{H}_p)_{jk} = 0 \end{cases}$$
(40)

which means the vectors  $\{\psi_{nk}\}_{k=1,\dots,L}$  and  $\{\phi_{nk}\}_{k=1,\dots,L}$  are, respectively, in the kernel of  $\mathcal{H}_0 - \mathcal{H}_p$  and  $\mathcal{H}_0 + \mathcal{H}_p$ .

# 4 TOPOLOGICAL PHASES

In this section, we will define two kinds of discrete topological invariants that can characterize our system. The value taken by the invariants, as a function of the entries of the matrices  $\mathcal{H}_0$  and  $\mathcal{H}_p$ , defines the *topological phase* of the system.

# 4.1 Boundary invariants

Let us further examine the meaning of  $\mathcal{H}_0$  and  $\mathcal{H}_p$ . In the index notation, the Hamiltonian takes the form

$$H = \sum_{i} \mathcal{H}_{0\,ii} \left( 2a_{i}^{\dagger}a_{i} - 1 \right) + 2 \sum_{i>j} \left( \mathcal{H}_{0\,ij} a_{i}^{\dagger}a_{j} + \mathcal{H}_{p\,ij} a_{i}^{\dagger}a_{j}^{\dagger} + h.c. \right) ; \tag{41}$$

where h.c. denotes the Hermitian conjugate; this means that:

- $\mathcal{H}_{0 \, ii}$  is coupled to the term  $2a_i^{\dagger}a_i 1$  and represents the chemical potential for the lattice site *i*,
- $\mathcal{H}_{0 i j}$  is coupled to the term  $a_i^{\dagger} a_j$  and represents the hopping amplitude between sites *i* and *j*,
- $\mathcal{H}_{p\,ij}$  is coupled to the term  $a_i^{\dagger}a_j^{\dagger}$  and represents the pairing amplitude between sites *i* and *j*.

If we assume that hopping and pairing act on a finite range r, i.e.

$$\mathcal{H}_{0\,ij} = 0$$
,  $\mathcal{H}_{p\,ij} = 0$  for  $|i - j| > r$ , (42)

then, under certain conditions, equations (39) can be used recursively to construct the vectors  $\{\psi_{nk}\}_{k=1,\dots,L}$  and  $\{\phi_{nk}\}_{k=1,\dots,L}$ .

# 4.1.1 Transfer matrix

The idea is the following: given the first r components of the vectors (  $\{\psi_{nk}\}_{k=1,...,r}$  and  $\{\phi_{nk}\}_{k=1,...,r}$  ), equations (39) for j = 1 give us  $\psi_{n,r+1}$  and  $\phi_{n,r+1}$ . Plugging these values in equations (39) for j = 2, we get  $\psi_{n,r+2}$  and  $\phi_{n,r+2}$  and so on up until  $\psi_{n,L}$  and  $\phi_{n,L}$ .

In general, given  $\{\psi_{nk}\}_{k=1,...,r}$  and formally setting  $\psi_{n,1-r} = \ldots = \psi_{n0} = 0$ , we can write:

$$\begin{pmatrix} \psi_{n,j+1} \\ \vdots \\ \psi_{n,j+2-2r} \end{pmatrix} = T_j^{\psi} \begin{pmatrix} \psi_{n,j} \\ \vdots \\ \psi_{n,j+1-2r} \end{pmatrix}, \quad j = r, \dots, L-1;$$
(43)

the  $2r \ge 2r$  matrix  $T_j^{\psi}$  is called a transfer matrix. Similarly, given  $\{\phi_{nk}\}_{k=1,\dots,r}$  and formally setting  $\phi_{n,1-r} = \dots = \phi_{n0} = 0$ , we get:

$$\begin{pmatrix} \phi_{n,j+1} \\ \vdots \\ \phi_{n,j+2-2r} \end{pmatrix} = T_j^{\phi} \begin{pmatrix} \phi_{n,j} \\ \vdots \\ \phi_{n,j+1-2r} \end{pmatrix}, \quad j = r, \dots, L-1.$$
(44)

For a finite number of lattice sites L, equations (39) for j = L - r + 1, ..., L represent a set of constraints on  $\mathcal{H}_0$  and  $\mathcal{H}_p$  that are needed for the solutions of (43) and (44) to actually represent Majorana zero modes; in other terms, these constraints grant the existence of the zero eigenvalue  $\varepsilon_n = 0$ , which we assumed (they are equivalent to requiring  $det\mathcal{H} = 0$ ).

In the thermodynamic limit  $L \to \infty$  with open boundary conditions on the left edge, the recursive procedure in (39) doesn't generate any constraint on  $\mathcal{H}_0$  and  $\mathcal{H}_p$ ; the only constraint we have, for the solutions of (43) and (44) to be Majorana zero modes, is that  $\tilde{c}_{2n-1}$  and  $\tilde{c}_{2n}$  must represent physical states, i.e. the vectors  $\{\psi_{nk}\}_{k=1,\dots,L}$  and  $\{\phi_{nk}\}_{k=1,\dots,L}$  need to be normalizable.

#### 4.1.2 Edge modes

The normalizability of  $\{\psi_{nk}\}_{k=1,...,L}$  and  $\{\phi_{nk}\}_{k=1,...,L}$  is related to the eigenvalues of the transfer matrices. Let us consider, for example, a periodic system with period *P*:

$$\mathcal{H}_{0\,ij} = \mathcal{H}_{0\,i+P,j+P}, \quad \mathcal{H}_{p\,ij} = \mathcal{H}_{p\,i+P,j+P}; \qquad (45)$$

focusing on the  $\psi$ -type variables for simplicity, equation (45) implies  $T_j^{\psi} = T_{j+P}^{\psi}$ , so we can define the transfer matrix over a single period as

$$T^{\psi} = \prod_{j=1}^{P} T_j^{\psi} , \qquad (46)$$

so that

$$\begin{pmatrix} \psi_{n,j+P} \\ \vdots \\ \psi_{n,j+1-2r+P} \end{pmatrix} = T^{\psi} \begin{pmatrix} \psi_{n,j} \\ \vdots \\ \psi_{n,j+1-2r} \end{pmatrix}.$$
(47)

We name  $\{\lambda_m\}_{m=1,\dots,M}$  the eigenvalues of  $T^{\psi}$  such that  $|\lambda_m| < 1$ , and  $\{v_m\}_{m=1,\dots,M}$  the corresponding eigenvectors; of course, M must be less than or equal to the total number of eigenvalues of  $T^{\psi}$ , which is at most equal to 2r. Any linear combination of  $\{v_m\}_{m=1,\dots,M}$  whose last r components are equal to zero can be plugged into equation (47) for j = r; by applying  $T^{\psi}$  recursively, this gives us a normalizable set of coefficients  $\{\psi_{nk}\}_{k=1,\dots,L}$ . At every application of the transfer matrix, the vector obtained has a smaller norm than the starting vector: this means that  $\{\psi_{nk}\}_{k=1,\dots,L}$  has an exponential decay for  $k \to \infty$ , meaning that the corresponding Majorana zero mode  $\tilde{c}_{2n}$  is localized at the left edge of the chain.

Let us define  $n^{\psi}$  as the maximum number of linearly independent combinations of  $\{v_m\}_{m=1,...,M}$  with the constraint of the last r entries being equal to 0. These combinations, through equation (47), generate the set  $\{\tilde{c}_{2n_s}\}_{s=1,...,n^{\psi}}$  of the even-index Majorana zero modes localized at the left edge of the chain. Notice that  $n^{\psi} > 2$  requires further degeneracy (than the one due to particle-hole symmetry) in the 0-eigenspace of  $\mathcal{H}$ .

Substituting  $\psi$  with  $\phi$ , the same procedure gives us the set  $\{\tilde{c}_{2n_s-1}\}_{s=1,\dots,n^{\phi}}$  of odd-index Majorana zero modes localized at the left edge of the chain.

We can also start by taking the inverse of equation (43): given  $\{\psi_{nk}\}_{k=L+1-r,\dots,L}$  and formally setting  $\psi_{n,L+1} = \dots = \psi_{n,L+r} = 0$ , we can write

$$\begin{pmatrix} \psi_{n,j-1} \\ \vdots \\ \psi_{n,j-2+2r} \end{pmatrix} = \begin{pmatrix} T_j^{\psi} \end{pmatrix}^{-1} \begin{pmatrix} \psi_{n,j} \\ \vdots \\ \psi_{n,j-1+2r} \end{pmatrix}, \quad j = , \dots, L+1-r.$$
(48)

In this case, we use the eigenvalues of  $T^{\psi} \{\lambda_{m'}\}_{=1,...,M'}$  such that  $|\lambda_{m'}| > 1$  and their eigenvectors  $\{v_{m'}\}_{m'=1,...,M'}$ . We define  $n'^{\psi}$  as the maximum number of linearly independent combinations of  $\{v_{m'}\}_{m'=1,...,M'}$  with the constraint of the last r entries being equal to 0 (same constraint as before); these combinations now generate the set  $\{\tilde{c}_{2n's}\}_{s=1,...,n'^{\psi}}$  of even-index Majorana zero modes localized at the right edge of the chain. Substituting  $\psi$  with  $\phi$ , the same procedure gives us the set  $\{\tilde{c}_{2n's-1}\}_{s=1,...,n'^{\phi}}$  of odd-index Majorana edge zero modes localized at the right edge of the chain.

We can show that  $2\max\{n^{\psi} + n'^{\psi}, n^{\phi} + n'^{\phi}\}$  is a lower bound for the degeneracy of the 0-eigenspace of  $\mathcal{H}$ . Furthermore, we can show  $n^{\psi} + n'^{\psi} \leq M + M' - r \leq r$ , meaning that the maximum range of hopping and pairing sets an upper bound for both the number of even-index and odd-index Majorana edge zero modes.

 $r - n^{\psi} + n'^{\psi}$  is the number of non-localized even-index Majorana zero modes that are suppressed by normalization. 2r - M - M' of these correspond to missing eigenvalues (when  $T^{\psi}$  is not diagonalizable) or eigenvalues with modulus 1. The others are due to the geometrical structure of the eigenvalues themselves. Let us say, for example, that r = 2 and  $T^{\psi}$  has two eigenvalues of modulus < 1,

corresponding to 
$$\begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}$$
 and  $\begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}$ , and two eigenvalues of modulus > 1 corresponding to  $\begin{pmatrix} 0\\1\\0\\0 \end{pmatrix}$  and  $\begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}$ ; the

first and the third eigenvectors generate a Majorana zero mode localized respectively at the left edge and at the right edge of the chain, while the second and the forth are not compatible with open boundary conditions and are discarded, thus we have 2 = r edge modes. Let us say, instead, that modulus < 1

eigenvalues correspond to 
$$\begin{pmatrix} 1\\0\\1\\0 \end{pmatrix}$$
 and  $\begin{pmatrix} 0\\1\\0\\1 \end{pmatrix}$  and modulus > 1 eigenvalues correspond to  $\begin{pmatrix} 1\\0\\-1\\0 \end{pmatrix}$  and  $\begin{pmatrix} 0\\1\\0\\-1 \end{pmatrix}$ :

in this case no combination of the first two eigenvectors, nor of the last two ones, is compatible with open boundary conditions, meaning there are no Majorana edge zero modes; to find a combination of eigenvectors compatible with open boundary conditions, we need to mix eigenvalues with modulus < 1, with eigenvalues with modulus > 1, but in that case the Majorana zero mode is suppressed by normalization.

Finally,  $n^{\psi}$ ,  $n^{\phi}$ ,  $n'^{\psi}$  and  $n'^{\phi}$  are examples of topological invariants. Later we will see how these values are related in the case of the Kitaev chain.

# 4.2 Bulk invariants

Another example of a topological invariant can be examined by considering the bulk properties of our system. To do so, we need to switch to the momentum representation: we define the *momentum* creation and annihilation operators as the Fourier transforms of their site counterparts presented in (1) and (2):

$$a_{k}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikj} a_{j}^{\dagger} , \quad a_{k} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ikj} a_{j} , \quad k \in K ;$$
(49)

the set of momenta *K* contains *L* elements in the interval  $(-\pi, \pi]$  and depends on the parity of *L* and on the boundary conditions we impose, such as periodic boundary conditions (PBC) or antiperiodic boundary conditions (ABC). Specifically, we find

$$K = \begin{cases} \{0, \pm k_m, \pi\}_{m=1,...,M}, & PBC, L even \\ \{0, \pm k_m\}_{m=1,...,M}, & PBC, L odd \\ \{\pm k_m\}_{m=1,...,M}, & ABC, L even \\ \{\pm k_m, \pi\}_{m=1,...,M}, & ABC, L odd \end{cases}$$
(50)

where

(51)

$$k_m = \begin{cases} \frac{2\pi}{L}m, & PBC\\ \frac{2\pi}{L}m - \frac{\pi}{L}, & ABC \end{cases}, \qquad M = \begin{cases} \left[\frac{L-1}{2}\right], & PBC\\ \left[\frac{L}{2}\right], & ABC \end{cases},$$

[ ] being the function that takes the integer part of a real number.

The site creation and annihilation operators are then the inverse Fourier transforms of the momentum operators, i.e.

$$a_j^{\dagger} = \frac{1}{\sqrt{L}} \sum_{k \in K} e^{-ikj} a_k^{\dagger} , \quad a_j = \frac{1}{\sqrt{L}} \sum_{k \in K} e^{ikj} a_k ; \qquad (52)$$

one can verify that (49) and (52) are equivalent due to the identities

$$\frac{1}{N} \sum_{k \in K} e^{ik(j-j')} = \delta_{jj'}, \quad \frac{1}{N} \sum_{j=1}^{L} e^{-i(k-k')j} = \delta_{kk'}.$$
(53)

From equations (2), (49) and (53) one can straightforwardly show that

$$\{a_k, a_{k'}\} = 0, \quad \{a_k^{\dagger}, a_{k'}\} = \delta_{ij},$$
 (54)

i.e. the transformation  $\{a_j\}_{j=1,\dots,L} \to \{a_k\}_{k=1,\dots,L}$  is canonical.

Plugging equations (52) into equation (1), we can write the general form of the Hamiltonian in the momentum representation:

$$H = \left(a_{k_{1}}^{\dagger} a_{-k_{1}} a_{-k_{1}}^{\dagger} a_{k_{1}} \dots a_{k_{M}}^{\dagger} a_{-k_{M}} a_{-k_{M}}^{\dagger} a_{k_{M}}\right) \hat{\mathcal{H}} \begin{pmatrix} a_{k_{1}} \\ a_{-k_{1}} \\ a_{k_{1}} \\ \vdots \\ a_{k_{M}} \\ a_{-k_{M}}^{\dagger} \\ a_{-k_{M}} \\ a_{k_{M}}^{\dagger} \end{pmatrix},$$
(55)

where, for the sake of simplicity, we considered ABC and *L* even, so as not to include special cases k = 0 and  $k = \pi$ .

# 4.2.1 Closed boundary conditions and diagonalization

To study the bulk properties of the system, we want  $\hat{\mathcal{H}}$  to be diagonal in blocks of  $2x^2$  matrices and that requires closed boundary conditions and translational symmetry (see Appendix). With these conditions, equation (55) reduces to:

$$H = \sum_{k \in K} (a_k^{\dagger} a_{-k}) \mathcal{H}_k \begin{pmatrix} a_k \\ a_{-k}^{\dagger} \end{pmatrix}.$$
 (56)

In terms of  $\mathcal{H}_k$ , observability and particle-hole symmetry translate into the following properties:

$$\mathcal{H}_{k} = \mathcal{H}_{k}^{\dagger}, \quad \sigma_{x} \mathcal{H}_{-k}^{*} \sigma_{x} = -\mathcal{H}_{k} , \qquad (57)$$

we also have time-reversal symmetry if the following condition is verified:

$$\mathcal{H}_{-k}^* = \mathcal{H}_k \,. \tag{58}$$

It is useful to decompose  $\mathcal{H}_k$  as a linear combination of the identity and the Pauli matrices:

$$\mathcal{H}_{k} = h_{k}^{0} \,\mathbb{1}_{2} + h_{k}^{x} \,\sigma_{x} + h_{k}^{y} \,\sigma_{y} + h_{k}^{z} \,\sigma_{z} = \begin{pmatrix} h_{k}^{0} + h_{k}^{z} & h_{k}^{x} + ih_{k}^{y} \\ h_{k}^{x} - ih_{k}^{y} & h_{k}^{0} - h_{k}^{z} \end{pmatrix},\tag{59}$$

where  $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ,  $\sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$ ,  $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ . In terms of  $h_k^0$ ,  $h_k^x$ ,  $h_k^y$ ,  $h_k^z$ , properties (57) become

$$\begin{cases} \left(h_{k}^{0}\right)^{*} = h_{k}^{0}, \quad h_{-k}^{0} = -h_{k}^{0} \\ \left(h_{k}^{x}\right)^{*} = h_{k}^{x}, \quad h_{-k}^{x} = -h_{k}^{x} \\ \left(h_{k}^{y}\right)^{*} = h_{k}^{y}, \quad h_{-k}^{y} = -h_{k}^{y} \\ \left(h_{k}^{z}\right)^{*} = h_{k}^{z}, \quad h_{-k}^{z} = h_{k}^{z} \end{cases}$$

$$\tag{60}$$

and property (58) adds the condition

$$h_k^0 = h_k^x = 0. (61)$$

From the explicit expression of  $\mathcal{H}_k$  in (59) we can extract its eigenvalues  $E_k^{\pm}$  and eigenvectors  $v_k^{\pm}$ :

$$E_{k}^{\pm} = h_{k}^{0} \pm \left| \overrightarrow{h_{k}} \right|, \quad v_{k}^{\pm} = \begin{pmatrix} e^{i\varphi_{k}}\chi_{k}^{\pm} \\ \pm e^{-i\varphi_{k}}\chi_{k}^{\mp} \end{pmatrix}, \quad (62)$$

where we defined

$$\chi_k^{\pm} = \sqrt{\frac{\left|\overrightarrow{h_k}\right| \pm h_k^z}{2\left|\overrightarrow{h_k}\right|}}, \quad e^{2i\varphi_k} = \frac{h_k^x + ih_k^y}{\left|h_k^x + ih_k^y\right|}; \tag{63}$$

if we call  $\Theta_k$  and  $\Phi_k$  the spherical coordinates of  $\overrightarrow{h_k}$  with respect to the *z*-axis, i.e.  $\Theta_k = \arccos\left(\frac{h_k^2}{|\overrightarrow{h_k}|}\right)$ and  $\Phi_k = \arg\left(h_k^x + ih_k^y\right)$ , we can easily see that  $\chi_k^+ = \cos\left(\frac{\Theta_k}{2}\right)$ ,  $\chi_k^- = \sin\left(\frac{\Theta_k}{2}\right)$  and  $\varphi_k = \frac{\Phi_k}{2}$ . Properties (60) imply that

$$\chi_{-k}^{\pm} = \chi_k^{\pm}, \quad e^{2i\varphi_{-k}} = -e^{2i\varphi_k}$$
 (64)

and that the eigenvalues  $E_k^{\pm}$  present the typical particle-hole symmetric structure we already saw in section 2:

$$E_{-k}^{\pm} = -E_k^{\mp} \,. \tag{65}$$

Now that we know the explicit form of its eigenvectors, we can diagonalize  $\mathcal{H}_k$  too:

$$H = \sum_{k \in K} \left( \tilde{a}_k^{\dagger} \, \tilde{a}_{-k} \right) diag \left( E_k^{+}, E_k^{-} \right) \left( \begin{array}{c} \tilde{a}_k \\ \tilde{a}_{-k}^{\dagger} \end{array} \right) = \sum_{k \in K} E_k^{+} \left( 2 \tilde{a}_k^{\dagger} \tilde{a}_k - 1 \right), \tag{66}$$

where we have defined the new creation and annihilation operators according to

$$\tilde{a}_{k}^{\dagger} = e^{i\varphi_{k}} \chi_{k}^{+} a_{k}^{\dagger} + e^{-i\varphi_{k}} \chi_{k}^{-} a_{-k}$$
(67)

and consistently with properties (64), which also grant the transformation  $\{a_k, a_{-k}^{\dagger}\} \rightarrow \{\tilde{a}_k, \tilde{a}_{-k}^{\dagger}\}$  is canonical.

#### 4.2.2 Winding number

Similarly to what we observed in section 4.1, in the case of a finite chain  $L < \infty$  we cannot say much about states with zero excitation energy. The existence of a zero eigenvalue simply translates into a constraint on the Hamiltonian matrices, namely  $|h_k^0| = |\overrightarrow{h_k}|$  for some  $k \in K$ . In the thermodynamic limit  $L \to \infty$ , though, we see the emergence of topological phases connected to the gap in the bulk energy spectrum.

First, in the limit  $L \rightarrow \infty$  we can think of the momentum as a continuous variable, i.e.

$$k \in K = (-\pi, \pi], \tag{68}$$

and all information on boundary conditions and parity of L are negligible. The bulk energy spectrum is given by the union of the images of the functions  $E_k^{\pm} = h_k^0 \pm |\vec{h_k}|$  over the full domain  $k \in (-\pi, \pi]$ ; due to (65), the spectrum must then be symmetric. For continuity, we have two cases:

- I. the bulk spectrum is gapped, i.e. it is given by two disconnected intervals, one with positive values and one with the opposite negative values,
- II. the bulk spectrum is given by one symmetric interval and admits zero energy states.

What we need to do then, is to construct a topological invariant that is sensitive to the closure of the gap. Let us first consider the case with time-reversal symmetry: from (60) and (61), we know that  $h_k^0$  vanishes and  $\overrightarrow{h_k}$  lies on the *yz*-plane; we can then define the winding number

$$\omega = \frac{1}{2\pi} \oint d\Theta_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\partial_k h_k^z}{h_k^y} dk$$
(69)

that counts how many laps around the origin  $\overrightarrow{h_k}$  does on the *yz*-plane. Notice that *w* doesn't change under small changes in  $\overrightarrow{h_k}$  unless  $\overrightarrow{h_k}$  crosses the origin for some  $\overline{k} \in (-\pi, \pi]$ , i.e.  $E_{\overline{k}}^{\pm} = 0$  and the bulk gap closes. Then, the winding number *w* can be used as a topological invariant; the phase transitions it identifies require a closure of the gap, and with it the appearance of zero energy states.

Now, we saw in section 4.1 that, in the thermodynamic limit, the zero energy states appear as Majorana modes localized at the edges of the chain, and their number is robust under small changes of the parameters of the system, i.e. its Hamiltonian. Notice that result was obtained considering open boundary conditions and then taking the limit  $L \rightarrow \infty$ , whereas the winding number was defined starting from closed boundary conditions; but, as we already mentioned, in the thermodynamic limit the properties of the system must be independent from the starting boundary conditions. The winding number  $\omega$ , instead, detects zero energy bulk states along the phase transitions. We can say, heuristically, that, when the system enters a phase transition, a bulk zero energy state appears and, as soon as the transition is completed, the state stabilizes as a Majorana edge mode.

#### 4.2.3 Broken time-reversal symmetry

When time-reversal symmetry is broken, we must take into account  $h_k^0$  and  $h_k^x$  too, so our parameters span four dimensions and a winding number is not definable. We can notice that, for  $\bar{k} = 0, \pi$ , the components  $h_k^0, h_k^x$  and  $h_k^y$  all vanish; we can use this to define the following topological invariant:

$$\nu = \operatorname{sgn}(h_0^z h_\pi^z) \,. \tag{71}$$

Similarly to  $\omega$ , a change of value of  $\nu$  requires a closure of the gap; the invariant  $\nu$ , though, can embed less information than the winding number w, since it has values in the cyclic group of order two ( $\mathbb{Z}_2$ ). We will see soon how these bulk invariants are related to the boundary ones in the case of the Kitaev chain.

# **5** APPLICATION: KITAEV CHAIN

The system proposed by Alexei Kitaev and its generalizations fit into the framework presented in sections 2, 3 and 4. The basic model corresponds to the homogeneous (i.e. symmetric under translations), and time-reversal symmetric case with nearest-neighbour interactions (i.e. range r = 1) so we can write

$$\mathcal{H}_{0\,ii} = -\frac{\mu}{2}, \qquad \mathcal{H}_{0\,i,i+l} = \begin{cases} -\frac{w}{2}, & l=1\\ 0, & l\geq 2 \end{cases}, \qquad \mathcal{H}_{p\,i,i+l} = \begin{cases} -\frac{\Delta}{2}, & l=1\\ 0, & l\geq 2 \end{cases}$$
(72)

the other parameters being set by properties (6). Then, as in (41), the Hamiltonian of the open chain is:

...

$$H = -\sum_{i=1}^{L} \mu \left( a_i^{\dagger} a_i - \frac{1}{2} \right) - \sum_{i=1}^{L-1} \left( w \; a_i^{\dagger} a_{i+1} + \Delta \; a_i^{\dagger} a_{i+1}^{\dagger} \right).$$
(73)

We can see that  $\mu$  is the chemical potential of a lattice site, w is the hopping amplitude between two neighbouring sites and  $\Delta$  is the relative pairing amplitude. Without loss of completeness, we can assume w > 0.

#### 5.1 Transfer matrix approach

According to (40), Bogoliubov equations for the open Kitaev chain are

$$\begin{cases} (w + \Delta)\psi_{n,j-1} + \mu\psi_{nj} + (w - \Delta)\psi_{n,j+1} = 0\\ (w - \Delta)\phi_{n,j-1} + \mu\phi_{nj} + (w + \Delta)\phi_{n,j+1} = 0 \end{cases}$$
(74)

so, referring to (43) and (44), we can compute the expression for the transfer matrices:

$$T_j^{\psi} = \sigma_x T^{-1} \sigma_x , \quad T_j^{\phi} = T = \begin{pmatrix} -\frac{\mu}{w+\Delta} & -\frac{w-\Delta}{w+\Delta} \\ 1 & 0 \end{pmatrix}.$$
(75)

The eigenvalues of T are

$$\lambda^{\pm} = \frac{-\frac{\mu}{2w} \pm \sqrt{\left(\frac{\mu}{2w}\right)^2 + \left(\frac{\Delta}{w}\right)^2 - 1}}{1 + \frac{\Delta}{w}}$$
(76)

and, according to section 4.1, we have phase transitions when the modulus of  $\lambda^+$  or  $\lambda^-$  crosses the value 1, i.e. in the following conditions:

a) 
$$\frac{\mu}{2w} = 1$$
: the eigenvalues are  $-1$  and  $-\frac{w-\Delta}{w+\Delta}$ ;  
b)  $\frac{\mu}{2w} = -1$ : the eigenvalues are 1 and  $\frac{w-\Delta}{w+\Delta}$ ;  
c)  $\begin{cases} -1 < \frac{\mu}{2w} < 1 \\ \frac{\Delta}{w} = 0 \end{cases}$ : the eigenvalues are  $-\frac{\mu}{2w} \pm i \sqrt{1 - (\frac{\mu}{2w})^2}$ .

We can then identify the following phases.

- Phase I:  $-1 < \frac{\mu}{2w} < 1$  and  $\frac{\Delta}{w} > 0$ . We have two eigenvalues with amplitude less than 1, as we can see for example in the case  $\mu = 0$ , where we have  $|\lambda^{\pm}| = \sqrt{\left|\frac{\Delta-w}{\Delta+w}\right|}$ .

- Phase II:  $-1 < \frac{\mu}{2w} < 1$  and  $\frac{\Delta}{w} < 0$ . We have two eigenvalues with amplitude more than 1; in the case  $\mu = 0$  we now have  $|\lambda^{\pm}| = \sqrt{\frac{|\Delta|+w}{|\Delta|-w|}}$ .
- Phase III:  $\frac{\mu}{2w} < -1$  or  $\frac{\mu}{2w} > 1$ . We have one eigenvalue with amplitude less than 1 and one with amplitude more than 1, as we can see setting  $\frac{\Delta}{w} = 0$ , so that we have  $\lambda^{\pm} = -\frac{\mu}{2w} \pm \sqrt{\left(\frac{\mu}{2w}\right)^2 1}$ .

To count Majorana edge modes, we have to find combinations of eigenvectors of the transfer matrix T that have the last r components equal to zero; in this case, r = 1 and the only vector that satisfies this constraint is  $\binom{1}{0}$ . Let us recall that applying T to  $\binom{1}{0}$  recursively gives us the non-normalized components  $\{\phi_{n,j}\}_{j=1,\dots,L}$  of an odd-index Majorana zero mode.  $\binom{1}{0}$  is not an eigenvector itself but can be decomposed as a combination of both eigenvectors of T: to have a normalizable Majorana zero mode, both eigenvalues of these two components need to have magnitude less than 1, or both greater than 1; in the former case, the Majorana zero mode is localized at the left edge of the chain, while in the latter case it is localized at the right edge of the chain.

For even-index Majorana zero modes the transfer matrix is  $\sigma_x T^{-1} \sigma_x$ , whose eigenvalues are the inverse of *T*'s eigenvalues: this ultimately means that an even-index Majorana edge zero mode always appears in couple with an odd-index one at the other edge of the chain.

According to the definitions given in section 4.1, we can conclude that:

- phase I is topological: we have an odd-index Majorana zero mode on the left edge of the chain and an even-index one on the right end of the chain, i.e.  $n^{\phi} = n'^{\psi} = 1$ ,  $n^{\psi} = n'^{\phi} = 0$ ;
- phase II is topological: we have an even-index Majorana zero mode on the left edge of the chain and an odd-index one on the right end of the chain, i.e.  $n^{\psi} = n'^{\phi} = 1$ ,  $n^{\phi} = n'^{\psi} = 0$ ;
- phase III is non-topological: we have no Majorana zero modes, i.e.  $n^{\psi} = n^{\phi} = n'^{\phi} = n'^{\psi} = 0$  .

# 5.2 Bulk spectrum approach

Returning to the Hamiltonian in (72), if we close the chain we can write the Hamiltonian in the momentum representation, as in (56) and (59) with

$$h_k^0 = h_k^x = 0$$
,  $h_k^y = \Delta \sin k$ ,  $h_k^z = -\left(\frac{\mu}{2} + w \cos k\right)$ ; (77)

the energy-momentum dispersion, as in (62), is

$$E_k^{\pm} = \pm \sqrt{\left(\frac{\mu}{2} + w \cos k\right)^2 + (\Delta \sin k)^2} .$$
 (78)

As we saw in section 4.2, in this approach phase transitions are characterized by a gap closure in the bulk spectrum. This happens when  $E_k^{\pm} = 0$  for some  $k \in (-\pi, \pi]$ , which exactly corresponds to the phase transitions found in the transfer matrix approach, in fact:

a) for  $\frac{\mu}{2m} = 1$  the gap closes at  $k = \pi$ ;

b) for 
$$\frac{\mu}{2w} = -1$$
 the gap closes at  $k = 0$ ;  
c) for  $\begin{cases} -1 < \frac{\mu}{2w} < 1\\ \frac{\Delta}{w} = 0 \end{cases}$  the gap closes at  $k = \cos^{-1}\left(-\frac{\mu}{2w}\right)$ .

This shows that the topological phases of the system can be identified consistently by either approach, corroborating the heuristic argument presented in 4.2.

To compute the winding number  $\omega$ , defined in (69), for each topological phase, we have to follow the curve traced by the winding vector  $(h_k^y, h_k^z)$ . This curve is a circle that goes clockwise for  $\frac{\Delta}{w} < 0$  (which means  $\omega \ge 0$ ) and counterclockwise for  $\frac{\Delta}{w} > 0$  (which means  $\omega \le 0$ ); the circle contains the origin for  $-1 < \frac{\mu}{2w} < 1$  (which means  $|\omega| = 1$  inside the interval and  $\omega = 0$  outside of it).

We can also directly compute the less sensitive  $\mathbb{Z}_2$ -invariant  $\nu$ , defined in (70): it is straightforward to show that  $\nu = 1$  when  $\left|\frac{\mu}{2w}\right| > 1$  and  $\nu = -1$  when  $\left|\frac{\mu}{2w}\right| < 1$ .

In conclusion:

- in phase I we have  $\omega = -1$  ,  $\nu = -1$  ,
- in phase II we have  $\omega = 1$  ,  $\nu = -1$  ,
- in phase III we have  $\omega = 0$  ,  $\nu = 1$  .

#### 5.3 Broken time-reversal symmetry

As we saw from property (7), breaking time-reversal symmetry means admitting complex non-diagonal entries in the Hamiltonian matrix  $\mathcal{H}$ . Without loss of completeness, we can take  $\Delta$  to be real and set

$$\mathcal{H}_{0\,il} = -\frac{\mu}{2}, \quad \mathcal{H}_{0\,i,l+l} = \begin{cases} -\frac{w}{2}e^{i\varphi}, \quad l=1\\ 0, \qquad l \ge 2 \end{cases}, \quad \mathcal{H}_{p\,i,l+l} = \begin{cases} -\frac{\Delta}{2}, \quad l=1\\ 0, \qquad l \ge 2 \end{cases}$$
(79)

so that the new Hamiltonian is:

$$H = -\sum_{i=1}^{L} \mu \left( a_i^{\dagger} a_i - \frac{1}{2} \right) - \sum_{i=1}^{L-1} \left( w e^{i\varphi} a_i^{\dagger} a_{i+1} + \Delta a_i^{\dagger} a_{i+1}^{\dagger} \right).$$

In the momentum representation we obtain

$$\begin{cases}
h_k^0 = w \sin\varphi \sink \\
h_k^x = 0 \\
h_k^y = \Delta \sink \\
h_k^z = -\left(\frac{\mu}{2} + w \cos\varphi \cosk\right)
\end{cases}$$
(80)

which leads to the energy-momentum dispersion:

$$E_k^{\pm} = w \sin\varphi \sin k \pm \sqrt{\left(\frac{\mu}{2} + w \cos\varphi \cos k\right)^2 + (\Delta \sin k)^2}.$$
 (81)

The condition for the gap closure is then

$$\left(\frac{\mu}{2w} + \cos\varphi \cos k\right)^2 + \left(\frac{\Delta}{w}\right)^2 \sin^2 k = \sin^2 \varphi \sin^2 k \tag{82}$$

for some  $k \in (-\pi, \pi]$  and it no longer identifies a 1-dimensional region in the space of parameters  $\frac{\mu}{2w}$ and  $\frac{\Delta}{w}$ . Pictorially, we can say that, starting from the time-reversal symmetric case  $\varphi = 0$  and moving to the maximal symmetry breaking case  $\varphi = \frac{\pi}{2}$ , the transition lines a) and b) (i.e.  $\frac{\mu}{2w} = \pm 1$ ) get progressively closer, squeezing phases I and II, while the transition line c) (i.e.  $\begin{cases} -1 < \frac{\mu}{2w} < 1\\ \frac{\Delta}{w} = 0 \end{cases}$ ), expands

into a 2-dimensional critical region that takes the form of a rectangle between lines a) and b) jointed with two elliptical segments cut along lines a) and b) and tangent to the starting lines  $\frac{\mu}{2w} = \pm 1$ .

The result is that topological phases I and II get smaller and smaller to the point of vanishing in the extreme limit of maximal symmetry breaking, while the non-topological phase III expands to the point of taking the whole parameter space, with the exception of an elliptical critical region centered on the origin.

# 5.4 Finite number of neighbours

We now extend Kitaev's model considering a greater but finite number of neighbours for hopping and pairing, i.e. r > 1. Setting

$$\mathcal{H}_{0\,ii} = -\frac{\mu}{2}, \quad \mathcal{H}_{0\,i,i+l} = \begin{cases} -\frac{w_l}{2}e^{i\varphi_l}, \ l \le r\\ 0, \qquad l \ge r+1 \end{cases}, \quad \mathcal{H}_{p\,i,i+l} = \begin{cases} -\frac{\Delta_l}{2}, \ l \le r\\ 0, \qquad l \ge r+1 \end{cases}$$
(83)

the Hamiltonian for the extended Kitaev chain is

$$H = -\sum_{i=1}^{L} \mu \left( a_i^{\dagger} a_i - \frac{1}{2} \right) - \sum_{l=1}^{r} \sum_{i=1}^{L-l} \left( w_l \ e^{i\varphi_l} \ a_i^{\dagger} a_{i+l} + \Delta_l \ a_i^{\dagger} a_{i+l}^{\dagger} \right).$$
(84)

In the momentum representation we find:

$$\begin{cases}
h_k^0 = \sum_{l=1}^r w_l \sin\varphi_l \sin(kl) \\
h_k^x = 0 \\
h_k^y = \sum_{l=1}^r \Delta_l \sin(kl) \\
h_k^z = -\left(\frac{\mu}{2} + \sum_{l=1}^r w_l \cos\varphi_l \cos(kl)\right)
\end{cases}$$
(85)

A study of topological phase diagrams of the extended Kitaev chain, assuming hopping and pairing parameters proportional to a power of l

$$w_l = w \ l^{-\alpha} , \quad \Delta_l = \Delta \ l^{-\beta} ,$$
 (86)

and using both bulk invariant and transfer matrix approaches, can be found in reference [20].

What we want to remark here, is the explicit relations that the topological invariants we introduced have in the extended Kitaev chain. For r = 1 we saw that

$$n^{\phi} = n^{\prime \psi}, \quad n^{\psi} = n^{\prime \phi}, \tag{87}$$

i.e. Majorana zero modes come in pairs with the odd-index one and the even-index one being localized at opposite edges of the chain, and this is due to the fact that the transfer matrix for the odd-index modes is the inverse of the one for the even-index modes and as such has inverted eigenvalues.

Equations (87) are true for the r > 1 time-reversal symmetric case too, since it is a consequence of the particular structure of the Bogoliubov equations

$$\begin{cases} \mu \psi_{nj} + \sum_{l=1}^{r} \left( (w_l + \Delta_l) \psi_{n,j-l} + (w_l - \Delta_l) \psi_{n,j+l} \right) = 0 \\ \mu \phi_{nj} + \sum_{l=1}^{r} \left( (w_l - \Delta_l) \phi_{n,j-l} + (w_l + \Delta_l) \phi_{n,j+l} \right) = 0 \end{cases}$$
(88)

that come from (40). In fact, we can see from (88) that after the substitutions  $\psi_{n,j-l} \leftrightarrow \psi_{n,j+l}$  the two equations are the same and lead to the same transfer matrix, i.e.

$$\begin{pmatrix} \psi_{n,j+1} \\ \vdots \\ \psi_{n,j-2+2r} \end{pmatrix} = T^{\phi} \begin{pmatrix} \psi_{n,j} \\ \vdots \\ \psi_{n,j-1+2r} \end{pmatrix},$$
(89)

where  $T^{\phi}$  is defined in (44) (we removed the index *j* since the system is homogeneous); thus we have

$$T^{\psi} = A \left( T^{\phi} \right)^{-1} A , \qquad (90)$$

where we have defined  $A = \operatorname{antidiag}(1, ..., 1)$ .  $T^{\psi}$  is similar to  $(T^{\phi})^{-1}$ , so it has inverted eigenvalues, which is the main point in proving (87).

We can also see from (88) that changing the sign of  $\Delta$  results in an exchange of the roles of odd-index modes with even-index modes, consistently to what we saw in the case r = 1 (transition between phase I and phase II); but changing the sign of  $\Delta$  also changes the winding of the vector  $(h_k^y, h_k^z)$ , as we can see in (85), and with it the sign of the winding number  $\omega$ . So, changing  $\omega$  to  $-\omega$  results in exchanging  $n^{\phi}$  with  $n^{\psi}$ : according to the phase diagram we studied for r = 1, we conclude that

$$\omega = n^{\psi} - n^{\phi} \,. \tag{91}$$

As for the  $\mathbb{Z}_2$ -invariant  $\nu$ , it must change sign anytime a new Majorana zero mode appears, so it must quantify the parity of the winding number ( $\nu = 1$  if  $\omega$  is even and  $\nu = -1$  if  $\omega$  is odd).

# 6 CONCLUSIONS

The Kitaev chain has been, and is still being, studied from a great variety of angles, which can also go beyond the applications of the framework we have presented. For example, experimental realizations of this system may have to deal with the presence of disorder and particle interactions. It already has been shown that moderate disorder supports the topological phase [27, 28] and that repulsive interactions tend to loosen the conditions on the chemical potential for the system to be in the topological phase [29-31].

The purpose of this work was to formulate a theoretical background to study the topological properties of a system of non-interacting spinless fermions and show how to apply it to various generalizations of the Kitaev chain. We have developed two independent tools, the first meant to study the boundary properties of the system and the localization properties of its states, the second meant to study its bulk properties. Both tools lead to the identification of topological phase transitions of the system, and by applying them to the Kitaev chain we saw how they are actually consistent and complementary.

# APPENDIX: SYMMETRIES

Let us consider a generic fermionic many-body system. In the occupation number notation, we define the state

$$\left|\left\{n_{j}\right\}_{j}\right\rangle = \prod_{j} \left(a_{j}^{\dagger}\right)^{n_{i}} \left|0\right\rangle, \tag{92}$$

where:

- the index *j* spans across a finite set {1, ..., *L*} and labels the single-particle states,
- $\left|\left\{n_{j}
  ight\}_{j}
  ight
  angle$  is the multi-particle state with occupation numbers  $\left\{n_{j}
  ight\}_{j}$ ,
- $|0\rangle$  is the empty state of the system,
- $n_i = 0.1$  means the single-particle state *j* is, respectively, empty or occupied,
- $a_i^{\dagger}$  is the creation operator of *j*.

 $\{|\{n_j\}_j\rangle\}_{\{n_j\}_j}$ , i.e. the set of states defined in (92) with given occupation numbers, is a basis for the Fock space F of the system. A linear or antilinear operator  $\mathcal{O}: F \mapsto F$  on the Fock space can be defined, according to elementary linear algebra, by setting how it acts on the vectors of a basis, in this case by defining  $\mathcal{O}|\{n_j\}_j\rangle$  for all  $\{n_j\}_j$ . Notice that, if  $\mathcal{O}$  is invertible, we can add a term  $\mathcal{O}^{-1}\mathcal{O}$  in (92) between each couple of neighbouring creation operators; therefore,  $\mathcal{O}$  can also be defined by setting how it acts on the creation operators and the empty state, i.e. by defining  $\mathcal{O}|0\rangle$  and  $\mathcal{O}a_j^{\dagger}\mathcal{O}^{-1}$  for all j.

The Fourier transform of  $a_i^{\dagger}$  is defined as

$$a_k^{\dagger} = \frac{1}{\sqrt{L}} \sum_j e^{ikj} a_j^{\dagger} , \qquad (93)$$

where k spans across a symmetrical set of L elements in the interval  $(-\pi,\pi]$ . Notice that, when we define  $\mathcal{O}$  through its applications  $\mathcal{O}a_j^{\dagger}\mathcal{O}^{-1}$  on the creation operators, if  $\mathcal{O}$  is linear then  $\mathcal{O}a_k^{\dagger}\mathcal{O}^{-1}$  will be the Fourier transform of  $\mathcal{O}a_j^{\dagger}\mathcal{O}^{-1}$ , whereas if  $\mathcal{O}$  is antilinear  $\mathcal{O}a_k^{\dagger}\mathcal{O}^{-1}$  will be the Fourier transform of  $\mathcal{O}a_i^{\dagger}\mathcal{O}^{-1}$ , whereas if  $\mathcal{O}$  is antilinear  $\mathcal{O}a_k^{\dagger}\mathcal{O}^{-1}$  will be the Fourier transform of  $\mathcal{O}a_i^{\dagger}\mathcal{O}^{-1}$ .

Symmetries in quantum mechanics are described by unitary or antiunitary operators. A unitary operator  $\mathcal{U}$  is such that  $\langle \psi | \mathcal{U}^{\dagger} \mathcal{U} | \varphi \rangle = \langle \psi | \varphi \rangle$ , i.e.  $\mathcal{U}^{\dagger} \mathcal{U} = \mathbb{1}$ . An antiunitary operator  $\mathcal{U}$  is such that  $\langle \psi | \mathcal{U}^{\dagger} \mathcal{U} | \varphi \rangle = \langle \varphi | \psi \rangle$ , i.e.  $\mathcal{U}^{\dagger} \mathcal{U}$  takes the complex conjugate both on its right and on its left. Unitary and antiunitary operators act like canonical transformations on the creation operators, i.e.  $\{\mathcal{U}a_{j}^{\dagger}\mathcal{U}^{-1} = \tilde{a}_{j}^{\dagger}\}_{j}$  will be a set of new creation and annihilation operators. This means that the new empty state  $|\widetilde{0}\rangle = \mathcal{U}|0\rangle$  is defined by  $\tilde{a}_{j}|\widetilde{0}\rangle = 0$  for every j and is not a degree of freedom in the construction of  $\mathcal{U}$ . As for the action of  $\mathcal{U}$  on the Fourier-transformed creation operators  $a_{k}^{\dagger}$ , this will be  $\mathcal{U}a_{k}^{\dagger}\mathcal{U}^{-1} = \tilde{a}_{k}^{\dagger}$  if  $\mathcal{U}$  is unitary and  $\mathcal{U}a_{k}^{\dagger}\mathcal{U}^{-1} = \tilde{a}_{-k}^{\dagger}$  if  $\mathcal{U}$  is antiunitary.

So we can construct a symmetry operator by defining its applications  $\mathcal{U}a_j^{\dagger}\mathcal{U}^{-1} = \tilde{a}_j^{\dagger}$  on the creation operators, and then choosing whether it acts on the Fourier transforms as  $\mathcal{U}a_k^{\dagger}\mathcal{U}^{-1} = \tilde{a}_k^{\dagger}$  (i.e. it is unitary) or as  $\mathcal{U}a_k^{\dagger}\mathcal{U}^{-1} = \tilde{a}_{-k}^{\dagger}$  (i.e. it is antiunitary). If we interpret *j* and *k* as, respectively, space and momentum indices, this process captures the physical meaning of the symmetry operator.

#### Time-reversal symmetry.

The physical meaning of a time-reversal operation is to leave space variables unchanged and invert momentum variables. Therefore, we can define the time-reversal operator T through

$$Ta_{j}^{\dagger}T^{-1} = a_{j}^{\dagger}, \qquad Ta_{k}^{\dagger}T^{-1} = a_{-k}^{\dagger}.$$
 (94)

This means that T is antilinear and acts on the Fock space as  $T: |\{n_j\}_j\} \mapsto |\{n_j\}_j\rangle$ , i.e. when T acts on a vector  $|\varphi\rangle$  it takes the complex conjugate of its components along the basis of vectors with given occupation numbers.

We define a system to be time-reversal symmetric if its Hamiltonian H is such that

$$THT^{-1} = H . (95)$$

If *H* has the structure of a one-body operator as in (1), i.e.

$$H = \left(a_{j_{1}}^{\dagger} \dots a_{j_{L}}^{\dagger} a_{j_{1}} \dots a_{j_{L}}\right) \mathcal{H} \begin{pmatrix} a_{j_{1}} \\ \vdots \\ a_{j_{L}} \\ a_{j_{1}}^{\dagger} \\ \vdots \\ a_{j_{L}}^{\dagger} \end{pmatrix},$$
(96)

then, by combining (95) and (96), we find  $THT^{-1} = H$ ; but H is a matrix made of scalars, so  $THT^{-1} = H^*TT^{-1} = H^*$ , which gives the condition on H for time-reversal symmetry:

$$\mathcal{H} = \mathcal{H}^* \,. \tag{97}$$

If H has the diagonalized form in (56), i.e.

$$H = \sum_{i=1}^{L} \left( a_{k_i}^{\dagger} a_{-k_i} \right) \mathcal{H}_{k_i} \begin{pmatrix} a_{k_i} \\ a_{-k_i}^{\dagger} \end{pmatrix},$$
(98)

then, by combining (95) and (98), we find  $T\mathcal{H}_{k_i}T^{-1} = \mathcal{H}_{-k_i}$ ; therefore, the condition on  $\mathcal{H}_{k_i}$  for time-reversal symmetry is:

$$\mathcal{H}_{k_i}^* = \mathcal{H}_{-k_i} \,. \tag{99}$$

#### Particle-hole symmetry.

The physical meaning of this operation is to swap particles with holes, leaving space and time variables unchanged. Therefore, we can define the particle-hole operator C through

$$Ca_{j}^{\dagger}C^{-1} = a_{j}, \qquad Ca_{k}^{\dagger}C^{-1} = a_{k}.$$
 (100)

One can show this means that *C* is antilinear and acts on the Fock space as  $C: |\{n_j\}_j\rangle \mapsto \xi_{\{n_j\}_j} |\{n_j\}_j\rangle$ , where  $\xi_{\{n_j\}_j}$  is a sign that depends on the occupation numbers of the state.

We define a system to be particle-hole symmetric if its Hamiltonian H is such that

$$CHC^{-1} = -C$$
 (101)

Notice that  $C(a_{j_1}^{\dagger} \dots a_{j_L}^{\dagger} a_{j_1} \dots a_{j_L})C^{-1} = (a_{j_1} \dots a_{j_L} a_{j_1}^{\dagger} \dots a_{j_L}^{\dagger}) = (a_{j_1}^{\dagger} \dots a_{j_L}^{\dagger} a_{j_1} \dots a_{j_L})\hat{\sigma}_x$ , where  $\hat{\sigma}_x = \sigma_x \otimes \mathbb{1}_L$ ; then, by combining (101) and (96), we find  $\hat{\sigma}_x C \mathcal{H} C^{-1} \hat{\sigma}_x = -\mathcal{H}$ , i.e.

$$\hat{\sigma}_{\chi} \mathcal{H}^* \hat{\sigma}_{\chi} = -\mathcal{H} \,. \tag{102}$$

We can also notice that  $C(a_{k_i}^{\dagger} a_{-k_i})C^{-1} = (a_{k_i} a_{-k_i}^{\dagger}) = (a_{-k_i}^{\dagger} a_{k_i})\sigma_x$ ; then, by combining (101) with (98), we find  $\sigma_x C \mathcal{H}_{-k_i} C^{-1} \sigma_x = -\mathcal{H}_{k_i}$ , i.e.

$$\sigma_{x}\mathcal{H}_{-k_{i}}^{*}\sigma_{x} = -\mathcal{H}_{k_{i}}.$$
(103)

# Translational symmetry.

We can define a translation operator as the unitary operator such that

$$S_l a_j^{\dagger} S_l^{-1} = a_{j+l}^{\dagger} ; (104)$$

according to (93), this means that  $S_l$  acts on the momentum creation and annihilation operators as

$$S_l a_k^{\dagger} S_l^{-1} = e^{-ikl} a_k^{\dagger}, \quad S_l a_k S_l^{-1} = e^{ikl} a_k.$$
(105)

Let us consider a generic Hamiltonian in the momentum representation as in (55), i.e.

$$H = \left(a_{k_{1}}^{\dagger} a_{-k_{1}} a_{-k_{1}}^{\dagger} a_{k_{1}} \dots a_{k_{M}}^{\dagger} a_{-k_{M}} a_{-k_{M}}^{\dagger} a_{k_{M}}\right) \widehat{\mathcal{H}} \begin{pmatrix} a_{k_{1}}^{\dagger} \\ a_{-k_{1}}^{\dagger} \\ a_{k_{1}}^{\dagger} \\ \vdots \\ a_{k_{M}} \\ a_{-k_{M}}^{\dagger} \\ a_{-k_{M}}^{\dagger} \\ a_{-k_{M}}^{\dagger} \end{pmatrix};$$
(106)

and write  $\widehat{\mathcal{H}}$  in blocks of  $2x^2$  matrices:

$$\widehat{\mathcal{H}} = \begin{pmatrix}
\widehat{\mathcal{H}}_{k_{1},k_{1}} & \widehat{\mathcal{H}}_{k_{1},-k_{1}} & \cdots & \widehat{\mathcal{H}}_{k_{1},k_{M}} & \widehat{\mathcal{H}}_{k_{1},-k_{M}} \\
\widehat{\mathcal{H}}_{-k_{1},k_{1}} & \widehat{\mathcal{H}}_{-k_{1},-k_{1}} & \cdots & \widehat{\mathcal{H}}_{-k_{1},k_{M}} & \widehat{\mathcal{H}}_{-k_{1},-k_{M}} \\
& \vdots & \ddots & \vdots \\
\widehat{\mathcal{H}}_{k_{M},k_{1}} & \widehat{\mathcal{H}}_{k_{M},-k_{1}} & \cdots & \widehat{\mathcal{H}}_{k_{M},k_{M}} & \widehat{\mathcal{H}}_{k_{M},-k_{M}} \\
& \widehat{\mathcal{H}}_{-k_{M},k_{1}} & \widehat{\mathcal{H}}_{-k_{M},-k_{1}} & \cdots & \widehat{\mathcal{H}}_{-k_{M},k_{M}} & \widehat{\mathcal{H}}_{-k_{M},-k_{M}}
\end{pmatrix}.$$
(107)

Applying  $S_l$  to H ultimately means transforming  $\hat{\mathcal{H}}_{k',k''}$  into  $e^{-i(k'-k'')l}\hat{\mathcal{H}}_{k',k''}$  in the expression of  $\hat{\mathcal{H}}$ . This shows that translational symmetry, i.e.

$$S_l H S_l^{-1} = H$$
, (108)

is equivalent to requiring  $\widehat{\mathcal{H}}$  to be diagonal in blocks of 2x2 matrices.

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