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Topological phases in disordered long-range Kitaev

chains

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Abstract

The aim of the thesis is to investigate the behaviour of the many-neighbours pairing Kitaev chain (and different dependencies of the Hamiltonian parameters on the distance), in the hypothesis of disorder associated with the chemical potential.

A proposal to a numerical resolution of the many-neighbours problem is lead through the Transfer Matrix method proposed by A. Alecce and L. Dell'Anna¹ for the calculation of the wave functions of the zero-energy Majorana edge modes in the basis of the Bogoliubov states, which diagonalize the Kitaev chain's Hamiltonian.

On the other hand, the study of the system in the hypothesis of disorder is carried out with the aim of generalizing the results proposed by N. M. Gergs, L. Fritz, and D. Schuricht² to the many-neighbours case, thus looking for the critical values of the chemical potential, typical for each amount of disorder (intended as standard deviation of a normal distribution) at fixed interaction parameters, above which a topological phase cannot exist.

In this study we show that, as happens in the nearest neighbour case, also in the general case there is an amount of disorder beyond which the critical chemical potential is zero (i.e., a topological phase is never possible), before which we show the presence of an enhancement of the edge modes.

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Figure 1: A representation of the Kitaev chain system. The black line is the chain itself, which lays over a p-wave superconductor (the blue block).

1 Introduction

1.1 The Kitaev chain

Implementing a full-scale quantum computer is a major challenge to modern physics and engineering. Theoretically, this goal should be achievable due to the possibility of fault-tolerant quantum computation³. It has been also suggested that fault-tolerance can be achieved at the physical level⁴, instead of using quantum error-correcting codes.

For example, Kitaev chain is a way to construct decoherence-protected degrees of freedom in one-dimensional systems ("quantum wires"). It was first proposed by A. Yu Kitaev in his article⁵ which titles "Unpaired Majorana Fermions in Quantum Wires" and consists in a row of equidistant sites which may be occupied by non-interacting spinless fermions in the presence of hopping between nearest lattice sites and superconducting pairing between nearest neighbors:

$$H = -\sum_{j=1}^{L} \mu \left(c_j^{\dagger} c_j - 1/2 \right) + \sum_{j=1}^{L-1} \left(-w c_j^{\dagger} c_{j+1} + \Delta c_j c_{j+1} + h.c. \right).$$
(1)

In the Hamilotonian above, L is the lenght of the chain (i.e. the number of fermionic sites) μ is the chemical potential, w the hopping parameter and Δ the superconductive pairing⁶ (both assumed to be real, so that the system is time-reversal symmetric, cfr. Appendix A.1.1), result of the presence of a p-wave superconductor⁷ under the fermionic chain, as one can see from figure 1.

It is useful, in order to investigate the properties of such a system, to reparametrize the Hamiltonian in terms of Majorana fermions, defined as:

$$\gamma_{2j-1} = c_j + c_j^{\dagger}, \quad \gamma_{2j} = \frac{1}{i} \left(c_j - c_j^{\dagger} \right), \tag{2}$$

and obeys the anti-commutative law:

$$\{\gamma_j, \gamma_k\} = 2\delta_{jk}.$$



Figure 2: The Majorana particles, here represented by cubes, are normally coupled as in the upper image, forming L fermions as defined by (2) (blue halos). However, sometimes they can couple with the other adjacent Majorana, forming L - 1 fermions (red halos in the bottom image) and leaving unpaired two Majoranas on the edges.

Majorana particles are fermions that are their own antiparticles. They were hypothesised by Ettore Majorana in 1937⁸, but they've never been observed (although the nature of the neutrinos is not settled yet⁹). However, in condensed matter physics, quasiparticle excitations can appear like bound Majorana fermions¹⁰¹¹. Though, instead of a single fundamental particle, they are the collective movement of several individual particles. Rewriting (1), the Hamiltonian becomes:

$$H = -\frac{i}{2} \sum_{j=1}^{L-1} \left[(w - \Delta)\gamma_{2j-1}\gamma_{2j+2} + (w + \Delta)\gamma_{2j+1}\gamma_{2j} \right] - \frac{i}{2} \sum_{j=1}^{L} \mu \gamma_{2j-1}\gamma_{2j}.$$

The simplest, but still most explanatory case we may consider is the one with $\mu = 0$ and $w = \Delta \equiv t$:

$$H = it \sum_{j=1}^{L-1} \gamma_{2j+1} \gamma_{2j}.$$
 (3)

Here we can re-compose the Hamiltonian in terms of new fermionic operators, defined by:

$$\tilde{c}_j = \frac{1}{2} (\gamma_{2j} + i\gamma_{2j+1}), \quad \tilde{c}_j^{\dagger} = \frac{1}{2} (\gamma_{2j} - i\gamma_{2j+1}),$$

giving out the Hamiltonian:

$$H = 2t \sum_{j=1}^{L-1} \left(\tilde{c}_j^{\dagger} \tilde{c}_j - \frac{1}{2} \right).$$
 (4)

The interpretation of what we have done is the following: as two Majorana particles form one fermion, we combined Majoranas belonging to adjacent sites, in order to compose new fermions out of them, as figure 2 shows.

However, in this way we take into account only L - 1 sites out of the original L, as one can see from equations (3) and (4). As a matter of fact, operators γ_1 and γ_{2L} , i.e. the first and the last Majoranas of the chain, are no longer considered. We can think at them as combined into a non-local fermion, the corresponding operator of which takes form:

$$f = \frac{1}{2} \left(\gamma_1 + i \gamma_{2L} \right). \tag{5}$$

As it does not appear in the Hamiltonian, it does not influence the energy of the system. Hence, our chain has two zero-energy states localized at its ends. Because of this, we see a ground state degeneracy: If $|\phi_0\rangle$ is a ground state with $f|\phi_0\rangle = 0$, then $|\phi_1\rangle = f^{\dagger}|\phi_0\rangle$ is also a ground state with the same energy. The configuration is such that these two Majorana quasi-particles, called *unpaired Majorana zero energy modes*, or MZM^{12} , form a two-state quantum system, which can incode a qubit information. Moreover, it is immune to classical error σ_x (that is the kind of error which transform a 0 in a 1 and vice versa) because the chain could be virtually infinite and such a transformation on Majorana edge modes is prevented. This is actually an advantage and is the mechanism which the possibility of using these systems to do fault-tolerant quantum computing is based on. For this reason, a great effort has been put on the study and realization of isolated Majorana fermions in 1-dimensional and 2-dimensional superconductors^{13\,14\,15}, both from a theoretical and an experimental ^{16 17 18} standpoint.

Despite the case studied above is very particular and at first glance it could appear as a bizarre thing due to a fine-tuning operation, in general one can find MZMs with less restrictive choices of parameters. MZMs thus defined are found to be distributed along the chain sites according to an exponential-decaying a wave function.

1.2 General case: a transfer matrix approach

It can be demonstrated ^{19 20} that, in addition to the degeneration of the ground state, the Kitaev chain presents, within a given domain of the parameters, the other conditions for the realization of the topological order, such as the opening of an energy gap in the bulk spectrum.

The topological order is generally characterized²¹ by the presence of edge excitations, which in the Kitaev chain we find as MZMs that, in general, decay exponentially in the bulk. There are several ways to find the aforementioned domain; the transfer matrix approach²²²³ also allows to verify the distribution of the Majorana modes along the chain. In order to construct the transfer matrix, we'd better to change notation, defining:

$$\gamma_{2j-1} = a_j, \quad \gamma_{2j} = b_j.$$

The Hamiltonian of the system will then become:

$$H = -\frac{i}{2} \sum_{n=1}^{L-1} \left[(w - \Delta)a_n b_{n+1} + (w + \Delta)a_{n+1} b_n \right] - \frac{i}{2} \sum_{n=1}^{L} \mu a_n b_n.$$

Then, supposing that the MZM we are looking for are distributed along, the chain, we can call them Q_a and Q_b and write them as:

$$Q_a = \sum_{j=1}^{L} \alpha_j \left(c_j + c_j^{\dagger} \right) = \sum_{j=1}^{L} \alpha_j a_j, \quad Q_b = \sum_{j=1}^{L} \frac{\beta_j}{i} \left(c_j - c_j^{\dagger} \right) = \sum_{j=1}^{L} \beta_j b_j.$$

The transfer matrix can be obtained from the Heisenberg equations of motion for the Majorana operators:

$$i\frac{da_{n}}{dt} = -[H, a_{n}] = -i(w + \Delta)b_{n+1} - i(w - \Delta)b_{n-1} - i\mu b_{n}$$
$$i\frac{db_{n}}{dt} = -[H, b_{n}] = i(w + \Delta)a_{n-1} + i(w - \Delta)a_{n+1} + i\mu a_{n}$$

Assuming that these operators depend on time as $a_n = \alpha_n e^{-iEt}$ and $b_n = \beta_n e^{-iEt}$, we can find the values of the energy E for which the above equations have solutions, given by:

$$(w - \Delta)\alpha_{n-1} + (w + \Delta)\alpha_{n+1} - \mu\alpha_n = -iE\beta_n$$

-(w + \Delta)\beta_{n-1} - (w - \Delta)\beta_{n+1} + \mu\beta_n = -iE\alpha_n
(6)

We then remember that we are looking for solutions which, as done by (5), create a degeneracy by commuting with the Hamiltonian. This is easily done setting E = 0, that is considering zero energy, hence the name MZM. The equations for α_n and β_n decouple, and they can be written in the transfer matrix form

$$\begin{pmatrix} \alpha_{n+1} \\ \alpha_n \end{pmatrix} = A \begin{pmatrix} \alpha_n \\ \alpha_{n-1} \end{pmatrix}, \quad \text{where } A = \begin{pmatrix} \frac{\mu}{\Delta + w} & \frac{\Delta - w}{\Delta + w} \\ 1 & 0 \end{pmatrix}$$
(7)

Similar expressions hold for the β_n s since the respective transfer matrices are related by $B = A^{-1}$. Knowing the behavior of the *a*-modes thus completely determines that of the *b*-modes.

The transfer matrix A has two eigenvalues, namely:

$$\lambda_{\pm} = \frac{\mu \pm \sqrt{\mu^2 - 4(\Delta^2 - w^2)}}{2(\Delta + w)}$$

Thus, one can always write:

$$\begin{pmatrix} \alpha_n \\ \alpha_{n-1} \end{pmatrix} = c_1 \begin{pmatrix} v_n \\ v_{n-1} \end{pmatrix} + c_2 \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix};$$
$$\begin{pmatrix} \alpha_{n+1} \\ \alpha_n \end{pmatrix} = A \begin{pmatrix} \alpha_n \\ \alpha_{n-1} \end{pmatrix} = A^n \begin{pmatrix} \alpha_1 \\ \alpha_0 \end{pmatrix} = c_1 \lambda_+^n \begin{pmatrix} v_1 \\ v_0 \end{pmatrix} + c_2 \lambda_-^n \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}.$$

This means that the MZM have an exponential behaviour along the chain (see figure 3). In particular, they are normalizable, thus they are allowed to exist, if in the thermodynamic limit (i.e. for $n \to \infty$) the wave function

$$\alpha_n = \text{const}_1 \cdot \lambda_+^{n-1} + \text{const}_2 \cdot \lambda_-^{n-1}$$



Figure 3: An example of the wave functions α_j and β_j for L = 200, $\mu = w$, $\Delta = 7w$ (separately normalized). For very big values of L, the two states decay long before there can be a significant overlap. This is not true for short chains, thus, the thermodynamic limit is necessary to prevent classical error.

converges to 0. This is possible only if both the eigenvalues are less than 1 in absolute value. Being the matrix B the inverse of A, the eigenvalues of B will have opposite behaviour of the ones of A, i.e. a MZM is allowed when both the eigenvalues of B diverge for $n \to \infty$, or, fixing β_n , converge with $n \to 0$. Moreover, if both the eigenvalues of A are greater than 1, that is α_n diverges, the eigenvalues of B will be less than 1 and MZMs are still allowed. For simplicity, we will henceforth call α the states located around the edge for n = 1 and β those around n = L.

In order to apply the transfer matrices, we first need to define an initial condition, given by the first vector (α_1, α_0) , choosing $\alpha_0 = 0$ as a border condition and α_1 is arbitrary until set by the normalization of the state. For the *b*-modes the initial state is (β_L, β_{L+1}) .

After this, one can do three simple observation:

a) the importance of having both a hopping and a superconductive pairing is now manifest, because it can be easily demonstrated that if only one of these parameters is non null, the eigenvalues of the transfer matrix will never be simultaneously smaller than or greater than 1 in absolute value (see figure 4);

b) setting $\mu = 0$ and $\Delta = w$ every value of α_n , but α_1 , is null, recovering the result described by equations (3),(4) and (5);

c) under these conditions, $\lambda_{-} = 0$ and $\lambda_{+} = \mu/(2w)$, meaning that MZM are allowed only if also $|\lambda_{+}| < 1$, that is $-2w < \mu < 2w$: this is the domain of the topological phase. We will see later that there are methods to derive this domain also for the general case.

Another important property that we can see again from the figure 3 is that, for sufficiently long chains, where the convergence of the eigenvalues is satisfied, there is a gap in the bulk



Figure 4: (a): Eigenvalues of the transfer matrix for w = 0. (b): eigenvalues for $\Delta = 0$. In both cases, Majorana edge excitations are forbidden.

of the chain, that is, the separation between the two end modes, although these decay exponentially in the bulk, is practically clear, i.e. there is no coupling between them. This implies that there is no continuous transformation capable of transforming one state into another. This is the mechanism by which MZMs are protected and immune to classical error, even in the most general case.

This is also a reflection of the symmetry properties of the system: the Hamiltonian of eq. (1) has a particle-hole symmetry (see Appendix A.1.2), which, as we will see in the next section, translates into a symmetrical distribution of the energy states with respect to the zero level of the energy, that is, for each state with energy E there is one with energy -E. The need to respect this symmetry implies two things:

a) first of all, the MZMs cannot move individually from the energy level 0 to an arbitrary value, but must do so simultaneously and towards opposite energies that are equal in absolute value; for this to happen, however, the MZMs are needed to be coupled, but as long as there is a gap in the bulk of the chain, this is not possible; this is very important, because the fact that the energy of the MZMs is protected and is 0 means that they have no influence on the Hamiltonian and the only way to obtain this condition is that they are unpaired and present at the ends of the chain, exactly as in the case depicted by the equation (3);

b) the presence of a gap in the bulk of the chain corresponds to a gap in the bulk energy spectrum; to transform one MZM into another it is necessary to excite (or de-excite) the system and then de-excite it (or excite it) again. This is certainly difficult if there is an energy gap, but if this gap closes, then the transition can take place continuously. This, in fact, is what happens for $|\mu/w| = 2$.

1.3 Bulk-edge correspondence

A way to characterize topological phases and determine the presence of MZM is by defining and finding the so called topological invariants, that is quantities which are strong against continuous variation of the properties of a system, but vary as the topological order changes. An 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:

$$c_{k}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikj} c_{j}^{\dagger}, \quad c_{k} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ikj} c_{j}.$$
 (8)

To do so, anyway, we need to consider a chain with periodic boundary conditions, that we can achieve if we think of bringing the two ends of the chain together to form a ring. The term $c_x^{\dagger}c_{x+1}$ transforms in:

$$\sum_{x} c_{x}^{\dagger} c_{x+1} = \sum_{x} \frac{1}{\sqrt{L}} \sum_{k'} c_{k'}^{\dagger} e^{-ik'x} \frac{1}{\sqrt{L}} \sum_{k} c_{k} e^{ik(x+1)}$$
$$= \sum_{x} \frac{1}{L} \sum_{k'} c_{k'}^{\dagger} e^{i(k-k')x} \sum_{k} c_{k} e^{ik}$$
$$= \sum_{k} \sum_{k'} \delta_{k,k'} c_{k}^{\dagger} c_{k'} e^{ik'}$$
$$= \sum_{k} c_{k}^{\dagger} c_{k} e^{-ik}.$$

Similarly, one can find that to Fourier transform the Hamiltonian (1) in the reciprocal space, it is sufficient to replace:

$$c_x^{\dagger}c_{x+1} \rightarrow c_k^{\dagger}c_k e^{ik}, \quad c_x^{\dagger}c_x \rightarrow c_k^{\dagger}c_k, \quad c_x c_{x+1} \rightarrow c_k c_{-k} e^{-ik}.$$

The Kitaev Hamiltonian becomes:

$$H = -\mu \sum_{k} \left(c_k^{\dagger} c_k - \frac{1}{2} \right) - \sum_{k} \left(w c_k^{\dagger} c_k e^{ik} + w c_k^{\dagger} c_k e^{-ik} - \Delta c_k c_{-k} e^{-ik} - \Delta c_{-k}^{\dagger} c_k^{\dagger} e^{ik} \right).$$

One can manipulate this expression. The first term becomes:

$$\mu \sum_{k} \left(c_{k}^{\dagger} c_{k} - \frac{1}{2} \right) = \frac{\mu}{2} \sum_{k} \left(c_{k}^{\dagger} c_{k} + c_{k} c_{k}^{\dagger} \right) = \frac{1}{2} \sum_{k} \left(\mu c_{k}^{\dagger} c_{k} + \mu c_{-k} c_{-k}^{\dagger} \right),$$

where we used the fermionic anti-commutative relations and, in the last passage, the fact that $k \to -k$ is a dumb index and the sum is over positive and negative ks. Similarly one can write:

$$\sum_{k} \left(wc_{k}^{\dagger}c_{k}e^{ik} + wc_{k}^{\dagger}c_{k}e^{-ik} \right) = \sum_{k} 2wc_{k}^{\dagger}c_{k}\cos k$$
$$= \frac{1}{2}\sum_{k} \left(2wc_{k}^{\dagger}c_{k}\cos k + 2w\underbrace{c_{-k}^{\dagger}c_{-k}}_{=1-c_{-k}c_{-k}^{\dagger}}\cos\left(-k\right) \right)$$
$$= \frac{1}{2}\sum_{k} \left(2wc_{k}^{\dagger}c_{k}\cos k + 2wc_{-k}c_{-k}^{\dagger}\cos k \right) + w\sum_{k}\cos k.$$

The second sum vanishes if we restrict our analysis to the first Brilluin zone, i.e. for k between $-\pi$ and π . Finally, for the terms with the Δ coefficient:

$$\sum_{k} \left(\Delta c_{k}c_{-k}e^{-ik} + \Delta c_{-k}^{\dagger}c_{k}^{\dagger}e^{ik} \right)$$
$$= \frac{1}{2}\sum_{k} \left(2\Delta c_{k}c_{-k}e^{-ik} + 2\Delta c_{-k}^{\dagger}c_{k}^{\dagger}e^{ik} \right)$$
$$= \frac{1}{2}\sum_{k} \left(\Delta c_{k}c_{-k}e^{-ik} + \Delta c_{-k}c_{k}e^{ik} + \Delta c_{-k}^{\dagger}c_{k}^{\dagger}e^{ik} + \Delta c_{k}^{\dagger}c_{-k}^{\dagger}e^{-ik} \right)$$
$$= \frac{1}{2}\sum_{k} \left(-\Delta c_{-k}c_{k}e^{-ik} + \Delta c_{-k}c_{k}e^{ik} + \Delta c_{-k}^{\dagger}c_{k}^{\dagger}e^{ik} - \Delta c_{-k}^{\dagger}c_{k}^{\dagger}e^{-ik} \right)$$
$$= \frac{1}{2} \left(2i\Delta c_{-k}c_{k}\sin k + 2i\Delta c_{-k}^{\dagger}c_{k}^{\dagger}\sin k \right).$$

Upon defining $C_k^{\dagger} = (c_k^{\dagger}, c_{-k})$, one can then write *H* in the Bogoliubov-de Gennes form²⁴:

$$H = \frac{1}{2} \sum_{k \in \mathbb{Z}} C_k^{\dagger} \mathcal{H}_k C_k, \quad \mathcal{H}_k = \begin{pmatrix} \epsilon_k & -i\tilde{\Delta}_k \\ i\tilde{\Delta}_k & -\epsilon_k \end{pmatrix}$$

with $\epsilon_k = -2w \cos k - \mu$ the kinetic energy and $\tilde{\Delta}_k = 2\Delta \sin k$ the Fourier-transformed pairing potential. In the limit of an infinite chain the sum becomes an integral over the Brillouin zone. The energy bulk spectrum is simply given by the eigenvalues of $\mathcal{H}_k/2$:

$$E^{\pm}_{\rm bulk}(k) = \pm \frac{1}{2} \sqrt{\epsilon_k^2 + \tilde{\Delta}_k^2}$$

As we said in the previous section, and as one can state by looking at figure 5, the energy levels are distributed symmetrically with respect to 0. This properties are due to the particle-hole invariance (Appendix A.1.2) of the system; in fact, applying a particle-hole exchange transformation to eq. (1) and doing again the previous calculations, one can obtain again the same energy spectrum found above. Briefly, given a solution with energy E and momentum k, particle-hole symmetry dictates in general the presence of a solution with energy -E and momentum -k.

In particular, under some choices of the parameters, such as the ones in figure 5 (a), the energy spectrum appear to be gapped. When the gap closes (figures 5 (b) and (c)), condition which we always find for $|\mu| = 2|w|$, Majorana modes are free to move along the chain, resulting in a transition which leads to a trivial phase (no edge modes). From a more rigorous point of view, we can think of this phase transition as follows: as long as



Figure 5: (a) Energy bulk spectrum for $\mu = 0$, $w = \Delta = 1$, presenting a gap at all k: since our chain does not have boundaries anymore, the energy spectrum does not contain the zero energy Majorana modes which we found in the previous section. However, for (b) $\mu = 2w$ and (c) $\mu = -2w$ the bulk gap closed for $k = \pm \pi$ and k = 0 respectively. At these points, Majorana modes are free to move along the chain and a phase transition occurs. Furthermore, by reproducing the energy spectrum diagrams also for other parameter values, it could be observed that the bulk always closes for $|\mu| = 2|w|$.

the energy gap does not close, the number of MZMs is protected and, therefore, from one opening of the gap to the next closure we know we are traveling through a domain which presents always the same number of MZMs. So we just need to look for this number for a particular point of each of these domains to get generic information. In fact, with the methods developed so far, we could look for edge excitations for any point that satisfies

$$|\mu| \ge 2|w|,\tag{9}$$

only to be disappointed to find that there are none. Since above (9) the domain doesn't close anymore, we can generalize and define it as a condition for the trivial phase.

In order to better investigate such a behaviour, it will be useful to define a vector $\mathbf{h}(k)$ such that:

$$\mathcal{H}_k = \mathbf{h}(k) \cdot \boldsymbol{\sigma},$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector whose components are the Pauli matrices. It is straightforward that:

$$h_x(k) = 0, \quad h_y(k) = \tilde{\Delta}, \quad h_z(k) = \epsilon_k.$$

We can always define and angle θ_k such that:

$$\cos \theta_k = rac{\mathbf{h}_y(k)}{|\mathbf{h}(k)|}$$
 and $\sin \theta_k = rac{\mathbf{h}_z(k)}{|\mathbf{h}(k)|}$,

which maps our system on a unitary ring. We can now define the winding number:

$$\mathcal{W} = \oint \frac{d\theta_k}{2\pi},\tag{10}$$

where the integral is done around the one-dimensional Brillouin zone, that is $k \in [-\pi, \pi)$. This quantity characterizes the number of times the vector $\hat{\mathbf{h}}(k)$ rotates in the yz plane around the one-dimensional Brillouin zone. It can be demonstrated²⁵ that the value of $|\mathcal{W}|$ is identical to the number of MZMs per edge for a given choice of system parameters. Both the winding number and the number of MZMs are *topological invariants*²⁶, which means that they are unaltered until a phase transition between different topological regimes occurs.

We now have a tool to compute the topological phase for a general choice of the parameters w and Δ . In fact, it is sufficient to know how many times the vector $\mathbf{h}(k)$ rotates around the origin and at which conditions. This is easily done if we count how many times the quantities $\sin \theta_k$ and $\cos \theta_k$ become null. Starting from:

$$\sin \theta_k = 2\Delta \sin k,$$

we can notice that for k spanning from $-\pi$ to π (excluded), the rhs annihilates twice, in correspondence to $k = -\pi$ and k = 0. The same number of zero points is found for the lhs with just one spanning of $\theta_k \in [0, 2\pi)$, in correspondence of $\theta_k = 0$ and $\theta_k = \pi$. If this spanning corresponds to a rotation around the origin of the yz plane, then \mathcal{W} will be 1, otherwise 0. In the first case, we should also find

$$\cos\theta_k = -2w\cos k - \mu \tag{11}$$

to be zero twice, that is for $\theta_k = \pi/2, 3\pi/2$. On the other hand, the rhs is null for:

$$\frac{\mu}{2w} = -\cos k = -\cos\left(-k\right).$$

Being $+\pi$ excluded from the domain, we will always find that the expression (11) will annihilate for two different values of k and for a fixed choice of μ and w only if:

$$\left|\frac{\mu}{2w}\right| < 1 \Rightarrow -2w < \mu < 2w \quad \text{(for } w > 0\text{)}.$$

Inside this region the system will display one MZM at each end, while outside, no MZMs are allowed.

In this section, we have found with two methods the same topological domain we obtained with the transfer matrix approach for the particular choice of parameters $\Delta = w$, demonstrating that it is valid in general.

2 Extended chain

In the study of the Kitaev chain and the formation of MZMs for quantum computing applications, it is appropriate to generalize the starting system and complicate it by involving a generic number of neighbors r in the hopping and superconducting coupling. In this section we will expand the study conducted so far to the extended model, with particular attention to the homogeneous case, following in the footsteps of Alecce and Dell'Anna¹. We will first obtain the winding number to know the topological phases, after which we will extend the application of the transfer matrices.

2.1 Extended topological phase

The extended time-reversal Kitaev chain $(EKC)^{2728}$ is defined by a Hamiltonian of the type:

$$H = -\sum_{j=1}^{L} \mu \left(c_j^{\dagger} c_j - \frac{1}{2} \right) + \sum_{\ell=1}^{r} \sum_{j=1}^{L-\ell} \left(-w_{\ell} c_j^{\dagger} c_{j+\ell} + \Delta_{\ell} c_j c_{j+\ell} + \text{ h.c.} \right).$$
(12)

The extended hopping and pairing coupling terms, w_l and Δ_l , can be generic variables for now. As we did before, we can rewrite the Hamiltonian in the Bogoliubov-de Gennes formalism:

$$H = \frac{1}{2} \sum_{k \in \mathbb{Z}} C_k^{\dagger} \mathcal{H}_k C_k,$$

being

$$\mathcal{H}_k = -\left(\mu + 2\sum_{\ell=1}^r w_\ell \cos(k\ell)\right)\sigma_z + \left(2\sum_{\ell=1}^r \Delta_\ell \sin(k\ell)\right)\sigma_y.$$

We can again define the winding number as done before, being:

$$h_z(k) = -\left(\mu + 2\sum_{\ell=1}^r w_\ell \cos(k\ell)\right), \quad h_y(k) = 2\sum_{\ell=1}^r \Delta_\ell \sin(k\ell).$$

In the homogeneous case, that is for $w_{\ell} \equiv w_0$, $\Delta_{\ell} \equiv \Delta \ \forall \ \ell$, one has:

$$h_y(k) = \Delta \sum_{\ell=1}^r \sin(\ell k) = \Delta \sin((r+1)k/2) \sin(rk/2) \csc(k/2),$$

$$h_z(k) = -\mu/2 - w_0 \sum_{\ell=1}^r \cos(\ell k) = -\mu/2 - w_0 \cos((r+1)k/2) \sin(rk/2) \csc(k/2).$$

The 2r zeros of $h_y(k)$, namely, k_n such that $h_y(k_n) = 0$, can be ordered, $k_0 < k_1 < k_2 < k_3 < \cdots < k_{2r-1}$, and are

$$k_{2n} = \frac{2\pi n}{r}, \quad k_{2n+1} = \frac{2\pi (n+1)}{r+1}.$$

The corresponding values of $h_z(k_n)$ are

$$h_z(0) = -\mu/2 - rw_0,$$

$$h_z(k_{2n}) = -\mu/2,$$

$$h_z(k_{2n+1}) = -\mu/2 - w_0.$$

In the regime of parameters where $h_z(k_n)$ has alternate signs for ordered $\{k_n\}$, varying k from 0 to 2π , the winding vector surrounds the origin r times. As a result, we get the following topological phases:

$$\mathcal{W} = 1 \quad \text{for } -2r < \mu/w_0 \le 0,$$

$$\mathcal{W} = r \quad \text{for } 0 < \mu/w_0 < 2,$$

$$\mathcal{W} = 0 \quad \text{otherwise.}$$
(13)

As we said before, the winding number is a topological invariant. The domain of definition of topological invariants is very important in the study of topological insulators and superconductors. In fact, through this, it is possible to classify these materials in real periodic tables²⁹, in which they are ordered according to the dimensionality of the system and its symmetry properties. For example, the domain \mathbb{Z} , to which the winding number belongs, corresponds, for a d = 1 dimensional system, to the Altland-Zirnbauer³⁰ BDI class, which has the time reversal, particle-hole and chiral symmetries (for more information see Appendix A.1).

However, for now and for our purposes, this outcome will serve us to verify the reliability of some results that we will obtain in the following of this work.

2.2 Bogoliubov equations

Transfer matrices are also a very powerful tool in the study of the topological phases of the extended system. In order to use it, however, it is necessary to find relations in which the wave functions of the Majorana modes are involved. To derive them, we must start from the Hamiltonian of the extended model (12) reparameterized in terms of Majorana fermions:

$$H = \frac{i}{2} \left\{ -\mu \sum_{j=1}^{L} \gamma_{2j-1} \gamma_{2j} + \sum_{\ell=1}^{r} \sum_{j=1}^{L-\ell} \left[(\Delta_{\ell} - w_{\ell}) \gamma_{2j-1} \gamma_{2(j+\ell)} + (\Delta_{\ell} + w_{\ell}) \gamma_{2j} \gamma_{2(j+\ell)-1} \right] \right\}.$$
(14)

The Hamiltonian in eq. (12), in the fermionic representation and real space, can be

generally written in the matrix form

$$H = \left(c_1^{\dagger} \dots c_L^{\dagger} c_1 \dots c_L\right) \mathcal{H} \begin{pmatrix} c_1 \\ \vdots \\ c_L \\ c_1^{\dagger} \\ \vdots \\ c_L^{\dagger} \end{pmatrix},$$

and can be diagonalized by means of a unitary transformation:

$$U^{\dagger}\mathcal{H}U = \operatorname{diag}\left(\epsilon_{1},\ldots,\epsilon_{L},-\epsilon_{1},\ldots,-\epsilon_{L}\right).$$

getting the typical spectrum of a particle-hole symmetric Hamiltonian. On the other hand, the Hamiltonian can be written in terms of Majorana operators as in eq. (14), which can be written quite in general as it follows:

$$H = i \sum_{i,j} \gamma_i A_{ij} \gamma_j, \tag{15}$$

where A is a real anti-symmetric matrix $(c_{ij}^* = c_{ij} = -c_{ji})$ such that

$$WAW^T = \operatorname{diag}\left(\left(\begin{array}{cc} 0 & \epsilon_1 \\ -\epsilon_1 & 0 \end{array}\right), \dots, \left(\begin{array}{cc} 0 & \epsilon_L \\ -\epsilon_L & 0 \end{array}\right)\right),$$

where $\{\pm \epsilon_n\}$ are eigenvalues of \mathcal{H} and W is a real orthogonal matrix, $WW^T = W^TW = I_L^{31}$.

Under the actions of U and W on respectively fermionic and Majorana operators

$$\begin{pmatrix} c_{1} \\ \vdots \\ c_{L} \\ c_{1}^{\dagger} \\ \vdots \\ c_{L}^{\dagger} \end{pmatrix} = U^{\dagger} \begin{pmatrix} c_{1} \\ \vdots \\ c_{L} \\ c_{1}^{\dagger} \\ \vdots \\ c_{L}^{\dagger} \end{pmatrix}, \quad \begin{pmatrix} b_{1} \\ \vdots \\ b_{2L} \end{pmatrix} = W \begin{pmatrix} \gamma_{1} \\ \vdots \\ \gamma_{2L} \end{pmatrix}$$
(16)

the Hamiltonian H can be written in the following forms:

$$H = \sum_{n=1}^{L} \epsilon_n \left(2\tilde{c}_n^{\dagger} \tilde{c}_n - 1 \right) = i \sum_{n=1}^{L} \epsilon_n b_{2n-1} b_{2n}.$$

$$\tag{17}$$

Assuming that U and W are canonical transformations we have $\left\{\tilde{c}_{n}^{\dagger}, \tilde{c}_{m}\right\} = \delta_{n,m}$ and $\{\tilde{c}_{n}, \tilde{c}_{m}\} = 0, \forall n, m = 1, \dots, L$, together with $\{b_{n}, b_{m}\} = 2\delta_{n,m}, \forall n, m = 1, \dots, 2L$. The two sets of new operators are linked by

$$b_{2n-1} = \tilde{c}_n + \tilde{c}_n^{\dagger},$$

$$b_{2n} = i \left(\tilde{c}_n^{\dagger} - \tilde{c}_n \right).$$
(18)

The quadratic Bogoliubov-de Gennes Hamiltonian H, written in terms of fermionic operators, can be diagonalized by Bogoliubov transformation, which is represented by the matrix U. We can write \tilde{c}_n as combination of the first set of operators c_j by means of two sets of functions $u_{n,j}$ and $v_{n,j}$:

$$\tilde{c}_n = \sum_{i=1}^{L} \left(u_{n,j}^* c_j + v_{n,j}^* c_j^\dagger \right)$$

with $\sum_{j=1}^{L} \left(|u_{n,j}|^2 + |v_{n,j}|^2 \right) = 1, \forall n = 1, \dots, L$. Thus we can write U^{\dagger} in the following way:

$$U^{\dagger} = \begin{pmatrix} u_{1,1}^{*} & \dots & u_{1,L}^{*} & v_{1,1}^{*} & \dots & v_{1,L}^{*} \\ \vdots & & \vdots & \vdots & & \vdots \\ u_{L,1}^{*} & \dots & u_{L,L}^{*} & v_{L,1}^{*} & \dots & v_{L,L}^{*} \\ v_{1,1} & \dots & v_{1,L} & u_{1,1} & \dots & u_{1,L} \\ \vdots & & \vdots & \vdots & & \vdots \\ v_{L,1} & \dots & v_{L,L} & u_{L,1} & \dots & u_{L,L} \end{pmatrix}$$

From equations (16) and (18), we can write

$$W_{2n-1,2j-1} = \frac{1}{2} \left(u_{n,j} + u_{n,j}^* + v_{n,j} + v_{n,j}^* \right),$$

$$W_{2n-1,2j} = \frac{i}{2} \left(-u_{n,j} + u_{n,j}^* + v_{n,j} - v_{n,j}^* \right),$$

$$W_{2n,2j-1} = \frac{i}{2} \left(u_{n,j} - u_{n,j}^* + v_{n,j} - v_{n,j}^* \right),$$

$$W_{2n,2j} = \frac{1}{2} \left(u_{n,j} + u_{n,j}^* - v_{n,j} - v_{n,j}^* \right)$$

or, vice versa,

$$u_{n,j}^* = \frac{1}{2} \left(W_{2n-1,2j-1} + W_{2n,2j} + i \left(W_{2n,2j-1} - W_{2n-1,2j} \right) \right),$$

$$v_{n,j}^* = \frac{1}{2} \left(W_{2n-1,2j-1} - W_{2n,2j} + i \left(W_{2n,2j-1} + W_{2n-1,2j} \right) \right).$$

Now using the Heisenberg equations, derived from eq. (17),

$$[H, b_{2n}] = 2i\epsilon_n b_{2n-1},$$

$$[H, b_{2n-1}] = -2i\epsilon_n b_{2n}$$

expressing b_n in terms of γ_j and using eq. (15), we can write

$$\epsilon_n W_{2n-1,2j-1} = 2 \sum_i W_{2n,i} A_{2j-1,i}$$

$$\epsilon_n W_{2n-1,2j} = 2 \sum_i W_{2n,i} A_{2j,i}$$

$$\epsilon_n W_{2n,2j-1} = 2 \sum_i W_{2n-1,i} A_{i,2j-1}$$

$$\epsilon_n W_{2n,2j} = 2 \sum_i W_{2n-1,i} A_{i,2j}$$

More specifically, using eq. (14), we get the following Bogoliubov equations of the wave functions for the extended Kitaev model:

$$\epsilon_{n}W_{2n-1,2j-1} = -\mu W_{2n,2j} + \sum_{\ell=1} \left[w_{\ell} + (\Delta_{\ell} - w_{\ell}) W_{2n,2(j+\ell)} - (\Delta_{\ell} + w_{\ell}) W_{2n,2(j-\ell)} \right],$$

$$\epsilon_{n}W_{2n-1,2j} = \mu W_{2n,2j-1} + \sum_{\ell=1}^{r} \left[w_{\ell} - (\Delta_{\ell} - w_{\ell}) W_{2n,2(j-\ell)-1} + (\Delta_{\ell} + w_{\ell}) W_{2n,2(j+\ell)-1} \right],$$

$$\epsilon_{n}W_{2n,2j-1} = \mu W_{2n-1,2j} + \sum_{\ell=1}^{r} \left[w_{\ell} - (\Delta_{\ell} - w_{\ell}) W_{2n-1,2(j+\ell)} + (\Delta_{\ell} + w_{\ell}) W_{2n-1,2(j-\ell)} \right],$$

$$\epsilon_{n}W_{2n,2j} = -\mu W_{2n-1,2j-1} + \sum_{\ell=1}^{r} \left[w_{\ell} + (\Delta_{\ell} - w_{\ell}) W_{2n-1,2(j-\ell)-1} - (\Delta_{\ell} + w_{\ell}) W_{2n-1,2(j+\ell)-1} \right].$$
(19)

However, being W real, we must consider only $u_{n,j}^* = u_{n,j}$ and $v_{n,j}^* = v_{n,j}$, therefore $W_{2n,2j-1} = W_{2n-1,2j} = 0$, while, calling $W_{2n-1,2j-1}$ the wave function $\phi_{\epsilon_{n,j}}$, and $W_{2n,2j}$ the wave function $\psi_{\epsilon_{n,j}}$,

$$\phi_{\epsilon_n,j} \equiv W_{2n-1,2j-1} = u_{n,j} + v_{n,j}, \psi_{\epsilon_n,j} \equiv W_{2n,2j} = u_{n,j} - v_{n,j}.$$

Thus, equations (19) reduce to:

$$\sum_{\ell=1}^{r} \left[(\Delta_{\ell} - w_{\ell}) \phi_{\epsilon_{n}, j-\ell} - (\Delta_{\ell} + w_{\ell}) \phi_{\epsilon_{n}, j+\ell} \right] - \mu \phi_{\epsilon_{n}, j} = \epsilon_{n} \psi_{\epsilon_{n}, j},$$

$$\sum_{\ell=1}^{r} \left[(\Delta_{\ell} - w_{\ell}) \psi_{\epsilon_{n}, j+\ell} - (\Delta_{\ell} + w_{\ell}) \psi_{\epsilon_{n}, j-\ell} \right] - \mu \psi_{\epsilon_{n}, j} = \epsilon_{n} \phi_{\epsilon_{n}, j},$$
(20)

which are the Bogoliubov-de Gennes equations and the *r*-neighbor generalization of equations (6). They are wave functions of the Majorana modes in the basis in which H is diagonal, therefore they are eigenfunctions of the energy. That is, they are the wave functions of quasi-particles created and destroyed by b_j . If we find them decoupled at the ends, we have the Bogoliubov quasi-particle \tilde{c} delocalized in a superposition of states.

2.3 Transfer matrix method

Still following Alecce and Dell'Anna, now we can define the transfer matrices.

Since we are interested in the zero energy states, we will consider the case where, for some n, we have $\epsilon_n = 0$.

In this case, the wave functions $\phi_{o,j}$ and $\psi_{o,j}$, related to zero energy, in eqs. (20) decouple and we can solve the equations separately. Supposing $\Delta_r + w_r \neq 0$, these equations, for $\epsilon_n = 0$, can be written in the following form:

$$\begin{pmatrix} \phi_{o,j+r} \\ \vdots \\ \phi_{o,j-r+1} \end{pmatrix} = T \begin{pmatrix} \phi_{o,j+r-1} \\ \vdots \\ \phi_{o,j-r} \end{pmatrix}, \quad \begin{pmatrix} \psi_{o,j-r} \\ \vdots \\ \psi_{o,j+r-1} \end{pmatrix} = T \begin{pmatrix} \psi_{o,j-r+1} \\ \vdots \\ \psi_{o,j+r} \end{pmatrix}$$
(21)

after introducing the following transfer matrix:

$$T = \begin{pmatrix} t_1 & \cdots & t_r & \cdots & t_{2r} \\ 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & 0 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 1 & 0 \end{pmatrix}$$

where

$$t_i = -\frac{\Delta_{r-i} + w_{r-i}}{\Delta_r + w_r}, \quad \text{for } i = 1, \dots, r-1$$

$$t_r = -\frac{\mu}{\Delta_r + w_r},$$

$$t_i = \frac{\Delta_{i-r} - w_{i-r}}{\Delta_r + w_r}, \text{ for } i = r+1, \dots, 2r.$$

It is straightforward to notice that $t_1 = \text{Tr}(T) = \sum_{i=1}^{2r} \lambda_i$, is the trace of T, and $t_{2r} = -\text{Det}(T) = -\prod_{i=1}^{2r} \lambda_i$, the determinant, where λ_i are the eigenvalues of T.

Using this approach, one can write the wave functions evaluated at some point from its value at another point by applying several times the transfer matrix, namely applying T to some power, say j, related to the space distance between the two points. What is relevant is therefore T^{j} , or, more conveniently, its diagonal form, so that T^{j} can be written as $T^{j} = SD^{j}S^{-1}$ were S diagonalizes $T(D = S^{-1}TS)$. The problem is reduced, therefore, to finding the eigenvalues (D) and the eigenstates (S) of T. In order to find the eigenvalues, one has to write the characteristic polynomial $p_{2r}(\lambda)$ of the $2r \times 2r$ matrix T, and find the solutions of $p_{2r}(\lambda) = 0$. One can easily prove that the polynomial $p_{2r}(\lambda) = \text{Det}(T - \lambda 1)$ is such that

$$p_{2r}(\lambda) = \lambda p_{2r-1}(\lambda) - t_{2r}$$

and, therefore, by iteration, and making it equal to zero, one has to solve the following eigenvalue equation

$$p_{2r}(\lambda) = \lambda^{2r} - \sum_{i=1}^{2r} t_i \lambda^{2r-i} = 0$$
(22)

in order to find the 2r eigenvalues of T, λ_s with $s = 1, \ldots, 2r$. One can easily check that the corresponding eigenfunctions are $\vec{v}_s = (\lambda_s^{2r}, \lambda_s^{2r-1}, \ldots, \lambda_s)^T$, which are the columns composing the matrix S. In fact, the first row of $T \cdot \vec{v}_s$ is:

$$\lambda_s^{2r} t_1 + \lambda_s^{2r-1} t_2 + \lambda_s^2 t_{2r-1} + \lambda_s t_{2r} =$$

= $\lambda_s \left(\lambda_s^{2r-1} t_1 + \lambda_s^{2r-2} t_2 + \lambda_s t_{2r-1} + t_{2r} \right) = (22)$
= λ_s^{2r+1} .

The subsequent components of the resulting vector are $\lambda_s^{2r}, \lambda_s^{2r-1}, \ldots, \lambda_s^2$, thus $T \cdot \vec{v}_s = (\lambda_s^{2r+1}, \lambda_s^{2r}, \ldots, \lambda_s^2)^T = \lambda_s \cdot \vec{v}_s$.

Taking into account expression (21), we can notice that one can write the first vector as a linear combination of the eigenvectors of T. In fact:

$$\begin{pmatrix} \phi_{o,j+r} \\ \vdots \\ \phi_{o,j-r+1} \end{pmatrix} = T \begin{pmatrix} \phi_{o,j+r-1} \\ \vdots \\ \phi_{o,j-r} \end{pmatrix} = T \sum_{s=1}^{2r} c_s \begin{pmatrix} \lambda_s^{2r} \\ \vdots \\ \lambda_s^{2r} \end{pmatrix} = \sum_{s=1}^{2r} c_s \lambda_s \begin{pmatrix} \lambda_s^{2r} \\ \vdots \\ \lambda_s^{2r} \end{pmatrix}.$$

In doing so, it is immediate to state that the first term is given by:

$$\phi_{0,j+r} = \sum_{s=1}^{2r} c_s \lambda_s^{2r} \lambda_s$$

Because it is possible to rewrite also the vector $(\phi_{0,j+r+1}, \cdot, \phi_{j-r+1})^T$ in terms of product of a transform matrix T times the vector $(\phi_{0,j+r}, \ldots, \phi_{j-r+1})^T$, thus having

$$\phi_{0,j+r+1} = \sum_{s=1}^{2r} c_s \lambda_s^{2r} \lambda_s^2,$$

one can conclude that in general exist a constant x worth to define a quantities $c_s^{\phi} = c_s \cdot \lambda_s^x$ such that:

$$\phi_{o,j} = \sum_{s=1}^{2r} c_s^{\phi} \lambda_s^j. \tag{23}$$

Similarly, one can write a similar expression for the state ψ_0 , noticing that:

$$\begin{pmatrix} \psi_{o,j-r} \\ \vdots \\ \psi_{o,j+r-1} \end{pmatrix} = T \begin{pmatrix} \psi_{o,j-r+1} \\ \vdots \\ \psi_{o,j+r} \end{pmatrix}$$

is equivalent to:



Figure 6: An example of two independent and normalized MZMs wave functions on the left edge for r = 2, $\mu/w_0 = 1$, $\Delta/w_0 = 1$, computed through the transfer matrix method. Plot (a) is calculated imposing $\phi_{0,1} = 0$ and $\phi_{0,2} > 0$; (b) with $\phi_{0,1} > 0$ and $\phi_{0,2} = 0$.

$$\begin{pmatrix} \psi_{o,j-r+1} \\ \vdots \\ \psi_{o,j+r} \end{pmatrix} = T^{-1} \begin{pmatrix} \psi_{o,j-r} \\ \vdots \\ \psi_{o,j+r-1} \end{pmatrix}.$$

In fact, being the eigenvalues of T^{-1} the reciprocals of the eigenvalues of T, it is immediate that:

$$\psi_{j+r} = \sum_{s=1}^{2r} c'_s \lambda_s^{-2r} \lambda_s^{-1}$$
$$\downarrow$$
$$\psi_{j+r+1} = \sum_{s=1}^{2r} c'_s \lambda_s^{-2r} \lambda_s^{-2},$$

i.e., as the index at the foot of ϕ increases, the exponent applied to λ_s decreases. As before, we can always define constant quantities c_s^{ψ} such that:

$$\psi_{o,j} = \sum_{s=1}^{2r} c_s^{\psi} \lambda_s^{-j}.$$
 (24)

Our aim is now to build the conditions to have the MZMs at every end. As we have seen for the r = 1 case, MZMs are allowed only if, in the thermodynamic limit, the wave function are normalizable. For example, if we are looking for MZMs on the left end of the chain, that is localized around j = 0, encoded in the wave function ϕ_0 , we must have that $j \to +\infty \Rightarrow |\phi_{0,j}| \to 0$ is necessary and sufficient condition. Being

$$\left|\phi_{0,j}\right| = \left|\sum_{s=1}^{2r} c_s^{\phi} \lambda_s^j\right| \le \sum_{s=1}^{2r} \left|c_s^{\phi}\right| \cdot \left|\lambda_s^j\right|,\tag{25}$$

and being the coefficients c_s^{ϕ} independent on j, the simplest way to have $|\phi_{0,j}|$ to be null as

 $j \to +\infty$ is to have all the $|\lambda_s|$ less then 1. However, this is not the only solution, because a part of the coefficients c_s^{ϕ} and c_s^{ψ} appearing in (23) and (24) can be fixed to 0 by imposing open boundary conditions. This will be clearer if we call $n^<$, $n^>$ and $n^=$ respectively the number of λ_s such that $|\lambda_s| < 1$, $|\lambda_s| > 1$ and $|\lambda_s| = 1$. Then, let us suppose the majority of $|\lambda_s|$ are smaller than 1, that is $n^< > n^> + n^=$. The open boundary conditions in the thermodynamic limit would require that:

$$\phi_{o,0} = \phi_{o,-1} = \dots = \phi_{o,1-r} = 0,$$

 $\psi_{o,L+1} = \psi_{o,L+2} = \dots = \psi_{o,L+r} = 0.$

However, the initial conditions are the entire vectors $(\phi_r, \phi_{r-1}, \ldots, \phi_0, \ldots, \phi_{1-r})^T$ and $(\psi_{L-r+1}, \psi_{L-r}, \ldots, \psi_{L+1}, \ldots, \psi_{L+r})^T$, leaving us with other r-1 free parameters per end (one condition is used while imposing normalization). We can use these free parameters to set to 0 the coefficients c_s^{ϕ} and c_s^{ψ} associated to the eigenvalues greater than or equal to 1, having thus normalizable states, provided that these eigenvalues are less than r. After this operation, we'll be left with $N = r - 1 - (n^> + n^=)$ degrees of freedom to construct the wave functions. This means that we can construct N + 1 different linear independent wave vectors at each edge, corresponding to N + 1 independent MZMs. The situation is analogous and reversed if, instead, $n^> > n^< + n^=$. In this case, we have to impose the following boundary conditions:

$$\phi_{o,L+1} = \phi_{o,L+2} = \dots = \phi_{o,L+r} = 0,$$

$$\psi_{o,0} = \psi_{o,-1} = \dots = \psi_{o,1-r} = 0,$$

verifying the existence of zero energy modes, which will be localized at the edges, $\psi_{o,j}$ on the left and $\phi_{o,j}$ on the right.

In both cases, we get at most N + 1 = r independent MZMs per edge (see, for example, figure (6), consistently with the winding number analysis done before and the results (13). We call this the *eigenvalue criterion* for the MZMs search.

3 Let's get dirty

Although the model treated so far is general, it is not sufficient to predict some peculiar characteristics of the Majorana modes present in superconducting chains. In fact, in systems of this type³² it is observed that a localization of the excitations is stronger than what the pure theoretical models suggest^{33,34}. The cause of this behavior is generally traced back to the presence of disorder, a moderate amount of which has been stated ^{35,36} to support the topological phase by narrowing the edge modes and pinning down quasiparticles associated with the transition to a non-topological phase. The effects of disorder on this kind of systems, such as the Kitaev chain and its extension, are therefore of great interest.

This section is devoted to the study of these effects. So let's get dirty and make some mess!

3.1 Disordered Kitaev chain

To introduce disorder into our system we must consider a random perturbation that applies to the Hamiltonian of the Kitaev chain. To do this, we consider² a variable chemical potential along the chain, the values of which are provided by a probability distribution, which for now we leave undefined. Thus, the equation 1 becomes:

$$H = -\sum_{j=1}^{L} \mu_j \left(c_j^{\dagger} c_j - 1/2 \right) + \sum_{j=1}^{L} \left(-w c_j^{\dagger} c_{j+1} + \Delta c_j c_{j+1} + h.c. \right).$$

The randomness of the chemical potential μ_j moves directly into the definition of the transfer matrices (7), which now become a very powerful tool to investigate the effects of the disorder on the domain of the topological phase and on the presence of MZMs. To explain what has just been said, let's show a first particular example, setting $t \equiv \Delta = w \neq 0$. We obtain the following transfer matrix, to be applied to the state $(\alpha_n, \alpha_{n-1})^T$ to compute $(\alpha_{n+1}, \alpha_n)^T$:

$$A_n = \begin{pmatrix} \frac{\mu_n}{2t} & 0\\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} \alpha_{n+1}\\ \alpha_n \end{pmatrix} = A_n \begin{pmatrix} \alpha_n\\ \alpha_{n-1} \end{pmatrix}$$

As we know, if α represents left-end excitation, in order to have a MZM, this wave function should converge to 0 (in modulus) as $n \to \infty$. Applying the transfer matrix repeatedly:

$$\begin{pmatrix} \alpha_{n+1} \\ \alpha_n \end{pmatrix} = \prod_{j=1}^n A_j \begin{pmatrix} \alpha_1 \\ \alpha_0 \end{pmatrix} = \begin{pmatrix} \prod_{j=1}^n \frac{\mu_j}{2t} & 0 \\ \prod_{j=1}^{n-1} \frac{\mu_j}{2t} & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_0 \end{pmatrix} \equiv \tilde{A}_n \begin{pmatrix} \alpha_1 \\ \alpha_0 \end{pmatrix},$$

meaning that:

$$\alpha_{n+1} = \alpha_1 \prod_{j=1}^n \frac{\mu_j}{2t}.$$

 α_1 is determined by the normalization condition and the behavior of α_{n+1} is linear with that of the product, which, upon careful glance, can be seen to be equal in absolute value to the absolute value of the only non-zero eigenvalue of the total transfer matrix:

$$|\lambda| = \prod_{j=1}^{n} \left| \frac{\mu_j}{2t} \right|,\tag{26}$$

meaning that the eigenvalue criterion, which we defined and studied in the previous chapter, is still valid.

Let's now rewrite the previous equation in absolute value:

$$|\alpha_1| \prod_{j=1}^n \left| \frac{\mu_j}{2t} \right| = |\alpha_1| \exp\left(\sum_{j=1}^n \log\left|\frac{\mu}{2t}\right|\right) = |\alpha_1| e^{n < \log\left|\frac{\mu}{2t}\right| >}.$$
 (27)

In the thermodynamic limit, the topological phase is determined by the behaviour of the mean logarithm $\langle \log \left| \frac{\mu}{2t} \right| \rangle$: if it is negative, the eigenvalue will converge to 0 and the MZM is allowed; otherwise, the eigenvalue will be ≥ 1 and the phase will be trivial. This means that we can get a phase transition curve if we impose $\langle \log \left| \frac{\mu}{2t} \right| \rangle = 0$.

For each probability distribution, this equation can be solved, a particularly simple job if we consider, by way of example, that the chemical potentials are randomized according to a box distribution. In fact, in this case the condition is:

$$\frac{1}{2\delta_{\mu}} \int_{\mu-\delta_{\mu}}^{\mu+\delta_{\mu}} d\mu' \log \left|\frac{\mu'}{2t}\right| = \frac{t}{\delta_{\mu}} \left[\frac{\mu+\delta_{\mu}}{2t} \left(\log \left|\frac{\mu+\delta_{\mu}}{2t}\right| - 1\right) - \frac{\mu-\delta_{\mu}}{2t} \left(\log \left|\frac{\mu-\delta_{\mu}}{2t}\right| - 1\right)\right] = 0.$$

By imposing it to be zero, we find an analytical formula for calculating the critical chemical potential μ^* , which is plotted in figure 7 for positive chemical potential (the plot is just horizontally mirrored for the negative ones).

The aforementioned image undoubtedly shows a peculiar behavior of the response of this system to the presence of disorder. In fact it is evident that, as the disorder increases, the topological phase also extends to previously forbidden chemical potentials, until the disorder reaches a critical value beyond which it prevails over the system and the presence of MZMs is inhibited for each potential.

It is possible to reproduce what has been done so far for the particular case in which we have set ourselves, also for a different choice of parameters, as we show in figure 8. However, in attempting it, one is faced with a problem. In fact, the eigenvalue criterion applies only if all the $|\alpha_{n+1}|$ have the same linear dependence on the related eigenvalues $\lambda_{n,\pm}$ of \tilde{A}_n :



Figure 7: These curves show the separation of phases for the disordered Kitaev chain with $\Delta = w$ with the disorder coming from (a) a normal distribution and (b) a box distribution. Below this curves, the eigenvalues of the transfer matrix are both less than 1, therefore the phase is topological with an MZM. Above, an eigenvalue becomes greater than 1 and therefore, according to the eigenvalue criterion, the phase is trivial, i.e. without MZM. In the images, the disorder is expressed in terms of the standard deviation of the distribution $\sigma = \delta_{\mu}/\sqrt{3}$.



Figure 8: The figure shows several critical curves for the Kitaev chain as the parameters w and Δ vary, calculated through the transfer matrix method, this time by extracting the random chemical potentials from a Gaussian distribution. On the numerical methods used for this and other graphs, see Appendix A.2.

$$\begin{pmatrix} \alpha_{n+1} \\ \alpha_n \end{pmatrix} = \tilde{A}_n \begin{pmatrix} \alpha_1 \\ \alpha_0 \end{pmatrix} = \tilde{A}_n \begin{bmatrix} v_{n,1} \\ v_{n,0} \end{pmatrix} + \begin{pmatrix} u_{n,1} \\ u_{n,0} \end{bmatrix} = \lambda_{n,+} \begin{pmatrix} v_{n,1} \\ v_{n,0} \end{pmatrix} + \lambda_{n,-} \begin{pmatrix} u_{n,1} \\ u_{n,0} \end{pmatrix}$$

 u_n and v_n are eigenvectors of \tilde{A}_n . In general, these vectors are different for different values of n, since the transfer matrices are not all the same ($\tilde{A}_n \neq A_1^n$), due to the randomness of the chemical potential. Our purpose is now to make a point, so let's take, for simplicity, $u_{n,1} = 0$.

$$|\alpha_{n+1}| = |\lambda_{n,+}v_{n,1}| \Rightarrow \sum_{n} |\alpha_{n+1}| = \sum_{n} |\lambda_{n,+}v_{n,1}|.$$

This sum must be normalizable. A necessary condition is then $|\lambda_{n,+}v_{n,1}| < 1$, which is quite different from the one deriving from eq. (25), because involving also the eigenvector entry $v_{n,1}$. However, the thermodynamic limit comes to our rescue and thanks to it we can recover a criterion that requires only the study of the eigenvalues. Let's take in consideration \tilde{A}_n as a product of infinite transfer matrices. We can separate this product into sub-products, say k < n sub-products, each involving a vary large number of matrices and the same number of matrices. Within the thermodynamic limit, all these products will converge, as a matter of self-averaging, to the same quantity, that is:

$$\tilde{A}_n = A_n \cdot A_{n-1} \cdot \ldots \cdot A_2 \cdot A_1 = B_k \cdot B_{k-1} \cdot \ldots \cdot B_2 \cdot B_1 \to B^k.$$

The *B* matrices obviously all have the same eigenvalues $\lambda_{B,\pm}$, again allowing us to rewrite the wave function in terms of the powers of these eigenvalues by means of a coefficient independent by *n*:

$$|\alpha_{n+1}| = \operatorname{const} \cdot \left| \lambda_B^k \right| = \operatorname{const} \cdot |\lambda_{B^k}| = \operatorname{const} \cdot \left| \lambda_{\tilde{A}_n} \right| \Rightarrow \sum_n |\alpha_{n+1}| = \operatorname{const} \sum_k |\lambda_B|^k.$$

Thus the eigenvalue criterion applies again: the wave function is normalizable if and only if the eigenvalues of matrices B, and, therefore, the eigenvalues of \tilde{A}_n , are less than 1. This result is generalizable to the extended Kitaev chain and the criterion can again be applied in the same modalities as expressed in section 2.3.

3.2 Disordered extended Kitaev chain

Applying disorder to the extended system translates into a Hamiltonian and a transfer matrix of the kind:

$$H = -\sum_{j=1}^{L} \mu_j \left(c_j^{\dagger} c_j - \frac{1}{2} \right) + \sum_{\ell=1}^{r} \sum_{j=1}^{L-\ell} \left(-w_\ell c_j^{\dagger} c_{j+\ell} + \Delta_\ell c_j c_{j+\ell} + \text{ h.c. } \right),$$
(28)

$$T_{n} = \begin{pmatrix} t_{1} & \cdots & t_{r,n} & \cdots & t_{2r} \\ 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & 0 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 1 & 0 \end{pmatrix}$$
(29)

where

$$t_i = -\frac{\Delta_{r-i} + w_{r-i}}{\Delta_r + w_r}, \quad \text{for } i = 1, \dots, r-1$$

$$t_{r,n} = -\frac{\mu_n}{\Delta_r + w_r},$$

$$t_i = \frac{\Delta_{i-r} - w_{i-r}}{\Delta_r + w_r}, \text{ for } i = r+1, \dots, 2r.$$

It is our purpose to investigate this system from many possible points of view. Now, it may therefore be essential to specify what kind of position dependence we expect from the parameters w_{ℓ} and Δ_{ℓ} in the non-homogeneous case. The most sensible option is to consider, as ℓ increases, a decrease in the intensity of these parameters, i.e. a reduction in the probability that there can be an exchange between two fermions, in the case of the hopping, or that a pair of fermions can leave the system or enter it, in the case of superconducting pairing. Therefore we assume an exponential decay of the form:

$$w_{\ell} = w_0 d_{\ell}^{-\alpha}, \quad \Delta_{\ell} = \Delta d_{\ell}^{-\beta}, \tag{30}$$

which couples the lattice site j with the site $(j + \ell)$. The hopping parameter w_{ℓ} can acquire a phase, $w_{\ell}e^{i\varphi_{\ell}}$, with φ_{ℓ} , w_0 , Δ real values, in the case of broken time-reversal symmetry (see Appendix A.1.1). The exponents α and β characterize the rate of decay for the parameters if they are assumed not negative. For $\alpha \to \infty$ and $\beta \to \infty$, one recovers the standard short-range Kitaev model. For $\alpha, \beta = 0$, the homogeneous condition is defined.

The index ℓ runs over the neighbor sites and d_{ℓ} is $d_{\ell} = \min(\ell, L - \ell)$ for closed boundary conditions and $d_{\ell} = \ell$ for open boundary conditions. For our purposes, we will assume open boundary condition and that time-reversal symmetry is preserved.

When using the transfer matrix method on this system, we come across very complicated calculations (in the next chapter we will give an idea with an example). The use of numerical calculus is therefore essential. In particular, the results that will be discussed in this section were obtained through python. For the problems that have arisen and the methods used to solve them, we refer to Appendix A.2.

One of the first and more important question one can do is about the extension of the topological order with respect to the Kitaev chain. As one can see from image



Figure 9: Critical curves for positive potentials and for different values of r for homogeneous a chain long L = 500 sites, with $w = \Delta$ and $\alpha = \beta = 0$. The curves are noisy due to the propagation of randomness on chains that are not actually infinite. By doing the calculations with longer chains, the noise should be mitigated. However, the shape of the topological phase is distinguishable.

9, as r increases, that is the range of extension of the pairing parameters in the equation (28), the total topological phase extends, both in terms of critical potentials, and as regards the maximum disorder and the topological order can support. In fact, larger topological domains are defined which incorporate those relating to smaller r values.

The considerations made up to now are valid for the overall topological phase, and the critical curves are found by imposing that all the degrees of freedom of the system are used, i.e. that the number of eigenvalues of the product transfer matrix which are, in absolute value, simultaneously greater (or less) or equal to 1, i.e. that lead to divergences and must be eliminated using the free parameters, is r - 1, so N = 0 and there is just N + 1 = 1 MZM (cfr. section 2.3). However, by allowing the system to have a greater number of free parameters N, it is possible to distinguish the topological phases characterized by different numbers of MZM. We report this type of phase diagram first for an example with r = 2 in figure 10. Here, the two different topological phases are distinguished: one with two MZM, which cannot go much beyond the domain defined by (13) (which we recognize for $\sigma = 0$) and dies at a relatively low value of the disorder; the other has an MZM and is indeed extremely resistant to disorder, which allows Majorana particles to survive even for previously forbidden chemical potentials.

This exact same work can be performed, by way of example, also for values of r greater than 2. We therefore report in figure 11 the phase diagrams obtained, by way of example, by setting r = 3 and r = 5. From these figures we observe that even for negative chemical potentials the topological domain expands more and more, assuming on the whole a



Figure 10: The graphs shown above represent the topological domain for r = 2 and choosing $\Delta = w_0$ as parameters. Figure (b) is a detail for positive chemical potentials of figure (a), which also includes negative potentials. In yellow the is represented the phase with two MZMs, in blue the phase with one.

peculiar "Latin America" shape. Furthermore, despite the fact that the topological order is increasingly fragmented by an increasing number of distinct phases, the phase with a MZM is always undoubtedly preponderant for most of the values of disorder, constituting the real conquest front of the topological order at the expense of the trivial phase.

Now we want to study the non-homogeneous system, that is the one with the exponent α and β figuring in equation (30) different from zero. We said before that in the limit that these exponent go to infinity, the system become the r = 1 Kitaev chain, whose topological phase is less extensive. So we expect that, as these parameters increase, the topological phase will shrink, tending to the one we have for r = 1. These assumptions are verified, as one can see from figure 12: as the exponents increase, the phase with two MZMs will shrinks and disappears at $\alpha, \beta = 1$ (see images (b) and (c) with exponents 0.8 and 0.9, respectively). The phase with one MZM at the beginning reduces too, but, for $\alpha, \beta > 1$, it widens again progressively (images (d), (e)) tending to the limit case of figure (f), that is the phase diagram of the Kitaev chain for r = 1.



Figure 11: (a) and (b): phase diagrams for r = 3. (d) and (e): phase diagrams for r = 5. (c): phase diagram for r = 3 and $\alpha = \beta = 0.1$.



Figure 12: These phase diagrams are obtained also for a chain of length L = 500 and for $\Delta_{\ell} = w_{\ell} \forall \ell$. Diagram (a) has been done for $\alpha = \beta = 0.5$. If confronted with diagram (b) in figure 10, it is evident that the topological area is reduced with respect to the case with null exponents. In particular, we can state the reduction of the critical potential for $\sigma = 0$. From figure (b) to figure (e) we are increasing the exponents up to $\alpha = \beta = 5$. Figure (f) is the r = 1 phase diagram. The normalization of the variables is done with respect to $w = w_0$.

4 A quick calculation: r=2 disordered EKC

In the following, we will try to give analytical legitimacy, at least for small disturbances, to the simulations of the previous chapter. To do this, we will still use the transfer matrix method and we will deal with a simplifying case, that is the one, already treated previously for the Kitaev chain at r = 1 (see section 3.1) of equality of the parameters w and Δ . Furthermore, we will assume that these are homogeneous along the whole chain. The homogeneous r = 2 transfer matrix (29) is:

$$T_i = \left(\begin{array}{cccc} -1 & -\frac{\mu_i}{\Delta + \omega} & \frac{\Delta - \omega}{\Delta + \omega} & \frac{\Delta - \omega}{\Delta + \omega} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right)$$

Applying the condition $t \equiv w = \Delta$:

$$T_i = \left(\begin{array}{rrrr} -1 & -\frac{\mu_i}{2t} & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right).$$

Matrix multiplication works as follows:

$$T_2 \cdot T_1 = \begin{pmatrix} 1 - \frac{\mu_2}{2t} & -\frac{\mu_1}{2t} & 0 & 0\\ -1 & -\frac{\mu_1}{2t} & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\vdots$$
$$\prod_{i=1}^n T_i = \begin{pmatrix} T_{11}^n & T_{12}^n & 0 & 0\\ T_{11}^{n-1} & T_{12}^{n-1} & 0 & 0\\ T_{11}^{n-2} & T_{12}^{n-2} & 0 & 0\\ T_{11}^{n-3} & T_{12}^{n-3} & 0 & 0 \end{pmatrix} \equiv T^n,$$

where we defined as T^n the product of transfer matrices (NB: it's not an exponentiation). We can then consider the division into blocks of the matrices:

$$T_{i} = \begin{pmatrix} A_{i} & 0(2) \\ \frac{\sigma_{x} + i\sigma_{y}}{2} & \frac{\sigma_{x} - i\sigma_{y}}{2} \end{pmatrix}$$
$$T^{n} = \begin{pmatrix} \tilde{A}_{n} & 0(2) \\ \tilde{A}_{n-2} & 0(2) \end{pmatrix}, \text{ with } 0(2) \equiv \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

From the block properties of these matrices we can infer that:

$$\tilde{A}_n = \begin{pmatrix} T_{11}^n & T_{12}^n \\ T_{11}^{n-1} & T_{12}^{n-1} \end{pmatrix} \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \prod_{i=1}^n A_i = \prod_{i=1}^n \begin{pmatrix} -1 & -\frac{\mu_i}{2t} \\ 1 & 0 \end{pmatrix}$$

It is easy to observe that the determinant of T^n is 0 and two eigenvalues of its are 0 too. The other two eigenvalues are fully determined by the characteristic polynomial of \tilde{A}_n :

$$p_{\tilde{A}_n} = \begin{vmatrix} a - \lambda & b \\ c & d - \lambda \end{vmatrix} = 0 \Rightarrow (a - \lambda)(d - \lambda) - bc = 0$$

$$\Rightarrow \lambda_{\pm} = \frac{1}{2} \left[(a + d) \pm \sqrt{(a + d)^2 - 4(ad - bc))} \right].$$
(31)

Where

$$ad - bc = \det \begin{pmatrix} a & b \\ c & c \end{pmatrix} = \prod_{i=1}^{n} \det \begin{pmatrix} -1 & -\frac{\mu_i}{2i} \\ 1 & 0 \end{pmatrix} = \prod_{i=1}^{n} \frac{\mu_i}{2t}.$$
 (32)

Since two eigenvalues of T^n are null and therefore less than 1, to have topological order it is necessary that at least one other eigenvalue among those appearing in the equation (31) is, in absolute value, less than 1 too.

Then, we can notice that the absolute value value of the determinant is exactly the eigenvalue of the r = 1 case under the same choice of parameters, which we have seen in eq. (26), and we yet know how to evaluate it, depending on the probability distribution. Moreover, the trace of matrix \tilde{A}_n can be written as:

$$a + d = (-1)^{n} \left\{ 1 + \sum_{i=2}^{n} m_{i} + \sum_{i_{1}=4}^{n} \sum_{i_{2}=2}^{i_{1}-2} m_{i_{1}} m_{i_{2}} + \sum_{i_{1}=6}^{n} \sum_{i_{2}=4}^{i_{1}-2} \sum_{i_{3}=2}^{i_{2}-2} m_{i_{1}} m_{i_{2}} m_{i_{3}} + \dots + \sum_{i_{1}=2\nu}^{n} \sum_{i_{2}=2\nu-2}^{i_{2}-2} \dots \sum_{i_{\nu}=2}^{i_{\nu-1}-2} m_{i_{1}} m_{i_{2}} \dots m_{i_{\nu}} + m_{1} \left[1 + \sum_{i=3}^{n-1} m_{i} + \sum_{i_{1}=5}^{n-1} \sum_{i_{2}=3}^{i_{1}-2} m_{i_{1}} m_{i_{2}} + \sum_{i_{1}=7}^{n-1} \sum_{i_{2}=5}^{i_{2}-2} m_{i_{1}} m_{i_{2}} m_{i_{3}} + \dots + \sum_{i_{1}=2\nu-1}^{n-1} \sum_{i_{2}=2\nu-3}^{i_{1}-2} \dots \sum_{i_{\nu-1}=3}^{i_{\nu-2}-2} m_{i_{1}} m_{i_{2}} \dots m_{i_{\nu-1}} \right] \right\},$$

$$(33)$$

being
$$m_i \equiv -\frac{\mu_i}{2t}$$
 and $\nu \equiv \begin{cases} \frac{n}{2} & \text{for } n \text{ even,} \\ \frac{n-1}{2} & \text{for } n \text{ odd.} \end{cases}$

A formal derivation of this formula is presented in Appendix A.3.

Before going on with the disordered analysis, it is convenient to verify that this method recovers, in the absence of disorder, the known result on the domain of the topological phase that we find in equations (13). The first section will be devoted to this task.

4.1 Non-disordered $w = \Delta$

Now let's try to derive the well-known domain of the topological phase:

$$-4t < \mu < 2t,$$

in the case of absence of disorder $\sigma = 0$:

$$\mu_{i} = \mu_{j} = \mu \quad \forall i, j$$

$$ad - bc = \left(\frac{\mu}{2t}\right)^{n} = (-m)^{n} \quad \text{with}$$

$$m = m_{i} = m_{j}$$
(34)

In general:

$$(-1)^{n}(a+d) =$$

$$= 1 + (n-1)m + m^{2} \sum_{i_{1}=n}^{n} (i_{1}-2-1) + \dots \quad (a) \quad \{\nu + 1 \text{ terms}\}$$

$$+ m \left[1 + (n-3)m + m^{2} \sum_{i_{1}=5}^{n-1} (i_{1}-4) + \dots \right] \quad (b) \quad \{\nu \text{ terms}\}.$$

The first term of the raw (a) is:

$$m^2 \sum_{i=4}^{n} (i-3) = m^2 \frac{(n-2)!}{(n-4)!2!}$$

The next term in the same raw is:

$$\sum_{i=6}^{n} \sum_{i=4}^{i_1-2} \sum_{i_3=2}^{i_2-2} m^3 = m^3 \frac{(n-3)!}{(n-6)!3!}.$$

In general we will have:

$$\sum_{i=2k}^{n} \sum_{i_2=2k-2}^{i_1-2} \cdots \sum_{i_k=2}^{i_{k-1}-2} m^k = m^k \cdot \frac{(n-k)!}{(n-2k)!k!} = m^k \binom{n-k}{k}$$

and:

(a) =
$$\sum_{k=0}^{\nu} m^k \begin{pmatrix} n-k \\ k \end{pmatrix}$$
.

Doing the same for the second raw, one has:

(b) =
$$\sum_{k=0}^{\nu-1} m^{k+1} \begin{pmatrix} n-2-k \\ k \end{pmatrix} = \sum_{k=1}^{\nu} m^k \begin{pmatrix} n-k-1 \\ k-1 \end{pmatrix}.$$

Thus we have:

$$a + d = (-1)^n \left\{ 1 + \sum_{n=1}^{\frac{n}{2}m^k} \left[\binom{n-k}{n} + \binom{n-k-1}{k-1} \right] \right\},\$$

where

$$\begin{pmatrix} n-k \\ k \end{pmatrix} + \begin{pmatrix} n-k-1 \\ k-1 \end{pmatrix} = \frac{(n-k)!}{(n-2k)!k!} + \frac{(n-k-1)!}{(n-2k)!(k-1)!} = \\ = \frac{(n-k)! + (n-k-1)! \cdot k}{(n-2k)!k!} = \frac{(n-k-1)!}{(n-2k)!k!} [n-k+k] = \\ = n\frac{(n-k-1)!}{(h-2k)!k!} = \left(\frac{n}{n-k}\right) \cdot \frac{(n-k)!}{(n-2k)!k!} = \\ = \frac{n}{n-k} \cdot \left(\frac{n-k}{k}\right) \\ \Rightarrow a+d = (-1)^n \left[1 + \sum_{k=1}^{\nu} \frac{nm^k}{n-k} \left(\frac{n-k}{k}\right)\right].$$

Moreover, we notice that, if k = 0 were admitted:

$$\frac{nm^0}{n} \binom{n}{0} = \frac{n}{n} = 1$$
$$\Rightarrow a + d = (-1)^n \sum_{k=0}^{\nu} \frac{nm^k}{n-k} \left(\frac{n-k}{k}\right),$$

or, equivalently:

$$(a+d)_{\sigma=0} = \sum_{k=0}^{\nu} \frac{n}{n-k} \left(\frac{\mu}{2t}\right)^k (-1)^{n+k} \left(\begin{array}{c} n-k\\k \end{array}\right).$$

We can manipulate it further:

$$= (-1)^{n} \sum_{k=0}^{\nu} (-1)^{k} \frac{n}{h-k} \frac{(n-k)!}{(n-2k)!k!} \cdot 2^{-2k} \cdot (4\tilde{\mu})^{k} \quad \left(\tilde{\mu} \equiv \frac{\mu}{2t}\right)$$

$$= (-1)^{n} \sum_{k=0}^{\nu} (-1)^{k} n \cdot (n-k-1)! \cdot \frac{1}{(n-2k)!k!} 2^{-2k} (4\tilde{\mu})^{k} =$$

$$= (-1)^{n} \sum_{k=0}^{\nu} (-1)^{k} \frac{n!}{(n-1)(n-2)\cdots(n-k)} \cdot \frac{1}{(n-2k)!k!} 2^{-2k} (4\tilde{\mu})^{k} = (*),$$

where

$$\begin{aligned} \frac{n!}{(n-2k)!} &= n(n-1)(n-2)\dots(n-2k+1) = \\ &= 2^{2k}\frac{n}{2}\left(\frac{n-1}{2}\right)\left(\frac{n-2}{2}\right)\dots\left(\frac{n+2}{2}-k\right)\left(\frac{n+1}{2}-k\right) = \\ &= 2^{2k}\left[\frac{n}{2}\left(\frac{n-2}{2}\right)\left(\frac{n-4}{2}\right) - \left(\frac{n+2}{2}-k\right)\right] \cdot \left[\left(\frac{n-1}{2}\right) - \dots\left(\frac{n+1}{2}-k\right)\right] = \\ &= (-1)^{2k}2^{2k}\left[-\frac{n}{2}\left(-\frac{n-2}{2}\right)\dots\left(-\frac{n+2}{2}+k\right)\right]\left[\left(-\frac{n-1}{2}\right)\dots\left(-\frac{n+1}{2}+k\right)\right] \Rightarrow \\ &\Rightarrow (*) = \\ &= (-1)^n\sum_{k=0}^{\nu} (-1)^k \frac{\left[-\frac{n}{2}\left(-\frac{n-2}{2}\right)\dots\left(-\frac{n+2}{2}+k\right)\right]\left[\left(-\frac{n-1}{2}\right)\dots\left(-\frac{n+1}{2}+k\right)\right]}{(n-1)\dots(n-k)\cdot k!} (4\tilde{\mu})^k. \end{aligned}$$

We can notice that the argument of this sum is always null for

$$k \ge \frac{n+2}{2} = \frac{n}{2} + 1 \Rightarrow k_{1, \max} = \frac{n}{2}$$

 $k \ge \frac{n+1}{2} = \frac{n}{2} + \frac{1}{2} \Rightarrow k_{2, \max} = \frac{n-1}{2}$

Depending on the parity of n, beyond these values of k one of the two terms in square brackets will be null. Therefore we can run the sum to infinity with impunity.

$$(a+d)_{\sigma=0} = (-1)^n \sum_{k=0}^{\infty} \frac{\left[-\frac{n}{2}\cdots\left(-\frac{n+2}{2}+k\right)\right] \left[\left(-\frac{n-1}{2}\right)\cdots\left(-\frac{n+1}{2}+k\right)\right]}{(-n+1)-\cdots(-n+k)\cdot k!} (4\tilde{\mu})^k.$$

In this expression, we can recognize a hypergeometric function:

$${}_{2}F_{1}(\tilde{a},b;c;z) = \sum_{k=0}^{\infty} \frac{(\tilde{a})_{k}(b)_{k}}{(c)_{k}} \frac{z^{k}}{k!}$$
with $(q)_{k} = \begin{cases} 1 & k = 0\\ q(q+1)\cdots(q+k-1) & k > 0 \end{cases}$
and $\tilde{a} = -\frac{n}{2}, \quad b = -\frac{n-1}{2}, \quad c = -n+1, \quad z = 4\tilde{\mu} = 4\frac{\mu}{2t}$

Thus, ultimately, we define:

$$(a+d)_{\sigma=0} = (-1)^n {}_2F_1\left(-\frac{n}{2}, -\frac{n-1}{2}, -n+1, 4\frac{\mu}{2t}\right) =: 2f_n(\mu, \sigma)\Big|_{\sigma=0}.$$

From eq. (31), after applying the no-disorder condition (34) also to the determinant (32), we have the expression for the eigenvalues:

$$|\lambda_{\pm}|_{\sigma=0} = \left| f_n(\mu, 0) \pm \sqrt{\left(f_n(\mu, 0) \right)^2 - \left(\frac{\mu}{2t} \right)^n} \right|.$$
(35)

As we said before, there is topological order if at least one of these quantities is less than

1. We can see under what conditions this occurs when we consider the thermodynamic limit. We first notice that (positive t):

$$\left|\frac{\mu}{2t}\right|^{n} \xrightarrow{n \to \infty} \begin{cases} 0 & \text{for } |\mu| < 2t, \\ 1 & \text{for } |\mu| = 2t, \\ +\infty & \text{for } |\mu| > 2t. \end{cases}$$

While, from taking the limit of the hypergeometric function, one can state that:

$$|f_n(\mu, 0)| \xrightarrow{n \to \infty} \begin{cases} 0 \quad \forall \ \mu > 0, \\ +\infty \quad \forall \ \mu < 0, \end{cases}$$

while in the limit for $\mu \to 0$, $f_n(\mu, 0)$ is always 1 $\forall n$. This means that for positive values of μ :

$$|\lambda_{\pm}|_{(\sigma=0,\ \mu>0)} \xrightarrow{n\to\infty} \begin{cases} 0 & \text{for } \mu < 2t, \\ 1 & \text{for } \mu = 2t, \\ +\infty & \text{for } \mu > 2t \end{cases}$$

i.e. the two eigenvalues coincide. Instead, for $\mu \to 0$, one eigenvalue is always ± 2 and the other one is 0, and for negative values we can have:

$$|\lambda_{\pm}|_{(\sigma=0, \ \mu<0)} \xrightarrow{n\to\infty} |f_n(\mu, 0) \pm |f_n(\mu, 0)|| = |f_n(\mu, 0) \pm f_n(\mu, 0)|$$

i.e. one eigenvalue is null, the other one diverges. This is certainly true until $\mu/t < -2$. Below this value, $(\mu/(2t))^n$ is no longer null and we can expect that, beyond a certain value, the power under the root in eq. (35) is decisive and also causes the initially null eigenvalue to diverge. This happens when:

$$\begin{cases} \left| |f_n(\mu, 0)| - \sqrt{(f_n(\mu, 0))^2 - \left(\frac{\mu}{2t}\right)^n} \right| \ge 1, \\ \mu < 0. \end{cases}$$

To proceed with the calculation we must distinguish between even and odd values of n. In fact, if n is odd, the system above is satisfied if:

$$\left| |f_n(\mu,0)| - \sqrt{(f_n(\mu,0))^2 + \left|\frac{\mu}{2t}\right|^n} \right| \ge 1 \iff |f_n(\mu,0)| - \sqrt{(f_n(\mu,0))^2 + \left|\frac{\mu}{2t}\right|^n} \le -1,$$

which admits solutions for:

$$\left|\frac{\mu}{2t}\right|^n \ge 2|f_n(\mu,0)| + 1 \sim 2|f_n(\mu,0)|.$$

If n is even, if $(\mu/(2t))^n$ is greater than $(f_n(\mu, 0))^2$, then we are dealing with complex



Figure 13: Topological phases for the homogeneous r = 2 EKC with $t = \Delta = w$.

numbers. However, even in this case we can prove that the eigenvalue is greater than 1 even before this happens. Indeed:

$$\left| |f_n(\mu,0)| - \sqrt{(f_n(\mu,0))^2 - \left|\frac{\mu}{2t}\right|^n} \right| \ge 1 \iff |f_n(\mu,0)| - \sqrt{(f_n(\mu,0))^2 - \left|\frac{\mu}{2t}\right|^n} \ge 1,$$

which is solved for:

$$\left|\frac{\mu}{2t}\right|^n \ge 2|f_n(\mu,0)| - 1 \sim 2|f_n(\mu,0)|.$$

which is certainly less than the divergent quantity $(f_n(\mu, 0))^2$. In both cases we have neglected a 1 to be subtracted or added, thus obtaining the same inequality, which is numerically verified for $\frac{\mu}{2t} < -4$.

In summary, so far we have seen that:

$$\begin{split} &\frac{\mu}{t} \geq 2 \Rightarrow \ |\lambda_{\pm}|_{(\sigma=0)} \geq 1 \Rightarrow \text{ NO MZMs} \\ &0 < \frac{\mu}{t} < 2 \Rightarrow \ |\lambda_{\pm}|_{(\sigma=0)} = 0 \Rightarrow \ 2 \text{ MZMs} \\ &-4 < \frac{\mu}{t} \leq 0 \Rightarrow \ |\lambda_{-}|_{(\sigma=0)} < 1, \ |\lambda_{+}|_{(\sigma=0)} = +\infty \Rightarrow \ 1 \text{ MZM} \\ &\frac{\mu}{t} \leq -4 \Rightarrow \ |\lambda_{\pm}|_{(\sigma=0)} = +\infty \Rightarrow \text{ NO MZMs.} \end{split}$$

These results, shown schematically in figure 13, are in agreement with the prevision of (13).

4.2 Introducing disorder

The existence of the MZM is determined by the conditions:

$$|\lambda_{\pm}| \equiv \left| f_n(\mu, \sigma) \pm \sqrt{\left(f_n(\mu, \sigma) \right)^2 - \prod_{i=1}^n \frac{\mu_i}{2t}} \right| < 1,$$
(36)

with the quantity $f_n(\mu, \sigma)$ defined as:

$$f_{n}(\mu,\sigma) = \frac{(-1)^{n}}{2} \left\{ 1 + \sum_{i=2}^{n} m_{i} + \sum_{i_{1}=4}^{n} \sum_{i_{2}=2}^{i_{1}-2} m_{i_{1}} m_{i_{2}} + \sum_{i_{1}=6}^{n} \sum_{i_{2}=4}^{i_{1}-2} \sum_{i_{3}=2}^{n} m_{i_{1}} m_{i_{2}} m_{i_{3}} + \dots + \sum_{i_{1}=2\nu}^{n} \sum_{i_{2}=2\nu-2}^{i_{2}-2} \dots \sum_{i_{\nu}=2}^{i_{\nu-1}-2} m_{i_{1}} m_{i_{2}} \dots m_{i_{\nu}} + m_{1} \left[1 + \sum_{i=3}^{n-1} m_{i} + \sum_{i_{1}=5}^{n-1} \sum_{i_{2}=3}^{i_{1}-2} m_{i_{1}} m_{i_{2}} + \sum_{i_{1}=7}^{n-1} \sum_{i_{2}=2\nu-3}^{i_{1}-2} \sum_{i_{2}=3}^{i_{1}-2} m_{i_{1}} m_{i_{2}} \dots m_{i_{\nu-1}} \right] \right\},$$

$$(37)$$

being
$$m_i \equiv -\frac{\mu_i}{2t}$$
 and $\nu \equiv \begin{cases} \frac{n}{2} & \text{for } n \text{ even,} \\ \frac{n-1}{2} & \text{for } n \text{ odd.} \end{cases}$

The condition applies as follows: if both values λ_+ and λ_- in equation (36) are less than 1, two MZM are found; if only one value is less than 1, then there is just one MZM; if both values are 1 or greater than 1, the phase is trivial.

A first consideration that we can make concerns the minimum extension that we expect the topological phase can have. In fact, in the formula (36) we recognize in $\prod \mu_i/(2t)$ the non-zero eigenvalue of the Kitaev chain for the same choice of parameters. The topological phase of the latter system, illustrated in figure 7 (b), exists, as we have seen in eq. (27), provided that $e^{n < \log(\frac{\mu_i}{2t})^{>}} < 1$. In the thermodynamic limit, depending on the sign of the mean value of the logarithm, this quantity is zero below the critical curve and diverges infinitely above. So, below the critical curve, eq. (36) becomes:

$$|\lambda_{\pm}| = |f_n(\mu, \sigma) \pm |f_n(\mu, \sigma)|| = |f_n(\mu, \sigma) \pm f_n(\mu, \sigma)|,$$

that is, one of the two eigenvalues is always zero. Hence the general topological phase for r = 2 is at least coinciding with that for r = 1, and eventually even more extended. This is certainly in agreement with the simulations seen in the previous chapter (see fig. 9). If we want to know something more, such as how the phases of one or two MZMs are arranged, it is worth doing a more in-depth study.

As we know, in absence of disorder, that is for $\sigma = 0$, the function (37) reduces to a hypergeometric function which, in the thermodynamic limit, tends to 0 for positive chemical potentials:

$$f_n(\mu, 0) = \frac{(-1)^n}{2} {}_2F_1\left(-\frac{n}{2}, -\frac{n-1}{2}, -n+1, 4\frac{\mu}{2t}\right) \xrightarrow{n \to \infty} \begin{cases} 0 \quad \forall \ \mu > 0, \\ \pm \infty \quad \forall \ \mu < 0. \end{cases}$$

The purpose of this section is to find the quantity $g_n(\mu, \sigma)$ such that:

$$\begin{cases} f_n(\mu,\sigma) = \frac{(-1)^n}{2} \left[{}_2F_1\left(-\frac{n}{2}, -\frac{n-1}{2}, -n+1, 4\frac{\mu}{2t}\right) - g_n(\mu,\sigma) \right], \\ g_n(\mu,0) = 0. \end{cases}$$

4.2.1 Moments of the distribution

We start studying how to write in a more simple way the quantity, figuring in (37),

$$\frac{1}{\substack{k=0\\k=0}} + \underbrace{\sum_{k=1}^{n} m_{i}}_{k=1} + \underbrace{\sum_{i_{1}=4}^{n} \sum_{i_{2}=2}^{i_{1}-2} m_{i_{1}} m_{i_{2}}}_{k=2} + \underbrace{\sum_{i_{1}=6}^{n} \sum_{i_{2}=4}^{i_{1}-2} \sum_{i_{3}=2}^{i_{1}-2} m_{i_{1}} m_{i_{2}} m_{i_{3}} + \dots}_{k=3} + \underbrace{\sum_{i_{1}=2\nu}^{n} \sum_{i_{2}=2\nu-2}^{i_{1}-2} \dots \sum_{i_{\nu}=2}^{i_{\nu}-1} m_{i_{1}} m_{i_{2}} \dots m_{i_{\nu}}}_{k=\nu}, \quad (38)$$

where k indicates the number of sums. It's simpler to treat this problem studying this terms separately. Our aim is to decouple the sums to obtain a function of the moments of any probability distribution. Let's start from k = 2 because the k = 0 and k = 1 terms are not affected by disorder, being the first one a constant and the second one the mean value multiplied by a constant, as we approach the thermodynamic limit.

k=2

As we can graphically state seeing figure 14, we can write the term k = 2 as:

$$\sum_{i_{1}=4}^{n} \sum_{i_{2}=2}^{i_{1}-2} m_{i_{1}} m_{i_{2}} = 1/2 \left[\left(\sum_{i=2}^{n} m_{i} \right)^{2} - \sum_{i=2}^{n} m_{i}^{2} - 2 \sum_{i=2}^{n-1} m_{i} m_{i+1} \right] = \frac{1}{2} \left[(n-1)^{2} \tilde{M}_{1}^{2} - (n-1) \tilde{M}_{2} \right] - (n-2) < m_{i} m_{i+1} >,$$
(39)

where we used the notation $\langle \ldots \rangle$ to indicate a correlator, and assumed the thermodynamic limit in n to define, in general:



Figure 14: Graphical representation of the term k = 2, which corresponds to one of the two equivalent yellow parts. Every square corresponds to one term of the kind $m_{i_1}m_{i_2}$, where i_1 and i_2 are the variables on the axes. The red-delimited area will then describe the sum of all possible combinations of products $m_{i_1}m_{i_2}$ for i_1 and $i_2 \in [2, n]$. For the significance of the other colours, see equation (39).

$$\tilde{M}_k \equiv \frac{1}{n-\eta+1} \sum_{i=\eta \in \mathbb{N}}^{n \gg \eta} m_i^k = \langle m_i^k \rangle.$$

We can already observe that for $\sigma = 0$ the quantities \tilde{M}_k reduce to \tilde{M}_1^k . Defining the moments of the distribution and rewriting the expression (39), we have:

$$M_k \equiv \tilde{M}_k - \tilde{M}_1^k, \tag{40}$$

$$\frac{1}{2} \left[(n-1)^2 \tilde{M}_1^2 - (n-1) \tilde{M}_1^2 \right] - (n-2) < m_i m_{i+1} > -\frac{1}{2} (n-1) M_2.$$

Now we can suppose that the distribution is such that the stochastic determination of the chemical potential associated to any fermionic site is independent from the potentials in the other sites. This is a fair assumptions and simplify our lives, because the correlator $\langle m_i m_{i+1} \rangle$ will reduce to \tilde{M}_1^2 . Simplifying first the notation calling $m \equiv \tilde{M}_1$, we write:

$$\sum_{i_1=4}^{n} \sum_{i_2=2}^{i_1-2} m_{i_1} m_{i_2} = \underbrace{\frac{(n-3)(n-2)}{2}m^2}_{\sigma=0} - \underbrace{\frac{(n-1)}{2}M_2}_{\text{in } g_n(\mu,\sigma)}.$$

It is immediate to notice that the second term of this expression, due to the definition of M_k , will vanish for $\sigma = 0$, meanwhile the first one won't be affected. Thus the second term contributes to the definition of the quantity $g_n(\mu, \sigma)$ we want to evaluate. In the next, we will estimate the other contributions.

k = 3

This term is too complicated to be treated graphically as the previous one. However, we could use what we learned from k = 2 to imagine step by step what we should discard from a 3-D cube of side n - 1 in order to obtain this term.

With this purpose, let's also observe that, as in the k = 2 diagram we have two equivalent areas corresponding to the k = 2 term and this is the reason why we have a factor 1/2, in the same way we can expect from a hypothetical 3-D representation of the k = 3 term to show 3! = 6 equivalent volumes. So write:

$$\sum_{i_1=6}^n \sum_{i_2=4}^{i_1-2} \sum_{i_3=2}^{i_2-2} m_{i_1} m_{i_2} m_{i_3} = \frac{1}{3!} \left[(\sum_{i=2}^n m_i)^3 - \ldots \right].$$

The first thing we should subtract from the cube and which doesn't appear in the term k = 3 is the sum of the cubes:

$$\sum_{i_1=6}^n \sum_{i_2=4}^{i_1-2} \sum_{i_3=2}^{i_2-2} m_{i_1} m_{i_2} m_{i_3} = \frac{1}{3!} \left[(\sum_{i=2}^n m_i)^3 - \sum_{i=2}^n m_i^3 - \dots \right].$$

Then, we subtract all the terms with squares: $\sum_{i=2}^{n} m_i \sum_{j=2}^{n} m_j^2$. However, we have to avoid repetitions with the previous term imposing $j \neq i$ and we must consider the possible permutations of the axes: we have 3 possibilities on the choice of m_i and then just one possibility on the choice of m_i^2 . Thus:

$$\sum_{i_1=6}^n \sum_{i_2=4}^{i_1-2} \sum_{i_3=2}^{i_2-2} m_{i_1} m_{i_2} m_{i_3} = \frac{1}{3!} \left[(\sum_{i=2}^n m_i)^3 - \sum_{i=2}^n m_i^3 - 3\sum_{i=2}^n m_i \sum_{j\neq i}^n m_j^2 - \dots \right].$$

The only terms we are left to subtract are combinations of correlators, which, as we know, are useless in the computation of $g_n(\mu, \sigma)$, which is our aim.

$$\sum_{i_1=6}^n \sum_{i_2=4}^{i_1-2} \sum_{i_3=2}^{i_2-2} m_{i_1} m_{i_2} m_{i_3} = \frac{1}{3!} \left[(\sum_{i=2}^n m_i)^3 - \sum_{i=2}^n m_i^3 - 3\sum_{i=2}^n m_i \sum_{j\neq i}^n m_j^2 - \langle \text{correlators} \rangle \right].$$

Using again the notation developed in the section ??, the previous expression can be rewritten as:

$$\frac{1}{3!} \left[(n-1)^3 m^3 - (n-1)\tilde{M}_3 - 3(n-1)(n-2)\tilde{M}_1\tilde{M}_2 - \langle \text{ correlators} \rangle \right] = \\ = Cm^3 - \left[\underbrace{\frac{(n-1)}{3!}M_3 + m\frac{(n-1)(n-2)}{2}M_2}_{\text{in } g_n(\mu,\sigma)} \right],$$

where C is a constant. Again, the second term would annihilate for $\sigma = 0$. We have just found another contribution to $g_n(\mu, \sigma)$.

k = 4

For k = 4 we have:

$$\sum_{i_1=8}^{n} \sum_{i_2=6}^{i_1-2} \sum_{i_3=4}^{i_2-2} \sum_{i_4=2}^{i_3-2} m_{i_1} m_{i_2} m_{i_3} m_{i_4} =$$

= $\frac{1}{4!} \left[(\sum_{i=2}^{n} m_i)^4 - \sum_{i=2}^{n} m_i^4 - 4 \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^3 - 4 \cdot 3 \sum_{i=3}^{n} m_i \sum_{j < i}^{n} m_j \sum_{k \neq i,j}^{n} m_j^2 - \dots \right].$

We must pay attention to the term with three sums, where the second sum is performed for j < i. This happens because, if we summed over all the js, then all the different terms would have been counted two times, while we want to count each term one time and only then take into account all the possible permutations with the coefficient $4 \cdot 3$. Of course, we can rewrite $\sum_{i=2}^{n} m_i \sum_{j < i} m_j = 1/2 \sum_{i=2}^{n} m_i \sum_{j \neq i} m_j$. The factor 1/2 could then be seen as a way to 'un-permute' the first two sums before 're-permuting' everything again.

$$\frac{1}{4!} \left[(\sum_{i=2}^{n} m_i)^4 - \sum_{i=2}^{n} m_i^4 - 4 \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^3 - \frac{4 \cdot 3}{2} \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j \sum_{k \neq i,j}^{n} m_k^2 - \langle \operatorname{corr.} \rangle \right].$$

We must now notice that the term with m_i^2 can be combined with another sum over m_i^2 . This time, the coefficient will be number of combinations of 2 dinstinct elements out of 4. Moreover, we must again 'un-permute', because we are dealing again with two changeable sums:

$$\frac{1}{4!} \left[(\sum_{i=2}^{n} m_i)^4 - \sum_{i=2}^{n} m_i^4 - 4 \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^3 - \frac{4 \cdot 3}{2} \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j \sum_{k \neq i,j}^{n} m_k^2 - \frac{1}{2} \binom{4}{2} \sum_{i=2}^{n} m_i^2 \sum_{j \neq i}^{n} m_j^2 - \langle \operatorname{corr.} \rangle = \right]$$

$$= Cm^{4} - \frac{1}{4!} \left[(n-1)\tilde{M}_{4} + 4(n-1)(n-2)\tilde{M}_{1}\tilde{M}_{3} + \frac{4\cdot 3}{2}(n-1)(n-2)(n-3)\tilde{M}_{1}^{2}\tilde{M}_{2} + \frac{1}{2} \binom{4}{2}(n-1)(n-2)\tilde{M}_{2}^{2} \right].$$

Higher k

For higher values of k we take into account other combinations of products of \tilde{M}_k . For example, for k = 5 we start from:

$$\frac{1}{5!} \left[(\sum_{i=2}^{n} m_i)^5 - \sum_{i=2}^{n} m_i^5 - 5 \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^4 - \dots \right].$$

In subtracting the terms with m_i^3 we must notice that they can be combined with two sums of m_i or one of m_i^2 :

$$\frac{1}{5!} \left[(\sum_{i=2}^{n} m_i)^5 - \sum_{i=2}^{n} m_i^5 - 5 \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^4 - c_1 \sum_{i=3}^{n} m_i \sum_{j \neq i}^{n} m_j \sum_{k \neq i,j}^{n} m_j^3 - c_2 \sum_{i=2}^{n} m_i^2 \sum_{j \neq i}^{n} m_j^3 \dots \right].$$

The coefficient c_1 is just, as seen before, $5 \cdot 4/2$. The coefficient c_2 is given by the combinations of 2 distinct elements out of 5. Completing with the other terms, we find the expression for k = 5:

$$\frac{1}{5!} \left[(\sum_{i=2}^{n} m_i)^5 - \sum_{i=2}^{n} m_i^5 - 5 \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^4 - {5 \choose 2} \sum_{i=2}^{n} m_i^2 \sum_{j \neq i}^{n} m_j^3 - \frac{5 \cdot 4}{2} \sum_{i=3}^{n} m_i \sum_{j \neq i}^{n} m_j \sum_{k \neq i,j}^{n} m_j^3 - \frac{5 \cdot 4 \cdot 3}{3!} \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j \sum_{k \neq i,j}^{n} m_k \sum_{l \neq i,j,k}^{n} m_l^2 - \frac{5}{2} {4 \choose 2} \sum_{i=2}^{n} m_i \sum_{j \neq i}^{n} m_j^2 \sum_{k \neq i,j}^{n} m_k^2 - \langle \operatorname{corr.} \rangle \right].$$

Terms affected by disorder (taken with positive sign):

$$\frac{1}{5!} \left[(n-1)\tilde{M}_5 + 5(n-1)(n-2)\tilde{M}_1\tilde{M}_4 + {\binom{5}{2}}(n-1)(n-2)\tilde{M}_2\tilde{M}_3 + 5\cdot4(n-1)(n-2)(n-3)\frac{\tilde{M}_1^2}{2}\tilde{M}_3 + 5\cdot4\cdot3(n-1)(n-2)(n-3)(n-4)\frac{\tilde{M}_1^3}{3!}\tilde{M}_2 + 5{\binom{4}{2}}(n-1)(n-2)(n-3)\tilde{M}_1\frac{\tilde{M}_2^2}{2} \right].$$

We can rewrite all the coefficients as binomial ones:

$$\frac{1}{5!} \left[(n-1)\tilde{M}_5 + {\binom{5}{1}}(n-1)(n-2)\tilde{M}_1\tilde{M}_4 + {\binom{5}{2}}(n-1)(n-2)\tilde{M}_2\tilde{M}_3 + {\binom{5}{1}}(n-1)(n-2)(n-3)\frac{\tilde{M}_1^2}{2}\tilde{M}_3 + {\binom{5}{1}}\binom{4}{1}\binom{4}{1}\binom{3}{1}(n-1)(n-2)(n-3)(n-4)\frac{\tilde{M}_1^3}{3!}\tilde{M}_2 + {\binom{5}{1}}\binom{4}{2}(n-1)(n-2)(n-3)\tilde{M}_1\frac{\tilde{M}_2^2}{2} \right].$$

Then, for a **generic** k we will have a sum of terms of the form:

$$\frac{B}{k!} \cdot \frac{(n-1)!}{(n-\gamma-1)!} \cdot \frac{\tilde{M}_1^{\alpha_1}}{\alpha_1!} \frac{\tilde{M}_2^{\alpha_2}}{\alpha_2!} \cdot \dots \cdot \frac{\tilde{M}_k^{\alpha_k}}{\alpha_k!}$$
(41)

where:

$$\gamma = \sum_{i=1}^{k} \alpha_i$$

The sum will run over every combination of $\{\alpha_i\}$ such that the conditions:

$$\sum_{i=1}^{k} i \cdot \alpha_i = k, \quad \alpha_1 \neq k, \tag{42}$$

are satisfied. Moreover, the coefficient B is given by products of binomial coefficients. For example, for k = 15 and a term displaying:

$$\tilde{M}_1^2 \cdot \tilde{M}_2^3 \cdot \tilde{M}_3 \cdot \tilde{M}_4,$$

the coefficient B is given by:

$$\binom{15}{1}\binom{14}{1}\binom{13}{2}\binom{11}{2}\binom{9}{2}\binom{7}{3} = \frac{15!}{14!}\frac{14!}{13!}\frac{13!}{11!\,2!}\frac{11!}{9!\,2!}\frac{9!}{7!\,2!}\frac{7!}{4!\,3!} = \frac{15!}{(1!)^2(2!)^3(3!)^1(4!)^1} = \prod_{p=1}^k \frac{k!}{(p\,!)^{\alpha_p}}.$$

With $\alpha_p = 0 \forall p > 4$.

So, for the generic k we can rewrite the term (41) as:

$$\frac{(n-1)!}{(n-\gamma-1)!} \prod_{p=1}^{k} \frac{\tilde{M}_{p}^{\alpha_{p}}}{\alpha_{p}! \, (p\,!)^{\alpha_{p}}},\tag{43}$$

and the whole term is of the form:

$$Cm^{k} - \sum_{\{\alpha_{i}\}:(42)} \frac{(n-1)!}{(n-\gamma-1)!} \prod_{p=1}^{k} \frac{\tilde{M}_{p}^{\alpha_{p}}}{\alpha_{p}! (p\,!)^{\alpha_{p}}}.$$
(44)

Remembering the definition (40) and using the Newton's expansion of binomial, we can write:

$$\tilde{M}_p^{\alpha_p} = (M_p + m^p)^{\alpha_p} = \sum_{q=0}^{\alpha_p} {\alpha_p \choose q} M_p^q m^{\alpha_p - q}$$

Of the sum above, the only term which won't vanish for $\sigma = 0$ is the one with q = 0. This means that we found the contribution to $g_n(\mu, \sigma)$ from every k:

$$\sum_{\{\alpha_i\}:(42)} \frac{(n-1)!}{(n-\gamma-1)!} \prod_{p=1}^k \frac{1}{(p!)^{\alpha_p}} \sum_{q=1}^{\alpha_p} \frac{M_p^q \, m^{\alpha_p-q}}{(\alpha_p-q)! \, q!}.$$
(45)

4.2.2 Same order approximation

We can try to evaluate the expression (43) taking into consideration, for each value of k, only the biggest term, according to the factor:

$$\frac{(n-1)!}{(n-\gamma-1)!}.$$
(46)

This means that, for every k, we are looking for the smallest γ . In order to do so, we are better to make another approximation, stating:

$$\tilde{M}_x^y \sim O(x+y),$$

which means that we suppose that the order of every factor \tilde{M}_x^y is given from the index and the exponent. We can try to state in which limit this approximation holds, for example using a **box distribution**:

$$\tilde{M}_x = \frac{1}{2\delta} \int_{-\delta}^{+\delta} (m+h)^x \mathrm{d}h = \frac{1}{2\delta} \int_{-\delta}^{+\delta} \sum_{p=0}^k \binom{x}{p} m^{x-p} h^p \mathrm{d}h = \frac{1}{2\delta} \sum_{p=0}^x \binom{x}{p} m^{x-p} \int_{-\delta}^{+\delta} h^p \mathrm{d}h = \sum_{p \text{ even}}^x \binom{x}{p} m^{x-p} \frac{\delta^p}{p+1}.$$

If our approximation holds, this term will be of the same order of:

$$\tilde{M}_x^{x-y} = \left(\sum_{p \text{ even}}^{y} \binom{y}{p} m^{y-p} \frac{\delta^p}{p+1}\right)^{x-y}.$$

This can be true only if the leading order is, for every x, the one with p = 0, because this is the only term in common to all the x. This term is the leading one if:

$$|m|^x > |m|^{x-p} \frac{|\delta|^p}{p+1} \binom{x}{p} \quad \forall p.$$

Using the Stirling's approximation:

$$\left|\frac{m}{\delta}\right|^p > \binom{x}{p}\frac{1}{p+1} \sim \frac{1}{(p+1)\sqrt{2\pi}}\sqrt{\frac{x}{(x-p)p}}\frac{x^x}{(x-p)^{x-p}p^p}$$

The rhs is maximized for $p \sim x/2$, so, supposing $m > \delta$ (this will be consistent with the conclusions), if we demonstrate this expression for this value, it will be always demonstrated. Thus we obtain:

$$\left|\frac{m}{\delta}\right|^{\frac{x}{2}} > \frac{1}{\frac{x}{2}+1}\sqrt{\frac{2}{\pi x}} \ 2^{x} \Rightarrow \left|\frac{m}{4\delta}\right|^{\frac{x}{2}} > \frac{1}{\frac{x}{2}+1}\sqrt{\frac{2}{\pi x}}.$$

Changing notation to $m = -\frac{\mu}{2t}$ and $|\delta| = \frac{|\delta_{\mu}|}{2t}$:

$$\Rightarrow \left|\frac{\mu}{4\delta_{\mu}}\right|^{\frac{x}{2}} > \frac{1}{\frac{x}{2}+1}\sqrt{\frac{2}{\pi x}}.$$

In order to be the last expression valid for all the values of x, it is necessary that (for positive values of μ and δ_{μ}) $\mu/(4\delta_{\mu}) > 1$. Being, the rhs of the previous expression always < 1, we have our condition:

$$\delta_{\mu} < \frac{\mu}{4} \Rightarrow \sigma_{\mu} < \frac{\mu}{4\sqrt{3}}.$$
(47)

This is the domain within which our approximation is expected to work. Under this condition, we have demonstrated that:

$$\tilde{M}_x \sim \tilde{M}_y^{x-y} \sim \tilde{M}_{x-z}^z.$$

So, from (42), it is:

$$\tilde{M}_1^{\alpha_1} \cdot \tilde{M}_2^{\alpha_2} \cdot \ldots \cdot \tilde{M}_{k-1}^{\alpha_{k-1}} \cdot \tilde{M}_k^{\alpha_k} \sim \tilde{M}_k$$

If we suppose that all the α_i are finite or very small if compared to n, we conclude that the order of the term (43) is given by the factor (46). So, summing over all the combinations of α_i , we will just consider the greatest terms. This is simple, because for every value of k, the value of γ which maximizes the factor (46) is $\gamma = \alpha_1 + \alpha_2$ with $\alpha_1 = k - 2$ (let's remember that it must be $\alpha_1 \neq k$), and $\alpha_2 = 1$, setting all the other α_i to zero. This choice will, in fact, satisfy both the conditions in (42). So we can rewrite (43) as:

$$\frac{(n-1)!}{(n-k)!} \cdot \frac{\tilde{M}_2}{2} \cdot \frac{\tilde{M}_1^{k-2}}{(k-2)!} = \frac{n-1}{2} \tilde{M}_2 \frac{(n-2)!}{[(n-2)-(k-2)]!(k-2)!} \tilde{M}_1^{k-2}$$

Summing over all the values of k and remembering that $\tilde{M}_k = M_k + m^k$ and $\tilde{M}_1 = m$, we finally obtain:

$$\frac{n-1}{2}(m^2 + M_2) \sum_{k=2}^{\nu} \binom{n-2}{k-2} m^{k-2} = \frac{n-1}{2}(m^2 + \sigma^2) \sum_{k'=0}^{\nu-2} \binom{n-2}{k'} m^{k'},$$
(48)

with k' = k - 2. We are interested only on the part of this expression which will annihilate in absence of disorder, that is for $\sigma = 0$. Moreover, we must find also the disorderdependent part associated to the second term appearing in (37):

$$m_{1}\left[1+\sum_{i=3}^{n-1}m_{i}+\sum_{i_{i}=5}^{n-1}\sum_{i_{2}=3}^{i_{1}-2}m_{i_{1}}m_{i_{2}}+\sum_{i_{1}=7}^{n-1}\sum_{i_{2}=5}^{i_{1}-2}\sum_{i_{3}=3}^{n}m_{i_{1}}m_{i_{2}}m_{i_{3}}+\ldots\right]$$
$$+\sum_{i_{1}=2\nu-1}^{n-1}\sum_{i_{2}=2\nu-3}^{i_{1}-2}\dots\sum_{i_{\nu-1}=3}^{i_{\nu-2}-2}m_{i_{1}}m_{i_{2}}\dots m_{i_{\nu-1}}\right].$$

Fortunately, it is almost identical to the first term. We can thus finally write:

$$g_n(\mu,\sigma) \sim \frac{n-1}{2} \sigma^2 \sum_{k=0}^{\nu-2} \binom{n-2}{k} m^k + m_1 \frac{n-3}{2} \sigma^2 \sum_{k=0}^{\nu-3} \binom{n-4}{k} m^k$$
(49)

Being these two quantities almost identical, in the following we will again first work out just the (48) and then extend the treatment to the second term.

4.2.3 Condition of convergence

In the expression (48), we can rewrite the binomial coefficient as:

$$\binom{n-2}{k} = \binom{\nu-2}{k} \frac{(n-2)(n-3)\dots(\nu-1)}{(n-2-k)(n-3-k)\dots(\nu-1-k)}$$
$$\approx \binom{\nu-2}{k} \frac{(n-2)\dots(n/2-1)}{(n-2-k)\dots(n/2-1-k)},$$

where we assumed n even, that is $\nu = n/2$ in order to simplify the notation from now on. The case n odd can be treated identically with the difference that $\nu = (n-1)/2$. As we now, the difference -1/2 between these two quantities won't affect the result in the thermodynamic limit. Going on, the quantity above is equal to:

$$\binom{\nu-2}{k}\prod_{x=2}^{n/2+1}\left(\frac{n-x}{n-x-k}\right) = \binom{\nu-2}{k}\exp\left(\sum_{x=2}^{n/2+1}\log\left(\frac{n-x}{n-x-k}\right)\right).$$

We can manipulate the exponent:

$$\sum_{x=2}^{n/2+1} \log\left(\frac{n-x}{n-x-k}\right) = \sum_{x=2}^{n/2+1} \log(n-x) - \sum_{x=2}^{n/2+1} \log(n-x-k)$$

Let's Taylor expand the second logarithm around k = 0:

$$\log(n-x-k) = \log(n-x) - \frac{1}{n-x} \cdot k - \frac{1}{2} \frac{1}{(n-x)^2} \cdot k^2 - \frac{1}{3!} \frac{2}{(n-x)^3} k^3 - \dots = \log(n-x) - \sum_{a=1}^{\infty} \frac{1}{a} \left(\frac{k}{n-x}\right)^a$$

Being the maximum value of k and the minimum value of n - x:

$$k_{\max} = \frac{n}{2} - 2, \quad (n - x)_{\min} = \frac{n}{2} - 1,$$

we can assume k/(n-x) < 1 and:

$$\sum_{a=1}^{\infty} \frac{1}{a} \left(\frac{k}{n-x}\right)^a < \sum_{a=1}^{\infty} \left(\frac{k}{n-x}\right)^a = \frac{1}{1-\frac{k}{n-x}} - 1 = \frac{k}{n-x-k} \Rightarrow$$
$$\sum_{x=2}^{n/2+1} \log\left(\frac{n-x}{n-x-k}\right) < k \sum_{x=2}^{n/2+1} \frac{1}{n-x-k} < k \sum_{x=2}^{n/2+1} \frac{1}{n-x} = k \left[\psi(n-1) - \psi(n/2-1)\right],$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the gamma function. Taking the thermodynamic limit for $n \to \infty$:

$$k[\psi(n-1) - \psi(n/2 - 1)] \rightarrow k \log 2.$$

Going back to the coefficient, this means that:

$$\binom{n-2}{k} = \binom{\nu-2}{k} \exp\left(\sum_{x=2}^{n/2+1} \log\left(\frac{n-x}{n-x-k}\right)\right) < \binom{\nu-2}{k} e^{k\log 2} = \binom{\nu-2}{k} 2^k.$$

And

$$\frac{n-1}{2}\sigma^2 \sum_{k=0}^{\nu-2} \binom{n-2}{k} m^k < \frac{n-1}{2}\sigma^2 \sum_{k=0}^{\nu-2} \binom{\nu-2}{k} (2m)^k = \frac{n-1}{2}\sigma^2 (2m+1)^{\nu-2},$$

which, in the thermodynamic limit, converges only if:

$$|2m+1| = \left|\frac{\mu}{t} - 1\right| < 1 \Rightarrow 0 < \frac{\mu}{t} < 2$$
(50)

and converges to 0. This means that, when both the conditions (47) and (50) are satisfied, the disordered part of $f_n(\mu, \sigma)$, that is $g_n(\mu, \sigma)$, vanishes. Being the not-affected-bydisorder part of $f_n(\mu, \sigma)$ null for $\mu > 0$, we find that the two eigenvalues coincide and there are two MZM. These results are proven by the simulations, as can be seen by figure 15.



Figure 15: The figure is a particular of the topological phases diagram 10 for the r = 2 extended Kitaev chain with $\Delta = w = t$. As in the aforementioned figure, blue dots mark the topological phase with one MZM, yellow dots with two MZMs. The green line corresponds to $\mu = 4\sqrt{3}\sigma_{\mu}$. Above this line, the condition (47) is satisfied. It is remarkable that the topological phase with one MZM arises from and beyond this line.

5 Conclusions

5.1 Overview

In this work we studied the effects of the disorder on the system known as the extended Kitaev chain (EKC). In the first chapter the Kitaev chain was presented, the reasons that led to its conception, that is the possibility of performing fault-tolerant quantum computing, and its main properties. In the second chapter the EKC was introduced, which differs from the original system in that the parametric coupling, both superconducting and hopping, also extends to non-adjacent fermionic sites, and decays in the chain with an exponential law.

In both chapters the problem of determining the domain of the topological order has been formalized, i.e. under which choice of parameters the existence of the Majorana unpaired zero energy modes is allowed, which are the essential ingredients for the aforementioned application to quantum computation. Furthermore, the transfer matrix, deriving from the Bogoliubov-de Gennes equations, was defined as a powerful means to obtain some information about the system.

The same tool was the protagonist of chapter 3, in which we used it to set up simulations regarding the topological phases of the EKC when adding disorder as an ingredient of the system. These simulations support, in their modesty, the engineering perspectives of the extended Kitaev chain for applications to quantum computation. In fact, it has been observed that the presence of disorder, regardless of the number of neighbors involved in the parametric coupling, not only does not compromise, within a certain threshold, the presence of MZMs, but also broadens the conditions of existence defined in equations (13). This may suggest that the inherent complexity of Nature beyond mathematical models and noise, which generally acts in antagonism to applications where precision is needed, could actually be aiding in the implementation of the much-desired fault-tolerant quantum computing and in the development of the Kitaev chain, or of a system inspired by it, as a topological qubit.

In the same chapter, moreover, we investigated the effects of the decay exponents of the coupling parameters and we qualitatively observed that they play an important role in the formation of the topological phases, noting that they tend to reduce them, even suppressing the phases with more than one MZM, when are less than 1, a value where the topological order reaches a minimum of extension. Beyond this point. the growth of the exponents makes the topological phase tend to that of the original Kitaev chain in disorderly conditions.

Finally, in the chapter 4, a calculation has been proposed for the analytic determination of a part of the phase diagram for the homogeneous disordered EKC in the simplifying case $w = \Delta$. The calculation first of all ensures that, by using the transfer matrices, already known results are obtained (see eq. (34)). Then, in the second part, some approximations are exploited to show that, for small values of the disorder, the topological phase with two MZMs and its conditions of existence are preserved. In particular, we have exploited the calculations considering a box distribution. This calculation helped us to partially verify the reliability of the simulations made in the previous chapter. With this aim, we hope that the calculation could also be extended to higher values of the disorder, with the prospect of being able to analytically derive the entire topological phase with two MZMs.

5.2 Future perspectives

As already said previously, a natural continuation of the work here present can be to try to develop the analytical calculation proposed in the chapter 4, in such a way as to recover the dividing line between the two MZM phase and the other phases for higher values of disorder, if not even the entire phase diagram of the r = 2 disordered homogeneous EKC for $w = \Delta$. Furthermore, we do not exclude that we can start from here to propose a similar calculation for the same EKC but with $r \geq 3$, that is, with coupling parameters involving three neighbors or more.

In addition to this, a work consequent to that addressed in the chapter ref would concern the development of other analytical and simulation methods to find new confirmation of the results of the simulations presented by us, in such a way as to validate the method of transfer matrices, in the modalities applied by us, as an efficient method for the study of disordered EKCs.

If we want to talk about new frontiers in which this method can be applied, it would be natural to continue to complicate the EKC trying to make it more and more likely as a real system, for example considering both the disorder and the role of interactions^{37 38 39} between fermions, of which a study for the chain of Kitaev, i.e. for r = 1, has already been addressed by Gergs, Fritz and Schuricht².

It is in fact our supposition and hope that superconducting chains continue to resist theoretical and experimental tests that attempt to refute the presence of MZMs and compromise their applicability to fault-tolerant quantum computing, so that, one day, they can finally be developed and used for this task.

A Appendices

A.1 Symmetries

A.1.1 Time reversal symmetry

Time reversal symmetry ⁴⁰ means invariance under the transformation $t \rightarrow -t$. In general, if one want to know the time-evolution of a quantum-mechanical state, he needs to look at the time-dependent Schrödinger equation.

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = \mathcal{H}\psi$$

which is satisfied by a time-dependent wave function of the form

$$\psi(\boldsymbol{r},t) = e^{\frac{-\mathrm{i}\mathcal{H}t}{\hbar}}\psi(\boldsymbol{r},0),$$

where $\exp[-i\mathcal{H}t/\hbar]$ is the time evolution factor. The effect of time reversal $t \to -t$ (which we denote by the operator \mathcal{T}) on the wave function is that of complex conjugation $\psi \to \psi^*$ so that

$$\mathcal{T}\psi(r,t) = \psi(r,-t) = \psi^*(r,t).$$

Two important properties of the time reversal operator \hat{T} are:

a) Energy conservation: $[\mathcal{T}, \mathcal{H}] = 0$. Because of energy conservation, the time reversal operator \mathcal{T} commutes with the Hamiltonian $\mathcal{TH} = \mathcal{HT}$. Since \mathcal{T} commutes with the Hamiltonian, eigenstates of the time reversal operator are also eigenstates of the Hamiltonian.

b) Anti-linearity: $\mathcal{T}i = -i$. From Schrödinger's equation, it is seen that the reversal of time corresponds to a change of $i \to -i$, which implies that $\mathcal{T}i = -i$. An operator is called antilinear if its operation on a complex number yields the complex conjugate of the number $\mathcal{T}a = a^*$ rather than the number itself.

The time reversal operator applies to particle operators as follows:

$$\mathcal{T}c_j^{\dagger}\mathcal{T}^{-1} = c_j^{\dagger}, \quad \mathcal{T}c_k^{\dagger}\mathcal{T}^{-1} = c_{-k}^{\dagger}$$

From what we have seen so far, it can be deduced that, if we apply the time reversal operator and its the energy conservation property to one-particle Hamiltonians such as those of eqs. (1) and (12), thus having the form:

$$H = \begin{pmatrix} c_{j_1}^{\dagger} & \dots & c_{j_L}^{\dagger} & c_{j_1} & \dots & c_{j_L} \end{pmatrix} \mathcal{H} \begin{pmatrix} c_{j_1} \\ \vdots \\ c_{j_L} \\ c_{j_1}^{\dagger} \\ \vdots \\ c_{j_L}^{\dagger} \end{pmatrix}$$

we find $\mathcal{THT}^{-1} = \mathcal{H}$; but \mathcal{H} is a matrix made of scalars, so, from the anti-linearity property on finds $\mathcal{THT}^{-1} = \mathcal{H}^*\mathcal{TT}^{-1} = \mathcal{H}^*$, which gives the condition on \mathcal{H} for time-reversal symmetry:

$$\mathcal{H} = \mathcal{H}^*.$$

In order to have a time-reversal-symmetric system, the entries of \mathcal{H} must be real. This property is verified for all the Hamiltonians considered in this work.

Generally, in extending the Kitaev chain and defining the EKC, it is usual¹ to consider first Hamiltonians which do not present time-reversal symmetry, and therefore have complex coefficients, of the type:

$$H = -\sum_{j=1}^{L} \mu \left(c_{j}^{\dagger} c_{j} - \frac{1}{2} \right) + \sum_{\ell=1}^{r} \sum_{j=1}^{L-\ell} \left(-w_{\ell} e^{i\phi_{\ell}} c_{j}^{\dagger} c_{j+\ell} + \Delta_{\ell} c_{j} c_{j+\ell} + \text{ h.c. } \right),$$

of which, in fact, the one studied in eq. (12) is a special case for $\phi = 0$.

A.1.2 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 $^{41} P$ through

$$\mathcal{P}c_j^{\dagger}\mathcal{P}^{-1} = c_j, \quad \mathcal{P}c_k^{\dagger}\mathcal{P}^{-1} = c_{-k},$$

where the transformation of the Fourier-transformed operator comes from the definition in eq. (8).

One can show that P is antilinear too and that anticommutes with Hamiltonians \mathcal{H} which presents this symmetry:

$$\mathcal{PHP}^{-1} = -\mathcal{H}$$

For example, one can verify it very easily applying the parity-hole transformation to the Kitaev Hamiltonian H defined in equation (1). It is easy, remembering the anticommutation laws of fermionic operators, to see that the coefficients of the Hamiltonian, and thus the Bogoliubov-de Gennes Hamiltonian \mathcal{H} , change sign.

Because of the minus sign in the particle-hole symmetry, the spectrum of \mathcal{H} must be symmetric around zero energy in order to show particle-hole invariance.

class	\mathcal{C}	\mathcal{P}	\mathcal{T}	d = 0	1	2	3	4	5	6	7
Α				\mathbb{Z}		\mathbb{Z}		\mathbb{Z}		\mathbb{Z}	
AIII	1				\mathbb{Z}		\mathbb{Z}		\mathbb{Z}		\mathbb{Z}
AI			1	\mathbb{Z}				$2\mathbb{Z}$		\mathbb{Z}_2	\mathbb{Z}_2
BDI	1	1	1	\mathbb{Z}_2	\mathbb{Z}				$2\mathbb{Z}$		\mathbb{Z}_2
D		1		\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}				$2\mathbb{Z}$	
DIII	1	1	-1		\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}				$2\mathbb{Z}$
AII			-1	$2\mathbb{Z}$		\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}			
CII	1	$^{-1}$	-1		$2\mathbb{Z}$		\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}		
С		$^{-1}$				$2\mathbb{Z}$		\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	
\mathbf{CI}	1	$^{-1}$	1				$2\mathbb{Z}$		\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}

Figure 16: The periodic table of topological insulators.²⁹

For completeness, we introduce the combined operator $C = \mathcal{P} \circ \mathcal{T}$, the so-called chiral symmetry operator. Necessarily, a chiral symmetry can only be present, if both of the aforementioned symmetries are fulfilled or both are absent.

All the aforementioned symmetries are demonstrated ^{42 29} to classify topological insulators and superconductors in a periodic table, reported in figure 16. In the Altland-Zirnbauer classification³⁰, the EKC studied in eq. (12) falls in the *BDI* class for the one-dimensional systems which presents all the three symmetries. The associated topological classification is \mathbb{Z} , which is the domain which the topological invariants of these systems belong to. Indeed, the time reversal symmetry breaking system of the last paragraph, defined for $\phi \neq 0$, belongs to the *D* class, corresponding to a \mathbb{Z}_2 topological classification: this means that the topological invariant can only assume two values. In fact, for this kind of system it is impossible¹⁹ to define the winding number (10).

A.2 Numerical methods

The transfer matrix method applied throughout the thesis bases its correctness mainly on the self-averaging properties of very long chains. This made it possible to obtain, with particular reference to the graphs of chapter 3, pretty defined simulations without the need to mediate on different runs, thus giving the advantage of not having to specify whether the disorder considered was *quenched* or not.

In observing the simulations, however, it can be seen that, as the disorder increases, the boundary of the topological phase is blurred. This is due to the fact that the self-averaging property, as well as the criterion for determining the number of MZMs based on the convergence of the eigenvalues, theoretically require infinitely-long chains. Obviously, this is impossible to deal with and the theory must come to terms with the practical needs of simulations. In our calculations, for example, we considered chains of 500 fermionic sites or more, where the number 500 was a good compromise between the need for short



Figure 17: Topological positive chemical potentials for r = 2, $\Delta = w_0$ with (a) L = 1000 sites and a float precision of 300 decimal points; (b) L = 500 and 1000 decimal points. Confronting these figures with figure 10 (b), it is evident that (a) is more defined and less confused on the edge of the topological phase for high values of the disorder.

run times and the observability of fairly defined topological phase boundaries. With this choice, however, for large disorders the boundaries of the topological phases are sometimes confused. This problem can in fact be solved if we consider a greater number of fermionic sites. An example of this is provided by figure 17 (a).

The simulations has been performed by using Python. Unfortunately, this programming language and, in particular, its library for scientific calculations are not optimized for performing operations between matrices. A multiplication of a few hundred matrices generally leads to a fatal loss of precision, which results in false convergences to zero and false divergences in the entries of the product matrices and their eigenvalues. To solve this issue we used the *mpmath*⁴³ library, which is a free Python library for real and complex floating-point arithmetic with arbitrary precision. In our simulations, we generally worked with setting the float precision to 300 decimal places. This made it possible not to lose precision in the calculations. It can be observed that increasing the precision for the same length of the chain, the resolution and the domain of the topological phase won't change significantly (see fig. 17 (b)), giving out, one more time, better results.

The method applied to our simulations was to define the random transfer matrices for the points of the plane (σ, μ) (normalized with respect to w_0), multiply them, calculate the eigenvalues and verify the criterion of existence of the MZMs. Depending on the number of MZMs that existed, a color marker defined for the different topological phases was plotted at the point of the plane under investigation.

A.3 Formal derivation of eq. (33)

We define the transfer matrix

$$A_i = \left(\begin{array}{cc} -1 & \frac{\mu_i}{2w} \\ 1 & 0 \end{array}\right)$$

Let's consider $\tilde{A}_n = A_n A_{n-1} \cdots A_2 A_1$, then we want to calculate it's trace. We define $a_i = \frac{\mu_i}{2w}$. There is the multiplication law

$$A_2A_1 = \text{diag}(a_2, a_1) - A_1$$

where diag (a_2, a_1) is the diagonal matrix with elements a_2 and a_1 . We consider the product $A_n A_{n-1} \cdots A_2 A_1$, for *n* even. By using the multiplication law, we get:

$$A_n A_{n-1} \cdots A_2 A_1 = d_{n,1} - A_n d_{n-1,1} - A_{n-1} d_{n-2,1} - \dots - A_3 d_{2,1} - A_1,$$

where $d_{2,1} = \operatorname{diag}(a_2, a_1)$, $d_{3,1} = \operatorname{diag}(a_3, a_1)$, $d_{4,1} = \operatorname{diag}(a_4, a_1) + \operatorname{diag}(a_4, a_3) \operatorname{diag}(a_2, a_1)$ and so on. In general $d_{i,1}$ is the diagonal matrix obtained by summing all the products of the form $\operatorname{diag}(a_i, a_{i_k}) \operatorname{diag}(a_{i_k-1}, a_{i_{k-1}}) \cdots \operatorname{diag}(a_{i_1-1}, a_1)$ where $i_j > i_{j-1} + 1$ and $i_1 > 2$. We aim to calculate the eigenvalues of $\tilde{A}_n = A_n A_{n-1} \cdots A_2 A_1$. The trace is

$$\operatorname{Tr}\left(\tilde{A}_{n}\right) = \operatorname{Tr}\left(d_{n,1}\right) - \operatorname{Tr}\left(A_{n}d_{n-1,1}\right) - \operatorname{Tr}\left(A_{n-1}d_{n-2,1}\right) - \cdots - \operatorname{Tr}\left(A_{3}d_{2,1}\right) - \operatorname{Tr}\left(A_{1}\right).$$

We have that $\operatorname{Tr}(A_i \operatorname{diag}(c, d)) = -c$, thus we get

$$\operatorname{Tr}\left(\tilde{A}_{n}\right) = \operatorname{Tr}\left(d_{n,1}\right) + d_{n-1,1}^{1} + d_{n-2,1}^{1} + \dots + d_{2,1}^{1} + 1,$$

where d^1 is the element (1,1) of the diagonal matrix d. In particular

$$d_{i,1}^1 = \sum_l \tilde{a}_{i,l}^1$$

where $\tilde{a}_{i,l}^1$ are all the products of the upper endpoints of the noncrossing partitions of $(a_i, a_{i-1}, \dots, a_1)$ with at least two elements, e.g., the noncrossing partitions of $(a_5, a_4, a_3, a_2, a_1)$ are $(a_5, a_4, a_3, a_2, a_1)$, $(a_5, a_4) \cup (a_3, a_2, a_1)$ and $(a_5, a_4, a_3) \cup (a_2, a_1)$, then $d_{5,1}^1 = a_5 + a_5a_3 + a_5a_2$. We get the relation

$$d_{i,1}^1 = a_i \left(1 + d_{i-2,1}^1 + d_{i-3,1}^1 + \dots + d_{2,1}^1 \right).$$

By defining $\tilde{a}_{i,l}^2$ as all the products of the lower endpoints, we get

$$d_{i,1}^2 = \sum_l \tilde{a}_{i,l}^2$$

and

$$\mathrm{Tr}\,(d_{i,1}) = d_{i,1}^1 + d_{i,1}^2.$$

The trace is

$$\operatorname{Tr}\left(\tilde{A}_{n}\right) = 1 + \sum_{i=1}^{n} a_{i} + \sum_{j=4}^{n} \sum_{i=2}^{j-2} a_{j}a_{i} + a_{1} \sum_{i=3}^{n-1} a_{i} + \cdots,$$

where we have omitted products with more than two terms. Replacing a_i with $-m_i$, one gets eq. (33).

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