

Impact of dissipation on the topological phase of the Kitaev chain

Auteur : Wilmotte, Nils

Promoteur(s) : Damanet, François

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IMPACT OF DISSIPATION ON THE TOPOLOGICAL PHASE OF THE KITAEV CHAIN

NILS WILMOTTE
SUPERVISOR: FRANÇOIS DAMANET



FACULTY OF SCIENCES
PHYSICS DEPARTMENT

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1 Introduction

Nowadays, a bunch of physical systems have been proposed to perform quantum computing such as trapped ions or superconducting qubits [1]. Unfortunately, the inherent coupling of these physical systems, constituting the qubits, with an external environment inevitably leads to dissipation and decoherence [2]. Hence, errors in the algorithms occur due to the vanishing of the memory stored in these states and the suppression of quantum superposition and entanglement across time. To attain fault-tolerance in quantum computing, several proposals of large-scale error correcting codes [3] or intrinsically bias-protected qubit [4] emerged along with their challenges in the hardware scalability and the implementation of gate operations, notably because those ways of implementing error protection and corrections require the use of many additional auxiliary qubits beyond the scope of current quantum computers.

Yet, low-dimensional (1D or 2D) topological phase of matter hosting quasiparticles excitations, known as non-Abelian anyons (not bosons, nor fermions), as collective fermionic modes seem to be a privileged candidate to perform quantum computing. Indeed, the information being encoded non-locally in the system's collective modes should make it naturally resilient against local noise. Furthermore, unitary gates based on the non-Abelian braiding statistics of the quasiparticles are less prone to errors, as long as perturbations do not affect the topology of quasiparticles' worldlines during the exchange [5, 6]. These two aspects of noise-resilience are known as the 'topological protection' of the encoded qubits and give rise to a parallel fault-tolerant quantum computing framework known as 'topological quantum computing'. While such non-Abelian anyons have been predicted in several topological phases of matter such as fractional quantum Hall effect [7, 8] and spin liquids [9], we focus on zero-energy collective modes known as *Majorana zero modes* (MZMs) occurring in topological insulators and superconductors [10, 11]. In these systems, two MZMs compose a delocalized zero-energy fermionic mode, called the *Majorana bound state* (MBS), which occupation can be used to build a logical qubit [5, 12]. These MZMs have been predicted, first, to appear in 2D p -wave superconductors at vortices [10] and then, at the edges of a 1D p -wave superconductor spinless fermionic chain, now known as the Kitaev chain [13]. The MZMs non-Abelian exchange statistics have been proven in both 2D [14] and 1D [15] schemes.

Whereas information stored in the Kitaev chain is usually considered topologically protected against noise due to its non-local encoding and the fermion parity conservation [13], this resilience can actually fail in some regimes when interactions with external environments (baths) are considered [16]. Hence, performing studies on the dissipative dynamics of topological systems such as the Kitaev chain through open quantum system approaches, which is the topic of this MSc thesis, is more than relevant. Dissipation and decoherence sources have already been widely surveyed: for examples, in the context of topological qubits, it has been shown that qubit memory undergoes a finite or complete exponential decay when considering both static and oscillating tunneling with a gapped fermionic environment [17], that quantum memory robustness against small perturbations in the chemical potential scales exponentially with the chain length but that this scalability is suppressed when we add quasiparticle poisoning [18], that the decoherence of the topological qubit due to the coupling with a gapped fermionic bath mediated by bosons (phonons) is exponentially suppressed at low temperature [19], that non-Markovian interaction with local charge fluctuations induces decoherence of the MBS but that, at sufficiently low temperature/charge fluctuations, coherences are weakly protected [20] and that qubit coherence and fermion parity under braiding operations decay due to charge fluctuation [21].

However, while all of these works focus on specific environments and particular experimental schemes, to the best of our knowledge, no general framework has yet been proposed to model the interaction between a Kitaev chain and a fermionic bath. This constitutes the main objective of this MSc thesis. We develop a general framework based on the GKSL master equation formalism [22] to investigate the impact of weak dissipation on the topological phase of the Kitaev chain, with applications to topological quantum computing. While our results are obtained for

a specific spectral density of the baths, the latter can be easily replaced to model other type of fermionic environment interaction. Although our analysis is currently limited to small chains, i.e., chains which are not topological since the topological properties of a Kitaev chain are rigorously defined only in the thermodynamic limit of an infinite number of sites, the results we obtain are systematic and can be generalized to larger systems. Furthermore, these results are of particular interest given that small Kitaev chains have recently been realized experimentally [23, 24].

This MSc thesis is structured as follows. The first part, entitled 'The Closed Part', begins with Section 2, where we review the fermionic tools required to develop the theory of the Kitaev chain, including second quantization and the theory of quadratic Hamiltonians. Next, Section 3 applies these tools to the BCS theory of superconductivity in order to familiarize the reader with superconducting systems, the Kitaev chain itself being a toy model of non-trivial superconductivity. Finally, this first part concludes with Section 4, which introduces the Kitaev model. We first establish its connection with superconductivity before defining its topological phase and the associated occupation of an MBS. The relevance of the Kitaev chain for topological quantum computing is then discussed, and the section concludes with an important introduction to finite-size effects together with the tools required to characterize topology in finite systems.

The second part, entitled 'The Open Part', begins with an introduction to open quantum systems. In this section, we introduce the notions of density operators and the interaction picture, which allow us to derive microscopically the GKSL master equation. We then introduce the concepts of thermal fermionic baths and spectral densities, which serve as the basis for the derivation of the master equations used throughout this work. Next, in Section 6, we apply this formalism to the study of a dissipative 2-site Kitaev chain. We investigate the impact of dissipation on both its topological properties and its transient dynamics by varying the baths temperature and the width of the Lorentzian spectral density. Although such a short chain is not directly relevant for quantum computing applications, the physical mechanisms identified in this minimal model can be generalized to larger dissipative chains. This generalization is carried out in Section 7. Finally, the main results and perspectives of this work are summarized in Section 8.

Part I

The Closed Part

2 Fermions

To properly address dissipation in the Kitaev chain, a solid understanding of fermionic physics is essential. Therefore, this section begins by introducing fermions through their characteristic exchange statistics. Then, we present the formalism of second quantization and the associated mathematical tools required to describe fermionic systems. This framework forms the foundation of the analysis developed throughout this work.

2.1 Exchange statistics

In quantum mechanics, a system of identical particles behaves differently than in classical mechanics. Indeed, while it is possible to 'number' a particle at all time in a classical system, this becomes impossible in quantum mechanics. This phenomenon comes from the *uncertainty principle* [25] which implies that the concept of the path of a particle completely lose its meaning. Hence, in a system of multiple identical particles, a single particle becomes untractable and lose all its 'individuality'. This principle is called the *indistinguishability of identical particles*. A system of N identical particles must, then, be described by a global wavefunction $\Psi(\xi_1, \dots, \xi_N) \in \mathcal{H}_N$, where $\mathcal{H}_N$ is the N -particle Hilbert space and $\{\xi_i : i = 1, \dots, N\}$ denotes the spatial coordinates and the spin projection for each particle. Recall that each particle carries an additional discrete degree of freedom called *spin*, denoted by s . Spin is an intrinsic angular momentum whose projection onto a chosen axis is quantized. The corresponding magnetic quantum number m_s can take $2s + 1$ distinct values ranging from $-s$ to s . In particular, electrons are spin- $\frac{1}{2}$ particles and therefore possess two possible spin states, $m_s = \pm\frac{1}{2}$, commonly denoted by $\uparrow$ and $\downarrow$.

Let's consider a system of two identical particles described by the wavefunction $\Psi(\xi_1, \xi_2)$. Since the particles are identical, the exchange of the two must not affect the physicality of the system, *i.e.*, the wavefunction can only change with a trivial phase factor as

$$\Psi(\xi_1, \xi_2) = e^{i\alpha} \Psi(\xi_2, \xi_1). \quad (2.1)$$

Performing twice the exchange, we obtain that $e^{2i\alpha} = 1$, or similarly that $e^{i\alpha} = \pm 1$, leading us to the two possible choices for the exchange behavior of the wavefunction:

$$\Psi(\xi_1, \xi_2) = \pm \Psi(\xi_2, \xi_1). \quad (2.2)$$

If the wavefunction is unchanged, it is called *symmetrical*, while if it changes sign, it is called *antisymmetrical*. This reasoning can be generalized for an arbitrary number of identical particles by imposing that all exchange between two particles must obey to the same exchange behavior (either symmetrical or antisymmetrical). Particles described by symmetrical wavefunction obey *Bose-Einstein statistics* and are named *bosons* and particles described by antisymmetrical wavefunction obey *Fermi-Dirac statistics* and are named *fermions*. It is worth noting that for a multiparticle fermionic state, the exchange statistics depend on the parity of the two-particle permutation: even parity leaves the wavefunction unchanged, whereas odd parity introduces a minus sign. In the following, we will only focus on fermionic particles since all physical states described in this Master's thesis will present fermionic statistics.

The general wavefunction of a system of N identical fermions is given by the *Slater determinant*,

$$\Psi(\xi_1, \dots, \xi_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{k_1}(\xi_1) & \psi_{k_1}(\xi_2) & \dots & \psi_{k_1}(\xi_N) \\ \psi_{k_2}(\xi_1) & \psi_{k_2}(\xi_2) & \dots & \psi_{k_2}(\xi_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{k_N}(\xi_1) & \psi_{k_N}(\xi_2) & \dots & \psi_{k_N}(\xi_N) \end{vmatrix}, \quad (2.3)$$

where $\{\psi_{k_i} : i = 1, \dots, N\}$ is a basis of the fermionic single-particle Hilbert space $\mathcal{H}_1$ and the indices k_i refer to the quantum state of the particle. From this determinant, it is straightforward

to see that two fermions cannot be in the same state with the same coordinates, otherwise the wavefunction would vanish (the determinant becomes null). This is known as the *Pauli's exclusion principle*.

2.2 Second quantization

For an isolated system of non-interacting particles, the occupation number of a quantum state k_i is conserved and the wavefunction (2.3) is relevant to describe the system, however if interaction between particles is considered the occupation numbers can vary. Furthermore, when the system is coupled to a reservoir, the total number of particles in the system is usually not conserved. Hence, one needs a new mathematical framework to account for a grand canonical system of fermions.

This is performed by introducing the *Fock space* $\mathcal{F}$ defined as [26]

$$\mathcal{F} = \bigoplus_{N=0}^{+\infty} \mathcal{H}_N. \quad (2.4)$$

The Fock space $\mathcal{F}$ is itself a Hilbert space and a basis is given by the set of vectors $\{|n_0, n_1, n_2, \dots\rangle = |\mathbf{n}\rangle : \forall k, n_k = 0, 1\}$, with the orthonormality relation [25]

$$\langle n_0, n_1, \dots | n'_0, n'_1, \dots \rangle = \delta_{n_0 n'_0} \delta_{n_1 n'_1} \dots \quad (2.5)$$

A vector from this basis simply enumerates the number of particles, labeled by the index n_k , in each quantum state, or *mode*, k . Moreover, the vector $|0, 0, \dots\rangle \equiv |0\rangle$ belongs to $\mathcal{F}$ and represents the *vacuum state*, *i.e.*, no particle in any of the mode k of the system.

Once this basis is defined, we can introduce the *fermionic operators* $\hat{c}_k$ and $\hat{c}_k^\dagger$ which act on a basis state as

$$\hat{c}_k |n_0, n_1, \dots, n_k, \dots\rangle = (-1)^{S_k} n_k |n_0, n_1, \dots, n_k - 1, \dots\rangle, \quad (2.6)$$

$$\hat{c}_k^\dagger |n_0, n_1, \dots, n_k, \dots\rangle = (-1)^{S_k} (1 - n_k) |n_0, n_1, \dots, n_k + 1, \dots\rangle, \quad (2.7)$$

where¹ $S_k = \sum_{j=0}^{k-1} n_j$. The operator $\hat{c}_k$, which removes a particle from state k , is called the *annihilation operator*, while $\hat{c}_k^\dagger$, which adds a particle to state k , is called the *creation operator*. We see from (2.6) that $\hat{c}_k$ annihilates the vacuum state $|0\rangle$, for all k . This definition of the fermionic operators accounts for the antisymmetrical exchange statistics of the particles. From this, we can show the *canonical anticommutation relations* (CAR)

$$\{\hat{c}_k, \hat{c}_{k'}^\dagger\} = \hat{c}_k \hat{c}_{k'}^\dagger + \hat{c}_{k'}^\dagger \hat{c}_k = \delta_{kk'}, \quad (2.8)$$

$$\{\hat{c}_k, \hat{c}_{k'}\} = \{\hat{c}_k^\dagger, \hat{c}_{k'}^\dagger\} = 0, \quad (2.9)$$

for all k, k' , and define the *number operator* $\hat{n}_k = \hat{c}_k^\dagger \hat{c}_k$, such that $\hat{n}_k |\mathbf{n}\rangle = n_k |\mathbf{n}\rangle$.

Notice that the fermionic operators are defined for a specific discrete basis of $\mathcal{F}$, representing a set of discrete quantum states. However, there exist observables which are not always discrete but still are represented by Hermitian operators acting on the Fock space which eigenvectors form a continuous basis $\{|\xi_0, \xi_1, \dots\rangle\}$ with ξ_i any continuous variable, *e.g.*, the position. Such states are also associated with their continuous annihilation and creation operator, $\hat{\psi}(\xi)$ and

¹Notice here that S_k is defined for a specific ordering of the quantum states numbering in the basis vectors, hence the definition of the fermionic operators is itself 'ordering-dependent'. However, it shows no physical impact.

$\hat{\psi}^\dagger(\xi)$ called *field operators*. They are defined from the previous discrete fermionic operators as follows,

$$\hat{\psi}(\xi) = \sum_{k=0}^{+\infty} \psi_k(\xi) \hat{c}_k, \quad (2.10)$$

$$\hat{\psi}^\dagger(\xi) = \sum_{k=0}^{+\infty} \psi_k^*(\xi) \hat{c}_k^\dagger, \quad (2.11)$$

with $\psi_k(\xi)$ the single-particle wavefunction introduced in (2.3). The inverse relations are given by

$$\hat{c}_k = \int d\xi \psi_k(\xi) \hat{\psi}(\xi), \quad (2.12)$$

$$\hat{c}_k^\dagger = \int d\xi \psi_k^*(\xi) \hat{\psi}^\dagger(\xi), \quad (2.13)$$

where $\int d\xi$ is defined as the integral over the continuous variable of ξ and the sum over its discrete elements. From this, it can be shown that the field operators obey the continuous CAR,

$$\{\hat{\psi}(\xi), \hat{\psi}^\dagger(\xi')\} = \delta(\xi - \xi'), \quad (2.14)$$

$$\{\hat{\psi}(\xi), \hat{\psi}(\xi')\} = \{\hat{\psi}^\dagger(\xi), \hat{\psi}^\dagger(\xi')\} = 0. \quad (2.15)$$

The operator $\hat{\psi}^\dagger(\xi)$ creates a particle of continuous state ξ , whereas $\hat{\psi}(\xi)$ removes a particle of state ξ in the system. Acting on the continuous basis of $\mathcal{F}$, the density operator, defined as $\hat{\psi}^\dagger(\xi)\hat{\psi}(\xi)$, gives the probability density of having a particle of continuous state ξ .

This procedure of defining the Fock space $\mathcal{F}$ and the associated fermionic operators is known as *second quantization*. This formalism is embedded in the more general framework of *quantum field theory* where particles are described as excitations of underlying fields [27]. In this theory, fields are quantized and become operators, in analogy with the quantization of position and momentum in non-relativistic quantum mechanics. Furthermore, we can show that the wavefunction of a fermionic particle in quantum mechanics can be obtained from the Dirac field in the non-relativistic limit [28]. When the field is quantized, the wavefunction is promoted to an operator, resulting in the field operators $\hat{\psi}(\xi)$ and $\hat{\psi}^\dagger(\xi)$, hence the name *second quantization*. In the following, we will mainly work in the second quantization framework enabling us to drop the $\hat{\cdot}$ on operators.

2.3 Nambu spinors and quadratic Hamiltonian

Having defined the concept of second quantization, this section introduces the formalism required to describe systems with *fermionic quadratic Hamiltonians*. This framework provides the essential tools for treating particle-hole symmetric systems such as BCS superconductivity (see Section 3).

Indeed, superconducting theories are described by pairing Hamiltonians which natural excitations consist of collective modes. These modes can be seen as superpositions of particle and hole states. In the context of band theory in condensed matter physics, a particle is defined as an eigenmode of the generic operator $c^\dagger c$, while a hole is an eigenmode of $cc^\dagger$. For such particle-hole coupling theories, it is convenient to introduce the *Nambu spinors* $\mathbf{c}$ and $\mathbf{c}^\dagger$ [29–31], which simply consist in the concatenation of all fermionic operators of the system in one vector living in the

Nambu space. Hence, we define

$$\mathbf{c} = \begin{pmatrix} c_1 \\ \vdots \\ c_N \\ c_1^\dagger \\ \vdots \\ c_N^\dagger \end{pmatrix} \text{ and } \mathbf{c}^\dagger = \begin{pmatrix} c_1^\dagger & \cdots & c_N^\dagger & c_1 & \cdots & c_N \end{pmatrix}, \quad (2.16)$$

for an N -mode Fock space. Recall from (2.6) and (2.7) that fermionic operators are defined through their action on a given Fock basis. Hence, we can introduce a new set of fermionic operators, defined similarly on another basis, by performing the *fermionic transformation*²

$$\mathbf{c} \rightarrow \mathbf{a} = \mathbf{U}\mathbf{c}, \quad (2.17)$$

where $\mathbf{a} = \begin{pmatrix} a_1 & \cdots & a_N & a_1^\dagger & \cdots & a_N^\dagger \end{pmatrix}^T$ is the Nambu spinor associated with the new operators and $\mathbf{U}$ is a $2N \times 2N$ matrix. In order to preserve the CAR for a_k and $a_k^\dagger$, the transformation matrix $\mathbf{U}$ must be unitary [30], *i.e.*, $\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbb{1}$. The annihilation operators a_k define a new vacuum state $|\Omega\rangle \neq |0\rangle$, such that $a_k|\Omega\rangle = 0$ for all k . The new fermionic states are generated by acting with $a_k^\dagger$ on $|\Omega\rangle$, following (2.7) for all k .

When $\mathbf{U}$ mixes the original creation and annihilation operators in defining the new ones, the transformation is referred to as a *Bogoliubov-de Gennes (BdG) transformation*. As explained previously, fermionic excitations generated by $a_k^\dagger$ are superpositions of original particles and holes states. These quasiparticle excitations are known as *Bogoliubons* and $|\Omega\rangle$ is called the *Bogoliubov vacuum*. Such transformations play a central role in fermionic quadratic systems with pairing terms in the Hamiltonian.

The most general *fermionic quadratic Hamiltonian* for N fermions is defined as [30]

$$H = \sum_{i,j=1}^N \left(A_{i,j} c_i^\dagger c_j - A_{i,j}^* c_i c_j^\dagger + B_{i,j} c_i c_j - B_{i,j}^* c_i^\dagger c_j^\dagger \right), \quad (2.18)$$

where $\mathbf{A}$ is a Hermitian complex matrix and $\mathbf{B}$ is a skew-symmetric complex matrix, *i.e.*, $\mathbf{B}^T = -\mathbf{B}$. The expression of the Hamiltonian can be simplified in a *BdG form* by the use of the *Nambu spinors* as

$$H = \mathbf{c}^\dagger \mathbf{H} \mathbf{c}, \quad (2.19)$$

with

$$\mathbf{H} = \left(\begin{array}{c|c} \mathbf{A} & -\mathbf{B}^* \\ \hline \mathbf{B} & -\mathbf{A}^* \end{array} \right), \quad (2.20)$$

the *BdG Hamiltonian*³ of dimension $2N \times 2N$. In order to obtain the spectrum of eigenenergies and their associated eigenstates by diagonalizing this Hamiltonian, we need to find the adequate unitary matrix $\mathbf{U}$ to perform a BdG transformation (2.17) on the c_k modes. This transformation

²In this work the vector are noted as lowercase bold letters as $\mathbf{v}$, while matrices are noted as capital bold letters as $\mathbf{M}$.

³Loosely speaking, the term 'Hamiltonian' is used imprecisely here, since $\mathbf{H}$ is simply a matrix rather than an operator acting on the Fock space.

diagonalizes the BdG Hamiltonian:

$$H = \mathbf{c}^\dagger \mathbf{H} \mathbf{c}, \quad (2.21)$$

$$= \mathbf{a}^\dagger \mathbf{U} \mathbf{H} \mathbf{U}^\dagger \mathbf{a}, \quad (2.22)$$

$$= \mathbf{a}^\dagger \mathbf{H}_\Delta \mathbf{a}, \quad (2.23)$$

$$= \sum_{k=1}^N \epsilon_k \left(a_k^\dagger a_k - a_k a_k^\dagger \right), \quad (2.24)$$

where $\mathbf{H}_\Delta = \mathbf{U} \mathbf{H} \mathbf{U}^\dagger = \text{diag}(\epsilon_1, \dots, \epsilon_N, -\epsilon_1, \dots, -\epsilon_N)$ and $\epsilon_1 \geq \dots \geq \epsilon_N$ are the eigenenergies of the Bogoliubon excitations⁴.

The necessary tools introduced, let us now apply them to a quadratic fermionic theory: the *BCS theory of superconductivity*.

3 Superconductivity

Before introducing the Kitaev model, it is relevant to first review the quantum theory of superconductivity to give a concrete example of fermionic system that can be set in a quadratic form under some approximations, but also because the Kitaev Hamiltonian describes a particular superconducting system. This theory was formulated in 1957 by J. Bardeen, L.N. Cooper and J.R. Schrieffer [32], and is now known as the *BCS theory*. In this Section, we focus on how the *pairing Hamiltonian* is derived, but not on the macroscopic properties of such a system. This section is based on [33].

3.1 Cooper pairs

The main idea of the *BCS theory* is that, if an attractive interaction exists between electrons near the Fermi level E_F , electrons can bind together to form pairs, called *Cooper pairs*, with energy lower than E_F . Thus, the Fermi sea⁵ is no longer stable and a new state of matter arises, the superconductivity.

First, let us add two interacting electrons to a Fermi sea at temperature $T = 0$. We consider that they interact with the Fermi sea only through Pauli's exclusion principle. Given Bloch's arguments, the ground state of such a system should be given by a 2-particle wavefunction $\psi_0(\mathbf{r}_1, \mathbf{r}_2)$ of zero total momentum,

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \sum_{k > k_F} g_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_1} e^{-i\mathbf{k} \cdot \mathbf{r}_2}, \quad (3.1)$$

where k_F is the Fermi wavevector, and the two exponentials correspond to the single-particle basis for each electron. Since electrons are spin- $\frac{1}{2}$ particles, they obey Fermi-Dirac statistics and the ground state must be antisymmetric. This can be reflected in two ways: either the spin wavefunction is antisymmetric, in which case the spatial part becomes symmetric and the product of exponentials is replaced by a cosine, or the spin wavefunction is symmetric, in which case the spatial part must be antisymmetric, leading to a sine function for the position wavefunction. However, the ground state being of zero-momentum, the cosine is the most probable state and the wavefunction reads

$$\psi_0(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{k > k_F} g_{\mathbf{k}} \cos(\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \quad (3.2)$$

⁴Note here that the ordering $\epsilon_1 \geq \dots \geq \epsilon_N$ is just a convention.

⁵In condensed matter theory, the Fermi sea is the many-electron ground state in which all single-particle energy states with energies below the Fermi energy E_F are occupied at $T = 0$.

Inserting the wavefunction in the stationary Schrödinger equation⁶

$$(-\nabla_{\mathbf{r}}^2 + V(\mathbf{r}))\psi_0(\mathbf{r}) = E\psi_0(\mathbf{r}), \quad (3.3)$$

with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and V is the interaction potential between the two electrons, we get a condition for each coefficient $g_{\mathbf{k}}$. Indeed, the coefficients obey

$$(E - 2\epsilon_{\mathbf{k}})g_{\mathbf{k}} = \sum_{k' > k_F} V_{\mathbf{k}\mathbf{k}'} g_{\mathbf{k}'} \quad (3.4)$$

where $\epsilon_{\mathbf{k}} = k^2/2m$ are the single-particle energies and

$$V_{\mathbf{k}\mathbf{k}'} = \Omega^{-1} \int d^3\mathbf{r} V(\mathbf{r}) e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} \quad (3.5)$$

is the $\langle \mathbf{k} | V | \mathbf{k}' \rangle$ matrix element (Ω being a normalization volume). If we find a set of $g_{\mathbf{k}}$ coefficients with $E < 2E_F$ for an attractive potential V , then a bound pair exists. Indeed, this would mean that the two electrons lower their energy by forming a stable bound pair rather than remaining in the Fermi sea.

An attractive potential can be defined as

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V, & \text{if } |\epsilon_{\mathbf{k}} - E_F|, |\epsilon_{\mathbf{k}'} - E_F| < \omega_c, \\ 0, & \text{otherwise.} \end{cases} \quad (3.6)$$

where ω_c is a cutoff frequency, which origin is explained later. Thus, for $\mathbf{k}$ -states within the cutoff region, we can rewrite (3.4) by summing the left-hand-side over all $\mathbf{k}$ as

$$\frac{1}{V} = \sum_{k > k_F} (2\epsilon_{\mathbf{k}} - E)^{-1}. \quad (3.7)$$

Then, by taking the continuous limit, we get

$$\frac{1}{V} = N(0) \int_{E_F}^{E_F + \omega_c} \frac{d\epsilon}{2\epsilon - E} = \frac{1}{2} N(0) \ln \left(\frac{2E_F - E + 2\omega_c}{2E_F - E} \right). \quad (3.8)$$

Therefore, in the *weak-coupling limit*, defined as $N(0)V \ll 1$, the ground state energy is

$$E \approx 2E_F - 2\omega_c e^{-2/N(0)V} < 2E_F, \quad (3.9)$$

which is lower than the Fermi energy. This implies that the ground state must be a bound pair of electrons, a *Cooper pair*.

At first sight, this attractive potential seems unnatural since it is well known that electrons repulse one another through the Coulomb interaction $V(\mathbf{r}) = e^2/r$. This Coulomb potential gives matrix elements,

$$V_{\mathbf{k}\mathbf{k}'} = \frac{4\pi e^2}{(\mathbf{k} - \mathbf{k}')^2 + k_s^2} > 0, \quad (3.10)$$

always positive, even when we consider the *screening length* $1/k_s$. In fact, superconductivity cannot be explained without considering the surrounding ion cores. A simple physical picture for the attractive potential arises from the polarization of the ion lattice by the first electron. The

⁶Throughout this work, we employ Planck units, setting $c = \hbar = k_B = G = 1$. As a consequence, quantities that ordinarily carry different physical dimensions can be expressed in units of energy. In particular, frequencies and temperatures are treated as energies.

resulting excess positive charge then attracts a second electron and, if this attraction exceeds the screened Coulomb repulsion, a bound pair can form. This picture also provides a justification for the cutoff frequency ω_c . The interaction coming from the deformation of the lattice, the phonon frequency plays a central role. If one of the electron is scattered from $\mathbf{k}$ to $\mathbf{k}'$, then, by momentum conservation, a phonon carrying momentum $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ with characteristic frequency $\omega_{\mathbf{q}}$ must be absorbed or emitted. The phonon spectrum being bounded by the Debye frequency⁷ ω_D , electrons with energies such that $\epsilon_{\mathbf{k}} - E_F > \omega_D$ do not play a role in the pairing interactions. This is the origin of the previous cutoff (3.6).

3.2 Model Hamiltonian

We have shown in the previous section that the Fermi sea is unstable against the formation of Cooper pairs. Hence, as long as the Fermi sea keeps its structure, we expect the electron to form pairs and condense until reaching an equilibrium point known as the *BCS ground state*. This equilibrium occurs when the binding energy for a new additional pair equals zero. However, finding the ground-state wavefunction, or *BCS wavefunction* is not an easy task. Indeed, in the framework of second quantization, the most general wavefunction for N electrons with Cooper pairing is

$$|\psi_N\rangle = \sum_{\{\mathbf{k}\}} g(\mathbf{k}_i, \dots, \mathbf{k}_l) c_{\mathbf{k}_i\uparrow}^\dagger c_{-\mathbf{k}_i\downarrow}^\dagger \dots c_{\mathbf{k}_l\uparrow}^\dagger c_{-\mathbf{k}_l\downarrow}^\dagger |0\rangle, \quad (3.11)$$

where $|0\rangle$ is the vacuum state with no particle in the system, operators $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$ create a pair of electron with opposite momentum and spins, just as the 2-electron wavefunction (3.2), and $\mathbf{k}_i$ and $\mathbf{k}_l$ corresponds to the first and last of the M momentum states occupied in the band. In fact, the number of ways for choosing the $N/2$ states for pair occupancy is [33]

$$\frac{M!}{(M - N/2)!(N/2)!} \approx 10^{10^{20}},$$

which results in the same number of coefficients $g(\mathbf{k}_i, \dots, \mathbf{k}_l)$ to determine. Consequently, the problem cannot be solved exactly without resorting to approximation methods, such as the *Hartree-Fock approach*, or imposing further mean-field assumptions to solve the problem by canonical transformation.

In the following, we focus on the second method, the canonical transformation approach. We start with the Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow}. \quad (3.12)$$

The first term of this Hamiltonian corresponds to the single-electron energy, while the second term represents the energy associated to Cooper pairing. This second term implies that, in superconductors, operators such as $c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ can have a non-zero expectation value $\langle b_{\mathbf{k}} \rangle = \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$. Yet, we can make the approximation that the fluctuations $\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - \langle b_{\mathbf{k}} \rangle \rangle$ are very small, which can be shown statistically given the high number of particles in the system. Hence, by rewriting

$$c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} = \langle b_{\mathbf{k}} \rangle + (c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - \langle b_{\mathbf{k}} \rangle), \quad (3.13)$$

the Hamiltonian becomes

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} \left(c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \langle b_{\mathbf{l}} \rangle + c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow} \langle b_{\mathbf{k}}^* \rangle - \langle b_{\mathbf{k}}^* \rangle \langle b_{\mathbf{l}} \rangle \right). \quad (3.14)$$

⁷The Debye frequency is the maximum phonon frequency in the Debye model of crystal vibrations. It serves as a cutoff that ensures the correct total number of vibrational modes [34].

Here, the bilinear in the second term of (3.13) vanishes given the previous argument about small fluctuations. Finally, by setting the 'zero energy' to be the chemical potential μ of the particles (equal to E_F at $T = 0$) and defining the *superconducting gap*

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{l}} V_{\mathbf{k}\mathbf{l}} \langle b_{\mathbf{l}} \rangle \quad (3.15)$$

$$= - \sum_{\mathbf{l}} V_{\mathbf{k}\mathbf{l}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle, \quad (3.16)$$

we find the *model Hamiltonian*

$$H_M = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger + \Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - \Delta_{\mathbf{k}} \langle b_{\mathbf{k}}^* \rangle \right), \quad (3.17)$$

with $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. This Hamiltonian does not conserve the number of particles anymore which is not a problem since we are working in a grand-canonical ensemble framework. Furthermore, we transition from a quartic initial Hamiltonian (3.12) to a quadratic one (3.17), which is much simpler to analyze.

In order to get a spectrum for the Hamiltonian and its fundamental excitation modes, let us diagonalize it using a Bogoliubov-de Gennes transformation of the fermionic operators (a canonical transformation) defined in (2.17). We consider the transformation

$$\underbrace{\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k}\downarrow} \\ c_{\mathbf{k}\uparrow}^\dagger \\ c_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix}}_{\mathbf{c}} = \underbrace{\begin{pmatrix} u_{\mathbf{k}}^* & 0 & 0 & v_{\mathbf{k}} \\ 0 & u_{\mathbf{k}}^* & -v_{\mathbf{k}} & 0 \\ 0 & v_{\mathbf{k}}^* & u_{\mathbf{k}} & 0 \\ -v_{\mathbf{k}}^* & 0 & 0 & u_{\mathbf{k}} \end{pmatrix}}_{\mathbf{U}} \underbrace{\begin{pmatrix} a_{\mathbf{k}0} \\ a_{\mathbf{k}1} \\ a_{\mathbf{k}0}^\dagger \\ a_{\mathbf{k}1}^\dagger \end{pmatrix}}_{\mathbf{a}}, \quad (3.18)$$

with the unitarity condition for $\mathbf{U}$: $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$. This can be rewritten as

$$c_{\mathbf{k}\uparrow} = u_{\mathbf{k}}^* a_{\mathbf{k}0} + v_{\mathbf{k}} a_{\mathbf{k}1}^\dagger, \quad (3.19)$$

$$c_{-\mathbf{k}\downarrow}^\dagger = -v_{\mathbf{k}}^* a_{\mathbf{k}0} + u_{\mathbf{k}} a_{\mathbf{k}1}^\dagger, \quad (3.20)$$

from which we notice that $a_{\mathbf{k}0}$ participates in both destroying an electron with $\mathbf{k} \uparrow$ and creating one with $-\mathbf{k} \downarrow$ with a net effect of decreasing the global momentum, while $a_{\mathbf{k}1}$ acts similarly but with a net effect of increasing the global momentum. This transformation performed, one can show that the Hamiltonian reduces to

$$H_M = \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}} \langle b_{\mathbf{k}}^* \rangle) + \sum_{\mathbf{k}} E_{\mathbf{k}} \left(a_{\mathbf{k}0}^\dagger a_{\mathbf{k}0} + a_{\mathbf{k}1}^\dagger a_{\mathbf{k}1} \right), \quad (3.21)$$

if $|v_{\mathbf{k}}|^2 = 1 - |u_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right)$, with $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$. The first term is a constant which represents the *BCS ground state energy*, which differs from the Fermi level by the condensation energy⁸. From this Hamiltonian, we can show that the ground state is given by the wavefunction

$$|BCS\rangle = \prod_{\mathbf{k}=\mathbf{k}_1, \dots, \mathbf{k}_M} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle, \quad (3.22)$$

where we can now interpret $v_{\mathbf{k}}$ as the probability amplitude of the pair $(\mathbf{k}, -\mathbf{k})$ to be occupied, while $u_{\mathbf{k}}$ represents the probability amplitude of the pair to be unoccupied. The probability density $|v_{\mathbf{k}}|^2$ is plotted in Figure 3.1 in which we observe that the probability of being occupied, *i.e.*, the probability of having a Cooper pair, approaches unity far from E_F (set to zero on the plot) confirming the energetic pairing advantage. Furthermore, $\Delta = |\Delta_{\mathbf{k}}|$ corresponds to the characteristic energy determining the range of $\mathbf{k}$ values involved in Cooper pairing.

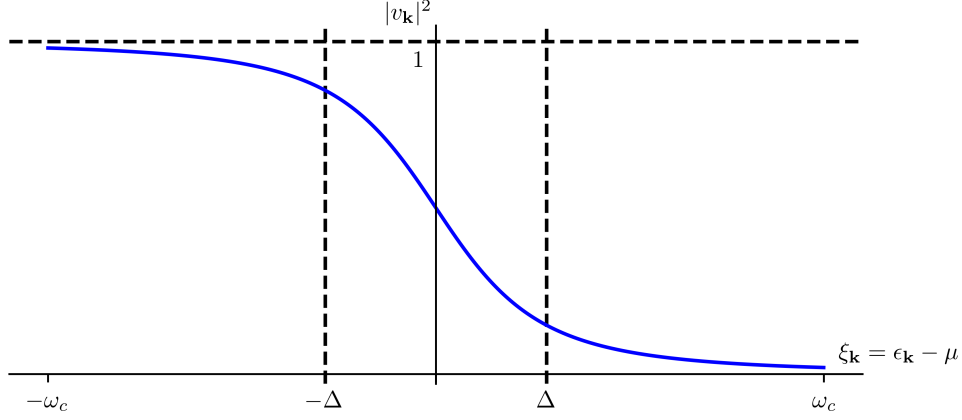


Figure 3.1: Plot of the probability density $|v_{\mathbf{k}}|^2$ with respect to $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$.

Finally, from (3.21) we see that the elementary excitations of the system are created by the collective modes $a_{\mathbf{k}0}$ and $a_{\mathbf{k}1}$ of energy $E_{\mathbf{k}}$, which are the previously defined *Bogoliubons* for this Hamiltonian. These excitations are of particular importance in this Master's thesis because, as we will see later, the zero-energy fermion composed of two Majorana zero modes is a zero-energy Bogoliubon of the Kitaev Hamiltonian. The first excitation energy branch of (3.21) is depicted in Figure 3.2 (blue branch), where the name *superconducting gap* for $\Delta_{\mathbf{k}}$ appears obvious. Indeed, in addition to represent the characteristic energy of electrons involved in the pairing process around E_F , it also gives the gap between the first excitation of the Hamiltonian and the BCS ground state at $\xi_{\mathbf{k}} = 0$, *i.e.*, at the Fermi level.

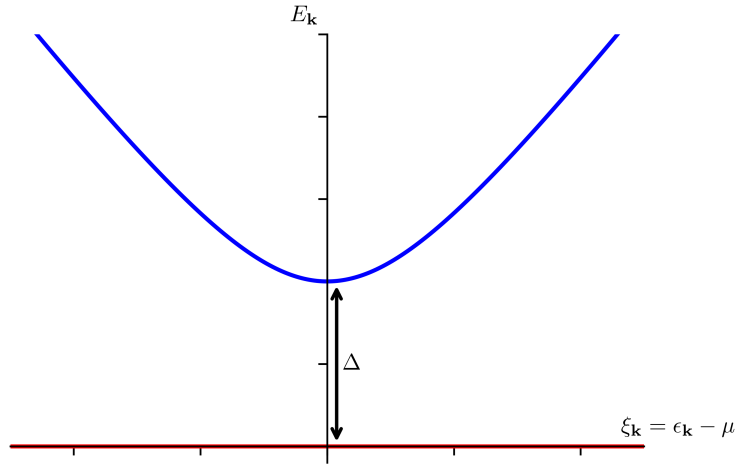


Figure 3.2: Plot of the first energy branch $E_{\mathbf{k}}$ (blue) with respect to $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. Here the BCS ground state energy (red) is set to zero.

4 The Kitaev chain

In 1937, Ettore Majorana proposed an alternative formulation of the Dirac equation [35] from which fermions arise as excitations of a field built from real fermionic operators. In this

⁸The condensation energy in superconducting systems is the difference between the internal energies of the superconducting s and the one of the normal n phases: $U_s(T) - U_n(T)$.

framework, such particles, known as Majorana fermions, are their own antiparticles since they are self-conjugate ($c = c^\dagger$). While no experimental evidence for their existence has been observed yet, it was proposed that such exotic particles could provide a description of neutrinos [36]. However, in condensed matter physics, such fermions can arise in the topological phase of topological insulators or superconductors [10, 11] as quasiparticle excitations of zero-energy, called *Majorana Zero Modes* (MZMs). These excitations arise as collective modes localized at boundaries between trivial and topological phases of the hosting system. Indeed, as we will show later, these two phases cannot be connected by a continuous transformation without closing an energy gap, which mandates the existence of a localized zero-energy mode at their boundary [31, 37]. For now, we can naively visualize this closed gap as $\Delta = 0$ in Figure 3.2 meaning that the excitation branch present a zero-energy mode. Such modes were proven to emerge at the edges of a one-dimensional chain of spinless electrons with p -wave superconducting pairing: the *Kitaev chain* [13], which Hamiltonian reads

$$H = - \sum_{n=1}^N \mu c_n^\dagger c_n - \sum_{n=1}^{N-1} \left(t c_n^\dagger c_{n+1} - \Delta e^{i\phi} c_n c_{n+1} + \text{h.c.} \right), \quad (4.1)$$

where μ is the on-site chemical potential, $t > 0$ is the hopping amplitude and $\Delta e^{i\phi}$ is the superconducting pairing. While this model corresponds to the tight-binding approximation of the 1D spinless p -wave superconducting Hamiltonian, it captures all the interesting topological properties of the latter and offers a simpler framework for applications in topological quantum computing. Indeed, it has been shown that MZMs exhibit non-Abelian braiding statistics under exchange in 2D [14] and in effective 1D [15] superconductors, and thus could be used as building blocks for logical qubits in a topological quantum computing scheme [5].

In this section, we first establish the connection between the Kitaev model and the underlying spinless p -wave superconducting Hamiltonian. We then introduce the notions of trivial and topological phases in the chain, leading thereafter to the demonstration of localized Majorana zero modes at its edges. Next, we highlight their relevance for quantum computation by discussing their non-Abelian braiding statistics, as well as the construction of qubits and logical gates. Finally, since the topological phase is formally defined in the thermodynamic limit of an infinite number of sites, we introduce the *end-to-end correlator* as a practical probe of topological features in finite-size Kitaev chains.

4.1 From continuous spinless topological superconductors to the Kitaev model

First, let us emphasize the differences between the *Kitaev Hamiltonian* (4.1) and the *model Hamiltonian* of BCS superconductivity in one dimension⁹

$$H_M = \underbrace{\sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma}}_{H_0} - \underbrace{\sum_k \left(\Delta c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta^* c_{-k\downarrow} c_{k\uparrow} \right)}_{H_1}. \quad (4.2)$$

While this Hamiltonian is expressed in the k -momentum space, the Kitaev Hamiltonian index n is referring to a position in the chain. In order to compare both Hamiltonian, we need to reexpress (4.2) in the x -position space using the relations (2.12) and (2.13). Considering that the single-particle wavefunctions for the electron are plane waves as in (3.1), (2.12) and (2.13)

⁹Here, we drop the constant term $-\Delta_{\mathbf{k}} \langle b_{\mathbf{k}} \rangle^*$ which only redefines the scale of the Bogoliubov vacuum state and we consider $\Delta_k = \Delta$ for simplicity.

become

$$c_{k\sigma} = \frac{1}{\sqrt{V}} \int dx e^{-ikx} \psi_\sigma(x), \quad (4.3)$$

$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{V}} \int dx e^{ikx} \psi_\sigma^\dagger(x), \quad (4.4)$$

with the normalization volume V . Furthermore, for $dk \rightarrow 0$ and $V \rightarrow \infty$, we employ the continuum limit, $\frac{1}{V} \sum_k \rightarrow \int \frac{dk}{2\pi}$. Let us plug this in the kinetic term H_0 and pairing term H_1 of (4.2):

$$H_0 \rightarrow \sum_\sigma \iiint \frac{dk}{2\pi} dx dx' e^{ik(x-x')} \psi_\sigma^\dagger(x) \left(\frac{k^2}{2m} - \mu \right) \psi_\sigma(x'), \quad (4.5)$$

$$H_1 \rightarrow - \iiint \frac{dk}{2\pi} dx dx' e^{ik(x-x')} \left(\Delta \psi_\uparrow^\dagger(x) \psi_\downarrow^\dagger(x') + \Delta^* \psi_\downarrow(x) \psi_\uparrow^\dagger(x') \right). \quad (4.6)$$

Thus, the Hamiltonian in k -space is rewritten in the x -position basis of the Hilbert space as

$$H_M = \sum_\sigma \int dx \psi_\sigma^\dagger(x) \left(-\frac{\partial_x^2}{2m} - \mu \right) \psi_\sigma(x) - \int dx \left(\Delta \psi_\uparrow^\dagger(x) \psi_\downarrow^\dagger(x) + \text{h.c.} \right), \quad (4.7)$$

which is the continuous Hamiltonian for BCS superconductivity. The detailed calculation is provided in Appendix A.

Recall that this Hamiltonian describes the Cooper pairing mediated by phonon interactions for wavefunctions of the form (3.2),

$$\psi_0(x_1 - x_2) = \phi(x_1 - x_2) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad (4.8)$$

with $\phi(x_1 - x_2) = \phi(x_2 - x_1)$ a symmetric spatial function. Here, the needed antisymmetry comes from the spin wavefunction called a *spin-singlet* and the resulting superconductivity is called *s-wave* superconductivity. Yet, in strongly correlated electron systems, new exotic type of pairing of general form

$$\psi_0(x_1 - x_2) = \phi_{11}(x_1 - x_2) |\uparrow\uparrow\rangle + \phi_{22}(x_1 - x_2) |\downarrow\downarrow\rangle + \phi_{12}(x_1 - x_2) (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad (4.9)$$

can arise as the ground state of the system, with antisymmetric spatial functions $\phi_{ij}(x_1 - x_2)$ [38, 39]. Given the symmetric nature of the spin wavefunctions, the antisymmetry of the spatial part is mandated to conserve global fermionic statistics for ψ_0 . These new symmetric spin wavefunctions appearing in each terms are called *spin-triplets*, and the resulting superconductivity for such pairing is known as *p-wave* superconductivity. By restraining ourselves in only one projected spin direction, we can consider the electron to be spinless, hence dropping the σ index on the fermionic operators that we have in (4.7). Such superconductivity for spinless electrons is described by the Hamiltonian [31]

$$H_p = \int dx \psi^\dagger(x) \left(-\frac{\partial_x^2}{2m} - \mu \right) \psi(x) + \int dx \left(\frac{i\Delta}{2m} \psi(x) (-i\partial_x) \psi(x) + \text{h.c.} \right). \quad (4.10)$$

Aside from the spinless character of the electrons, the key distinction between (4.7) and (4.10) lies in the presence of a derivative in the pairing term of (4.10). This feature gives rise to nontrivial topological effects, which we will not explore here. However, similar effects also emerge in the Kitaev model, whose Hamiltonian (4.1) can be viewed as a tight-binding discretization of Hamiltonian (4.10).

Indeed, a continuous Hamiltonian as (4.10) can be discretized by performing the tight-binding approximation which consists in considering only discrete positions $x_n = na$ on a 1D lattice for electrons, with a the distance between two closest neighbors on the lattice [31, 40]. In

this approximation, the field operators are replaced by discrete fermionic operators, and the derivatives by finite differences, as

$$\psi(x) \rightarrow c_n, \quad (4.11)$$

$$-i\partial_x\psi(x) \rightarrow -\frac{i}{2a}(c_{n+1} - c_{n-1}), \quad (4.12)$$

$$-\partial_x^2\psi(x) \rightarrow -\frac{1}{a^2}(c_{n+1} - 2c_n + c_{n-1}), \quad (4.13)$$

with $c_n = \psi(na)$. Let us employ these relations on (4.10) to obtain the Kitaev Hamiltonian:

$$H \rightarrow \sum_n \left(c_n^\dagger (-\mu) c_n - \frac{1}{2ma^2} c_n^\dagger (c_{n+1} - 2c_n + c_{n-1}) + \frac{\Delta}{2} c_n \frac{1}{2a} (c_{n+1} - c_{n-1}) + \frac{\Delta^*}{2} c_n^\dagger \frac{1}{2a} (c_{n+1}^\dagger - c_{n-1}^\dagger) \right), \quad (4.14)$$

which finally gives

$$H = - \sum_{n=1}^N \tilde{\mu} c_n^\dagger c_n - \sum_{n=1}^{N-1} \left(t c_n^\dagger c_{n+1} - |\tilde{\Delta}| e^{i\phi} c_n c_{n+1} + \text{h.c.} \right), \quad (4.15)$$

where the hopping amplitude is given by $t = 1/2ma^2$, the on-site chemical potential is $\tilde{\mu} = \mu - 2t$ and the superconducting pairing amplitude is now $\tilde{\Delta} = \Delta/2a$. Thus, as wanted, we get the Kitaev Hamiltonian from the continuous p -wave Hamiltonian (4.10). In the following, we drop the ' $\sim$ ' and we consider $\phi = 0$ without a loss of generality. Indeed, the superconducting phase can always be absorbed in the fermionic operators by a global $U(1)$ gauge transformation $c_n \rightarrow e^{-i\phi/2} c_n$, allowing us to choose $\Delta > 0$ without loss of generality.

4.2 Topology in the Kitaev chain

Now that the link between p -wave superconductivity and the Kitaev model has been highlighted, let us introduce the meaning behind topologically trivial or non-trivial phases in the Kitaev chain, and their consequences. In the following sections, up to Section 4.5, we closely follow the methodology presented in [31].

Without already defining properly the topology in the chain, let us look at the energy dispersion of the Hamiltonian and at how we can already conclude from it that there should exist two different parameter regimes. We obtain the energy dispersion by adding an extra site $n = 0$, and by imposing periodic boundaries for the chain such that $c_0 = c_N$. This being, we can switch to the k -momentum space by performing the Fourier expansion

$$c_n = \frac{1}{\sqrt{N}} \sum_k e^{ikna} c_k, \quad (4.16)$$

where we get that $k = 2\pi m/N$ with $|m| = 0, 1, \dots, N$ from the periodic boundary conditions. From this, we can get the form of the Hamiltonian (4.1) in the k -momentum space:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{\Delta_k}{2} c_{-k} c_k + \frac{\Delta_k^*}{2} c_k^\dagger c_{-k}^\dagger \quad (4.17)$$

with $\epsilon_k = -(\mu + 2t \cos(ka))$ and $\Delta_k = 2i\Delta \sin(ka)$, which can be rewritten in its more compact BdG form¹⁰ as

$$H = \frac{1}{2} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \mathbf{H}(k) \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \quad (4.18)$$

¹⁰Instead of expressing H as in (2.19), we retain the summation over k which leads to a smaller BdG Hamiltonian that still fully captures the k -dependence.

with the BdG Hamiltonian $\mathbf{H}(k) = \begin{pmatrix} \epsilon_k & \Delta_k^* \\ \Delta_k & -\epsilon_k \end{pmatrix}$. Hence, we get the two energy dispersions for single particles ($E_k > 0$) and holes ($E_k < 0$) from the eigenvalues of $\mathbf{H}(k)$, *i.e.*,

$$E_k = \pm \sqrt{\epsilon_k^2 + |\Delta_k|^2}, \quad (4.19)$$

$$= \pm \sqrt{(\mu + 2t \cos(ka))^2 + 4\Delta^2 \sin^2(ka)}. \quad (4.20)$$

In Figure 4.1, we observe that, for $|\mu| > 2t$, we always have a particle-hole gap for the bare electron dispersion ϵ_k , *i.e.*, the dispersion when there is no superconducting coupling ($\Delta = 0$), whereas it is gapless for $|\mu| \leq 2t$. In comparison, the superconducting electrons branches are always gapped for $|\mu| \neq 2t$ and the gap closes only at $k = 0, \pm\pi$ for $\mu = \pm 2t$. For $|\mu| > 2t$ (Fig. 4.1(a) and Fig. 4.1(f)), the superconducting energy branches E_k can be smoothly deformed into the bare electron ones as $\Delta \rightarrow 0$, without the gap ever closing. In contrast, for $|\mu| < 2t$ (Fig. 4.1(c) and Fig. 4.1(d)), such a deformation necessarily involves a closing of the gap.

These distinct gap behaviors, separated by the gapless points $\mu = \pm 2t$ (Fig. 4.1(b) and Fig.

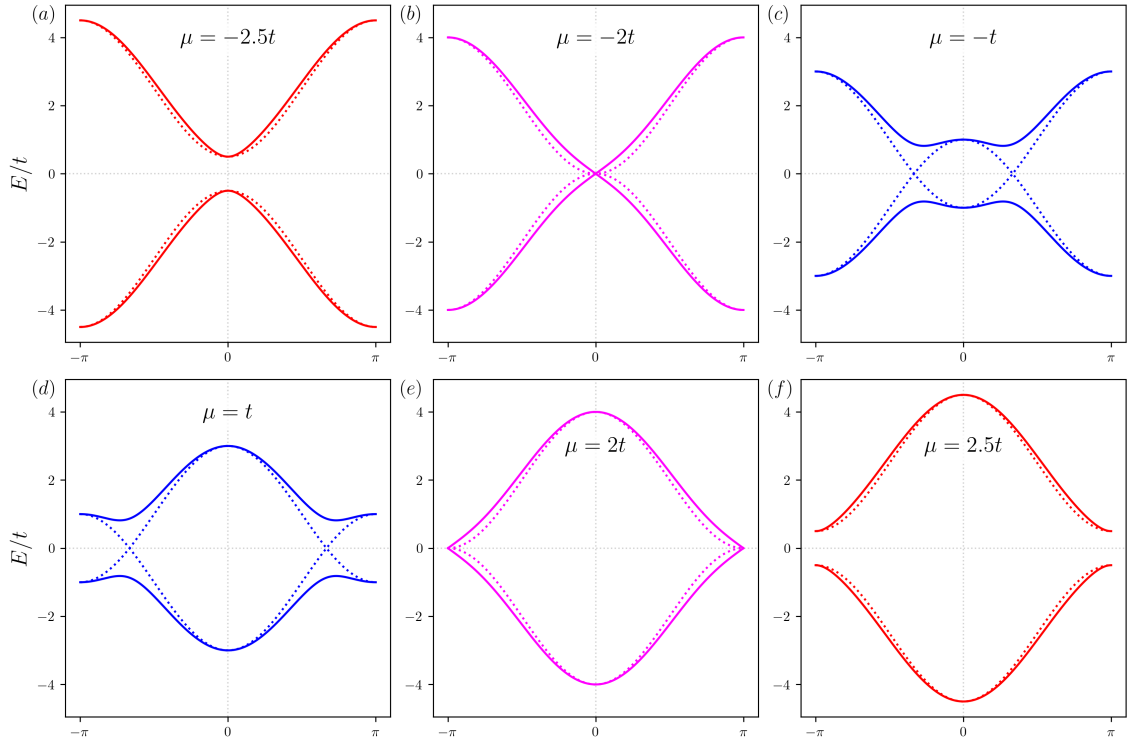


Figure 4.1: Energy dispersion (solid line) E_k of the Kitaev chain for different values of the chemical potential μ and with $\Delta = t/2$. We can compare the dispersion of the superconducting electrons to the bare electron dispersion ϵ_k (dotted line). For $|\mu| > 2t$ ((a) and (f)), the system is in the strong-coupling phase, whereas, for $|\mu| < 2t$ ((c) and (d)), it is in the weak-coupling phase. The phase transition between the two occurs when the particle-hole gap closes at $|\mu| = 2t$ ((b) and (e)). (Figure reproduced from [31]).

4.1(e)), enable us to distinguish between two different regimes of the Kitaev chain: the *strong-pairing* ($|\mu| > 2t$) and *weak-pairing* ($|\mu| < 2t$) phases¹¹. Figure 4.2 shows the phase space of the Kitaev model. In the following, we will show that the strong-pairing phase is topologically trivial, as it can be smoothly deformed into the bare electron vacuum (the state where all particle states are occupied) in the limit $\Delta \rightarrow 0$. In contrast, this is no longer possible for the weak-pairing phase, which is therefore topologically non-trivial.

¹¹This phase designation originates from [10] in which N. Read and D. Green discriminate two phases with respect to their different behaviors as $\mathbf{k} \rightarrow 0$.

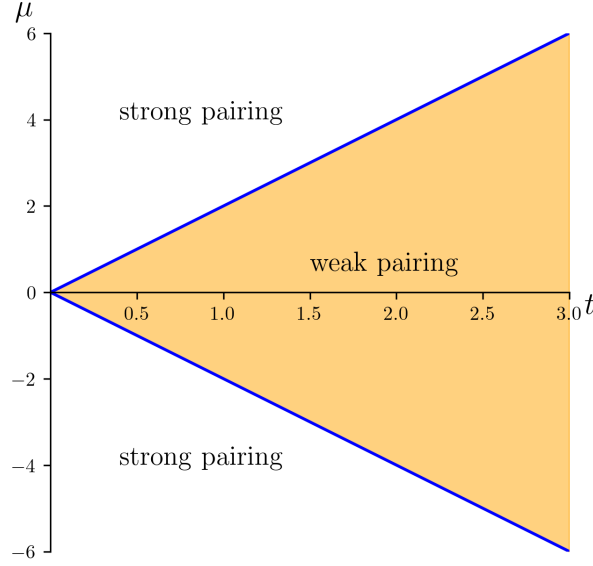


Figure 4.2: Phase diagram $\mu - t$ for the Kitaev chain. The transition between the weak- and strong-pairing phases occurs when the particle-hole gap closes at $|\mu| = 2t$. (Figure reproduced from [31]).

Therefore, let us introduce how is topology defined in the Kitaev chain. Roughly speaking, topology is a branch of mathematics which classes geometrical objects in distinct topological sector characterized by an integer number: a *topological invariant*¹². Two objects are said to be topologically equivalent if they share the same value of a topological invariant. In that case, it is always possible to continuously deform one object to the other without any cutting or tearing. An overused example is the comparison between a doughnut (a torus) and a coffee cup: one can convince oneself that each object can be smoothly deformed to the other, and vice versa. On the other hand, one would need to tear a hole in a pool ball before deforming it into a torus shape, which makes the two objects topologically distinct, as depicted on Figure 4.3. While the doughnut and the coffee cup have the same topological invariant, this latter differs for the pool ball.

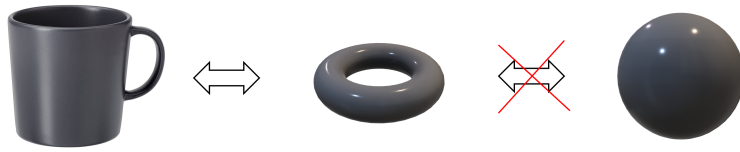


Figure 4.3: In topology, a doughnut is equivalent to a cup, but not to a pool ball. (The picture of the cup comes from [41]).

The geometrical object characterizing the Kitaev model is the trajectory of a unit vector on the unit sphere that we define through the BdG Hamiltonian in the k -momentum space. Indeed, in (4.18), we have defined the BdG Hamiltonian as

$$\mathbf{H}(k) = \begin{pmatrix} \epsilon_k & \Delta_k^* \\ \Delta_k & -\epsilon_k \end{pmatrix}, \quad (4.21)$$

with $\epsilon_k = -(\mu + 2t \cos(ka))$ and $\Delta_k = 2i\Delta \sin(ka)$. The eigenvalues of this matrix give us the energy dispersion of the system for all k and therefore, entirely characterize the phase of the

¹²There exist multiple topological invariants to characterize a system, and their relevance depends on the symmetry of the latter.

system (weak- and strong-coupling). Then, we rewrite the BdG Hamiltonian (4.21) as

$$\mathbf{H}(k) = \mathbf{h}(k) \cdot \boldsymbol{\sigma}, \quad (4.22)$$

where we define the Hamiltonian density vector $\mathbf{h}(k) = (0 \quad 2\Delta \sin(ka) \quad \epsilon_k)^T$ of norm $|\mathbf{h}(k)| = E_k$, and the Pauli matrices vector $\boldsymbol{\sigma} = (\sigma_x \quad \sigma_y \quad \sigma_z)^T$ ¹³. From $\mathbf{h}(k)$, we build the unit vector $\mathbf{u}(k) = \mathbf{h}(k)/|\mathbf{h}(k)|$ which evolves on the yz plane of the unit sphere. As said previously, the geometrical object which defines the topological phase of the system is the trajectory followed by this unit vector on the unit sphere when k evolves from $-\pi$ to π . For $|\mu| > 2t$, this trajectory is a circular arc that never enclose the origin, as depicted in Figure 4.4. Indeed, if $\mu > 2t$ ($\mu < -2t$), the bare electron dispersion ϵ_k , *i.e.*, the z -component of $\mathbf{u}(k)$, is always negative (positive) for all k . Thus, the trajectory for this phase never loops around the origin. On the other hand, if $|\mu| < 2t$, the trajectory corresponds to a closed loop encircling the origin of the sphere. We can already convince ourselves that these two trajectories are topologically distinct from one another by visual reasoning: a circle is topologically distinct from a line since we need to cut the first to get the second. To probe the topology of the system in a more accurate way, we define a topological invariant called the *winding number* W as [42]

$$W = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta(k), \quad (4.24)$$

with $\tan(\theta(k)) = u_z(k)/u_y(k) = h_z(k)/h_y(k)$. This topological invariant counts the number of turns that the unit vector $\mathbf{u}(k)$ makes around the origin of the unit sphere. For $|\mu| > 2t$, $W = 0$, while for $|\mu| < 2t$, $W = 1$. Therefore, these two parameter regimes, with different values of W , are topologically distinct.

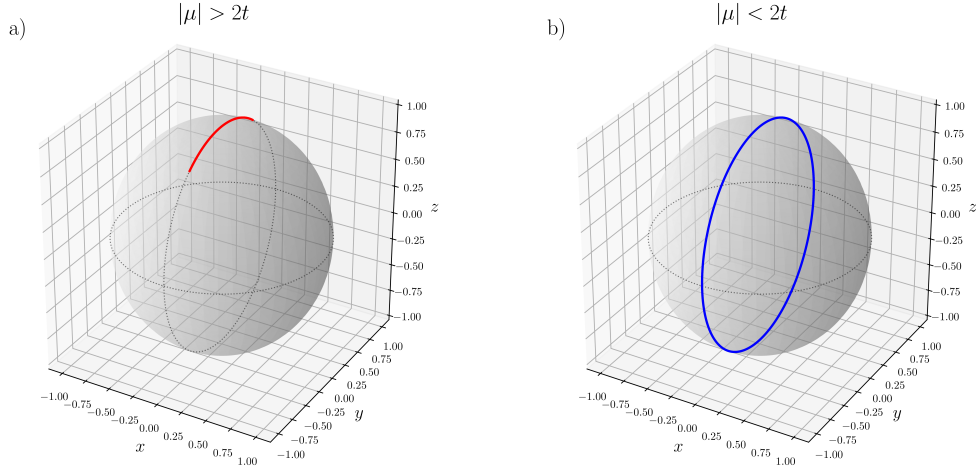


Figure 4.4: Trajectories of the unit vector $\mathbf{u}(k)$ on the unit sphere. a) For $|\mu| > 2t$, the trajectory does not encircle the origin, resulting in a winding number $W = 0$. b) For $|\mu| < 2t$, the trajectory encircle the origin, resulting in a winding number $W = 1$. The two trajectories, showing a distinct W , represent two topologically distinct phases of the Kitaev chain.

A fundamental result of this theory is that, in order to have a smooth transition between two topologically distinct phases in the real space, the particle-hole gap must close at their shared

¹³As a reminder, the *Pauli matrices* are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.23)$$

boundary, as illustrated in Figures 4.1 and 4.2. Thus, there must exist a state of zero-energy localized at the boundary [37]. For the Kitaev model with open boundaries condition, this state will be a zero-energy *Bogoliubon*, called a *Majorana bound state* (MBS), delocalized at each edge of the chain. Indeed, considering the chain in its topological phase, the edges correspond to boundaries between a topologically non-trivial system (the chain) and a trivial one (the vacuum). In the next section, we prove the existence of such a state in the chain. Furthermore, from now on, we often call the trivial (strong pairing) and non-trivial (weak pairing) topological regimes, the *trivial* and *topological* phases.

4.3 Majorana bound state and Majorana zero modes

Particular phases:

Any complex fermionic operator can be decomposed into its Hermitian and anti-Hermitian parts as

$$c_n = \frac{1}{2} (\gamma_{A,n} + i\gamma_{B,n}), \quad (4.25)$$

where we introduce the *Majorana operators*

$$\gamma_{A,n} = c_n^\dagger + c_n \quad \text{and} \quad \gamma_{B,n} = i(c_n^\dagger - c_n). \quad (4.26)$$

From (4.25), we see that any fermionic mode is composed of two so-called *Majorana modes*, as depicted on Figure 4.5. These new operators are self-adjoint $\gamma_{\alpha,n}^\dagger = \gamma_{\alpha,n}$, idempotent $\gamma_{\alpha,n}^2 = 1$, and follow anticommutation relations $\{\gamma_{\alpha,m}, \gamma_{\beta,n}\} = 2\delta_{\alpha,\beta}\delta_{m,n}$. From the self-adjoint and idempotent properties, we notice that it is no longer possible to define a number operator for Majorana modes since $\gamma^\dagger\gamma = \gamma\gamma^\dagger$ always gives the identity. We can interpret this result as follows: a Majorana mode is half a fermion and half a hole, thus it is always occupied and unoccupied simultaneously [43]. Now, by expressing the Kitaev Hamiltonian (4.1) in terms of the Majorana operators, we get

$$H = -\frac{1}{2} \sum_{n=1}^N \mu (1 + i\gamma_{A,n}\gamma_{B,n}) + \frac{1}{2} \sum_{n=1}^{N-1} (i(\Delta + t)\gamma_{B,n}\gamma_{A,n+1} + i(\Delta - t)\gamma_{A,n}\gamma_{B,n+1}). \quad (4.27)$$

If we consider $\Delta = t$, the Hamiltonian becomes

$$H = -\frac{1}{2} \sum_{n=1}^N \mu (1 + i\gamma_{A,n}\gamma_{B,n}) + \frac{1}{2} \sum_{n=1}^{N-1} 2it\gamma_{B,n}\gamma_{A,n+1}. \quad (4.28)$$

This Hamiltonian describes a chain of $2N$ Majorana modes coupled to their nearest-neighbors and sitting on two sub-lattices A and B . If $|\mu| > 2t$, the neighbor coupling on same site n dominates, whereas the coupling for neighbors on different sites dominates for $|\mu| < 2t$. Once more, this is an insight in the behaviors of the chain for two different phases.

Before giving a general proof for the existence of the zero-energy mode in the topological phase, let us focus on two extreme regimes occurring for sweet spots of parameters.

In the parameter sweet spot $\Delta = t = 0$ and $\mu \neq 0$, we get the 'perfect non-topological phase' for which the Hamiltonian reads

$$H = -\frac{1}{2} \sum_{n=1}^N \mu (1 + i\gamma_{A,n}\gamma_{B,n}) = -\sum_{n=1}^N \mu c_n^\dagger c_n. \quad (4.29)$$

Hence, in this particular phase, the eigenexcitations correspond simply to the bare electrons, or equivalently to two Majorana modes coupled on the same site, as represented on Figure 4.5(a).

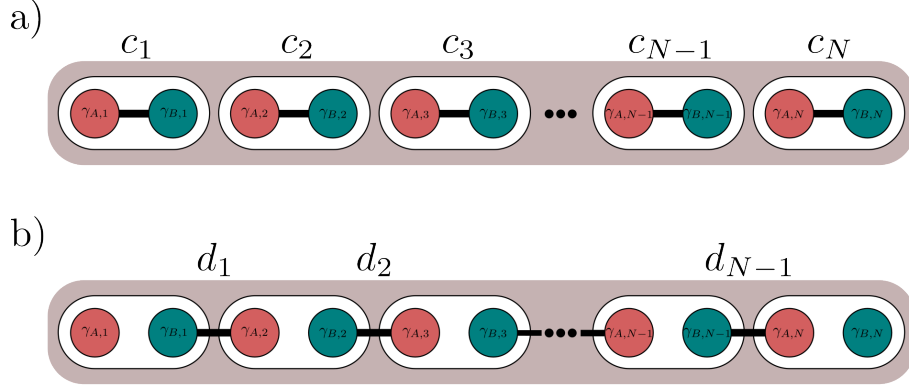


Figure 4.5: Sketches of the Kitaev chain in two extreme parameter regimes. Here, the white boxes correspond to the N physical electronic modes. Furthermore, an eigenexcitation of the system is represented as the coupling of two Majorana modes linked by a black line. a) The Kitaev chain in the sweet spot $\Delta = t = 0$ and $\mu \neq 0$: each fermionic mode c_i is decoupled from its neighbor. b) The Kitaev chain in the sweet spot $\Delta = t \neq 0$ and $\mu = 0$: the eigenexcitations of the chain are new fermionic modes corresponding to the coupling of Majorana modes from neighboring physical sites. This phase leaves two unpaired Majorana modes at each edge, corresponding to two MZMs.

This parameter regime is, of course, topologically trivial since $|\mu| > 2t = 0$.

On the other hand, the 'perfect topological phase' occurs when we set $\Delta = t \neq 0$ and $\mu = 0$, which results in the Hamiltonian

$$H = \sum_{n=1}^{N-1} it \gamma_{B,n} \gamma_{A,n+1}. \quad (4.30)$$

Then, we can define new fermionic operators¹⁴

$$d_n = \frac{1}{2} (\gamma_{B,n} + i\gamma_{A,n+1}) \quad (4.31)$$

which describe fermionic excitations composed of two Majorana modes from different neighboring sites. Using these new fermionic operators, we rewrite (4.30) as

$$H = \sum_{n=1}^{N-1} it \gamma_{B,n} \gamma_{A,n+1} = 2t \sum_{n=1}^{N-1} \left(d_n^\dagger d_n - \frac{1}{2} \right), \quad (4.32)$$

which eigenexcitations are the previously cited fermionic excitations composed of two Majorana modes from different neighboring sites, as shown on Figure 4.5(b). Obviously, given the parameter choice $\mu = 0 < 2t$, the chain is in a topological phase. A key result from (4.32) is the number $N - 1$ of terms in the Hamiltonian, which means that the two edge Majorana modes $\gamma_{A,1}$ and $\gamma_{B,N}$ are missing from it. Hence, we define an additional fermionic mode from these missing Majorana modes as

$$d_M = \frac{1}{2} (\gamma_{B,N} - i\gamma_{A,1}), \quad (4.33)$$

which commutes with H , i.e., $[H, d_M] = 0$. Therefore, this mode describes a perfectly delocalized fermionic excitation which occupation is associated with zero energy. This is an instance of a Majorana bound state present in the Kitaev chain, and the two Majorana modes composing the

¹⁴This is equivalent as a fermionic transformation (2.17) from c_n to d_n .

MBS are the previously introduced *Majorana zero modes* (MZMs)¹⁵. Moreover, the Bogoliubov vacuum of the Kitaev chain $|0\rangle$, defined as $d_n|0\rangle = 0$, for all n , is also associated to the null energy. Thus, the Kitaev chain is showing a 2-fold degenerate ground state. This degenerate ground state is separated from the non-zero energy excitation by the gap $2t$, as shown on Figure 4.6.

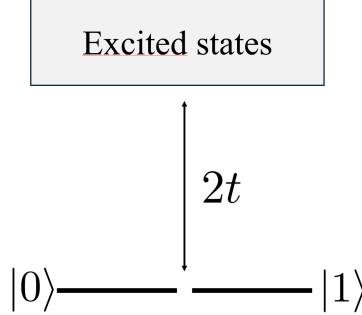


Figure 4.6: Representation of the 2-fold degenerate ground state composed of the Bogoliubov vacuum $|0\rangle$, and the MBS $|1\rangle$. The degenerate ground state is separated by a gap $2t$ from the other fermionic excitations of the system. (Figure adapted from [44].)

Parity of the degenerate ground state:

The two ground states, $|0\rangle$ (the vacuum) and $|1\rangle = d_M^\dagger |0\rangle$ (the MBS), have different fermionic parities. Indeed, defining the parity operator

$$P = (-1)^F = \prod_n (1 - 2c_n^\dagger c_n) = \prod_n (-i \gamma_{A,n} \gamma_{B,n}) = \prod_n (1 - 2d_n^\dagger d_n), \quad (4.34)$$

where $F = \sum_n c_n^\dagger c_n$, we have that $P|0\rangle = 1$ and $P|1\rangle = -1$. This parity operator simply tells us whether the state contains an even (+1) or odd (-1) number of fermions in the system. Thus, we will call $|0\rangle$, the even parity ground state and $|1\rangle$, the odd parity ground state. In the Kitaev Hamiltonian (4.1), the pairing terms do not conserve the number of fermions, but preserve the state parity. Thus, internal dynamics ruled by the Kitaev Hamiltonian never couple the two ground states $|0\rangle$ and $|1\rangle$, and hence, no transition between these two is allowed.

As we will see later, the energy gap $2t$ and the conservation of parity within the ground-state subspace are central to what is known as the *topological protection* of *Majorana qubits*. Indeed, the degenerate ground-state manifold allows the definition of a qubit that is protected against excitations by the energy gap $2t$, while its parity, and therefore its computational basis, is preserved. Since this degenerate ground state originates from the topological phase of the Kitaev chain, this protection is referred to as *topological*.

Existence of an MBS for $|\mu| < 2t$:

Until now, we have observed the emergence of an MBS only for the sweet spot $\Delta = t \neq 0$ and $\mu = 0$, but what about the whole topological region $|\mu| < 2t$? Here, we show that it is always possible to define an MBS in the topological phase, even though the wavefunctions of its composing MZMs are not perfectly localized at the edge of the chain anymore. Let us generically

¹⁵In the literature, there is no universally adopted convention for the designation of these modes. Therefore, throughout this work, we refer to the two uncoupled edge Majorana modes as *Majorana Zero Modes*, while the fermionic mode formed by their combination is referred to as the *Majorana Bound State*.

define a fermionic mode composed of multiple Majorana modes as

$$d_M^\dagger = \sum_{n=1}^N (i\psi_{A,n}\gamma_{A,n} + \psi_{B,n}\gamma_{B,n}), \quad (4.35)$$

where $\psi_{A,n}$ and $\psi_{B,n}$ are respectively the amplitudes (discrete wavefunctions) of the Majorana modes $\gamma_{A,n}$ and $\gamma_{B,n}$ in the decomposition of $d_M^\dagger$. We can show that the operators

$$\gamma_A = \sum_n \psi_{A,n}\gamma_{A,n} \quad \text{and} \quad \gamma_B = \sum_n \psi_{B,n}\gamma_{B,n}, \quad (4.36)$$

are themselves Majorana operators since they are self-adjoint, idempotent, and obey to anticommutation relations. The goal now is to find the wavefunctions $\psi_{A,n}$ and $\psi_{B,n}$ of such Majorana modes so that $d_M^\dagger$ corresponds to a zero-energy mode. Recall that this feature is realized only if $Hd_M^\dagger|0\rangle = 0$, or equivalently, if $[H, d_M^\dagger] = 0$. This is translated in (4.35) as

$$\sum_{n=1}^N \psi_{A,n}[H, \gamma_{A,n}] + \psi_{B,n}[H, \gamma_{B,n}] = 0. \quad (4.37)$$

Given that all Majorana operators are linearly independent, by developing the commutators, we can show, for $n = 2, \dots, N-1$, that the wavefunctions need to obey to the equations

$$\mu\psi_{A,n} + (\Delta + t)\psi_{A,n+1} + (t - \Delta)\psi_{A,n-1} = 0, \quad (4.38)$$

$$\mu\psi_{B,n} + (\Delta + t)\psi_{B,n-1} + (t - \Delta)\psi_{B,n+1} = 0, \quad (4.39)$$

which can be rewritten in matrix form as

$$\begin{pmatrix} \mu & 0 \\ 0 & \mu \end{pmatrix} \psi_n + \begin{pmatrix} t - \Delta & 0 \\ 0 & t + \Delta \end{pmatrix} \psi_{n-1} + \begin{pmatrix} t + \Delta & 0 \\ 0 & t - \Delta \end{pmatrix} \psi_{n+1} = 0, \quad (4.40)$$

with the Majorana spinors $\psi_n = (\psi_{A,n} \ \psi_{B,n})^T$. In order to consider all modes $n = 1, \dots, N$ in (4.40), we have to add two additional fermionic modes c_0 and c_{N+1} to the chain with the imposed open boundary conditions

$$\psi_0 = \psi_{N+1} = 0. \quad (4.41)$$

Since we are interested by localized MZMs, we want their wavefunction to decay exponentially in the chain, which leads to the ansatz

$$\psi_n = z^n \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (4.42)$$

as a solution for (4.40). Inserting this ansatz in (4.40), we get the equation

$$\begin{pmatrix} \mu + (t + \Delta)z + (t - \Delta)/z & 0 \\ 0 & \mu + (t - \Delta)z + (t + \Delta)/z \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0, \quad (4.43)$$

which has a non-trivial solution if and only if the matrix is singular, *i.e.*, has a null determinant. The matrix being diagonal, the determinant is zero if only one of the diagonal elements is null. Equating the first element to zero, we get the two solutions

$$z_{\pm} = \frac{-\mu \pm \sqrt{\mu^2 - 4(t^2 - \Delta^2)}}{2(t + \Delta)}, \quad (4.44)$$

with the spinor $(\alpha \ \beta)^T \propto (1 \ 0)^T$. And equaling the second one to zero, we get

$$z'_\pm = 1/z_\mp = \frac{-\mu \pm \sqrt{\mu^2 - 4(t^2 - \Delta^2)}}{2(t - \Delta)}, \quad (4.45)$$

with the spinor $(\alpha \ \beta)^T \propto (0 \ 1)^T$. Therefore, the two orthogonal zero-energy solutions for the Majorana spinors are

$$\psi_n^A = (A_+ z_+^n + A_- z_-^n) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (4.46)$$

$$\psi_n^B = (B_+ z_+^{-n} + B_- z_-^{-n}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (4.47)$$

where $A_\pm$ and $B_\pm$ coefficients must be determined by the boundary conditions (4.41). Notice here that if $|z_\pm| < 1$, then ψ_n^A decreases and ψ_n^B increases with n , as depicted on Figure 4.7. This is the wanted behavior for MZM wavefunctions localized exponentially at each edge of the chain. Furthermore, in the limit $N \rightarrow \infty$, the boundary conditions $\psi_0^B = \psi_{N+1}^A = 0$ can be satisfied, whereas the conditions $\psi_{N+1}^B = \psi_0^A = 0$ are satisfied if $B_+ z_+^{-N-1} = -B_- z_-^{-N-1}$ and $A_+ = -A_-$. Thus, we get the final solutions for the spinors

$$\psi_n^A = \frac{1}{Z} (z_+^n - z_-^n) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \phi_n \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (4.48)$$

$$\psi_n^B = \frac{1}{Z} (z_+^{N+1-n} - z_-^{N+1-n}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \phi_{N+1-n} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (4.49)$$

with the normalization factor

$$Z = \sqrt{\frac{t}{\Delta} \frac{\mu^2 - 4(t^2 - \Delta^2)}{(4t^2 - \mu^2)}}. \quad (4.50)$$

Hence, the final zero-energy solution for the fermionic mode d_M is given by

$$d_M^\dagger = \frac{1}{2} (\gamma_B + i\gamma_A), \quad (4.51)$$

where

$$\gamma_A = \sum_n \phi_n \gamma_{A,n} \quad \text{and} \quad \gamma_B = \sum_n \phi_{N+1-n} \gamma_{B,n}. \quad (4.52)$$

From this, it is obvious to visualize that the MBS is composed of two MZMs, γ_A and γ_B , which are spread over multiple Majorana modes. These MZMs exponentially localizes at the left and right edges of the chain respectively, as shown on Figure 4.7. Moreover, the exponential decay towards the center of the chain, going as $|\phi_n| \propto e^{-n/\xi_M}$, shows a typical *localization length*

$$\xi_M = \max \left(\frac{1}{|\ln |z_+||}, \frac{1}{|\ln |z_-||} \right), \quad (4.53)$$

as shown in Appendix B. An interesting result is that for $\Delta = t$ and $\mu = 0$, we have $z_\pm = 0$ and $\xi_M = 0$, which corresponds to perfectly localized MZMs in accordance with the previously defined 'perfect topological phase'.

As enunciated above, in order to satisfy the boundary conditions (4.41), these solutions are realized only if $|z_\pm| < 1$. Indeed, if one of these was bigger than one, it would imply that both ψ_n^A and ψ_n^B solutions contain exponentially increasing and decreasing terms respectively with n , which makes impossible to satisfy (4.41). To summarize, the Kitaev chain shows a zero-energy solution only if the boundary conditions (4.41) are satisfied, *i.e.*, only if $|z_\pm| < 1$. In the

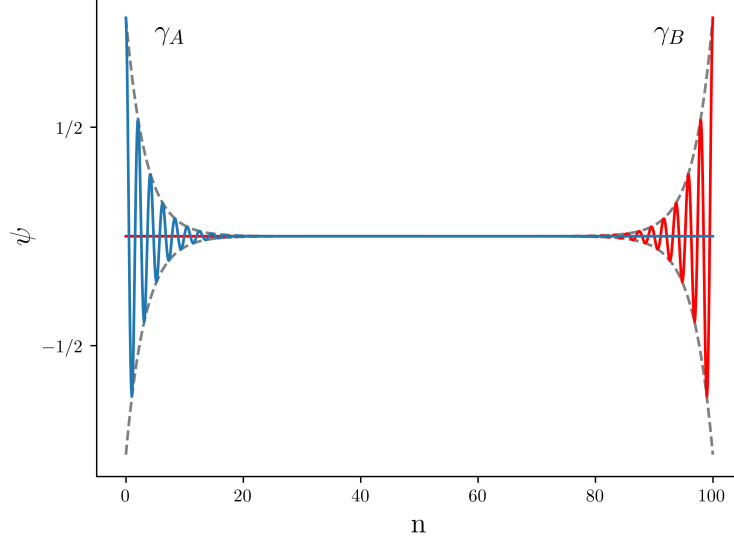


Figure 4.7: Wavefunctions exponentially localized at the left edge (blue) for γ_A and at the right edge (red) for γ_B in a 100-site Kitaev chain. The MBS wavefunction is the superposition of these two, resulting in a highly delocalized fermion. (Figure reproduced from [31]).

following, we show that this conditions on $z_{\pm}$ is equivalent to the parameter regime $|\mu| < 2t$, in other words the topological phase. Indeed, from the Vieta's formula for quadratic equations, we know that

$$z_+ z_- = \frac{t - \Delta}{t + \Delta}, \quad (4.54)$$

and therefore, $|z_+ z_-| < 1$. This mandates that at least one of the two $z_{\pm}$ must be smaller than one. There are two different cases from (4.44), either $z_{\pm}$ are complex conjugate numbers, which is realized when $\mu^2 < 4(t^2 - \Delta^2) < (2t)^2$ (topological phase), or $z_{\pm}$ are real and distinct numbers, which is realized when $\mu^2 > 4(t^2 - \Delta^2)$ (trivial or topological phases). In the first (topological) case, we have $|z_+ z_-| = |z_+|^2 = |z_-|^2 < 1$. Since both $z_{\pm}$ are smaller than one, a solution for the MBS exists. On the other hand, for the second (trivial and topological) case we only know that $|z_+| |z_-| < 1$. To have both $z_{\pm}$ lower than one, we may impose¹⁶ $(z_+^2 - 1)(z_-^2 - 1) > 0 \Leftrightarrow (4t^2 - \mu^2)/(t + \Delta)^2 > 0$. Thus, we have $|z_{\pm}| < 1$, only if $|\mu| < 2t$ for both cases. Thus, we conclude that the chain can host an MBS only in its topological phase. A final remark is that the boundary conditions leading to the solutions (4.48) and (4.49) are only valid in the thermodynamic limit, $N \rightarrow \infty$. As we will see later, a finite chain length gives rise to nontrivial effects that can be detrimental to the topological phase of the Kitaev chain.

4.4 Exchange statistics and topological quantum computing

While in a tridimensional space, the argument (2.2) for the exchange of two identical particles always holds (for point-like particles [45]), lower dimensional spaces lead to much more exotic exchange statistics than the bosonic and fermionic ones [5, 44]. Indeed, performing an exchange analysis through a Feynman path integral method [46] leads to *Abelian (commutative)*, and *non-Abelian anyonic* exchange statistics. The first corresponds to the multiplication of the system wavefunction by a phase factor $e^{i\phi}$ where ϕ is any rational multiple of 2π , whereas the second mandates the existence of a degenerate ground state for the system. In this case, exchanges of particles correspond to a unitary transformation U applied on the system wavefunction and

¹⁶If $x < 1$ and $y < 1 \Rightarrow (x^2 - 1)(y^2 - 1) > 0$.

inducing a non-trivial evolution in the degenerate ground state subspace. Furthermore, two different exchanges are represented by two distinct unitary transformations. Since the operators acting on a Hilbert space are, in general, non-commutative, the order in which the particles are exchanged matters for the final exchange result, hence the label *non-Abelian*. The non-Abelian anyons and their exotic exchange statistics are at the center of topological quantum computing. Indeed, as we will show later, it is possible to define a logical qubit in some parity sector of the degenerate many-body ground state. The gates needed to perform quantum algorithms are built from the unitary transformation resulting from the exchange of these particles. The exchange of particle in low-dimensional systems is also referred to as *braiding*.

Multiple effective 2D or 1D systems have been shown to host these anyons as quasiparticle excitations [7–9, 47], among which are Majorana zero modes. Indeed, it has been shown that MZMs emerging at vortices in 2D p -wave superconductors show non-Abelian anyonic statistics [14], as well as in effective 1D systems [15]. In the following section, we show that a system hosting more than two MZMs obeys non-Abelian exchange statistics, then we define a qubit from the degenerate ground state spanned by these MZMs and finally, we define the unitary gates needed for topological quantum computation.

First, let us consider two MZMs, γ_1 and γ_2 , hosted in some low-dimensional (1D or 2D) system. In the previous section, we have seen that these MZMs correspond to zero-energy excitations of the system. In the energy spectrum, they are separated from the next excitations by some energy gap. As long as the exchange time is longer than the characteristic time associated with the gap frequency, we can suppose that the system will remain at the same zero energy after exchange. Thus, the resulting state will still be a ground state of the system and the two modes remain MZMs. Such exchange procedure is called *adiabatic*. Considering that the fermion parity is not impacted during the exchange, we can consider that the Majorana operators are interchanged by some unitary matrix U as

$$U\gamma_1U^\dagger = \chi_2\gamma_2 \quad \text{and} \quad U\gamma_2U^\dagger = \chi_1\gamma_1, \quad (4.55)$$

where $\chi_{1,2}$ are phase factors. From the idempotent property of Majorana operators, we have that

$$1 = \left(U\gamma_mU^\dagger\right)^2 = \chi_n^2, \quad (4.56)$$

which yields $\chi_{1,2} = \pm 1$. Furthermore, we have seen previously that we can define a fermionic mode $d_M = (\gamma_1 + i\gamma_2)/2$ from these two MZMs, which occupation operator reads

$$n_M = d_M^\dagger d_M = \frac{1}{2}(1 + i\gamma_1\gamma_2). \quad (4.57)$$

Under exchange, this operator evolves as

$$Un_MU^\dagger = \frac{1}{2} \left(1 + iU\gamma_1\gamma_2U^\dagger\right) \quad (4.58)$$

$$= \frac{1}{2} (1 - i\chi_1\chi_2\gamma_1\gamma_2). \quad (4.59)$$

Since the fermion parity must be conserved for the 2-particle exchange, the number operator must be constant under such transformation which implies that $\chi_1\chi_2 = -1$. Therefore, either $\chi = \chi_1 = 1$ and $-\chi = \chi_2 = -1$, or the inverse.

Now, considering $2K$ MZMs in the system, the fermionic ground state is 2^K -fold degenerate and the exchange between two of them is once more defined by an unitary operator as

$$U_{nm}\gamma_nU_{nm}^\dagger = -\chi\gamma_m \quad \text{and} \quad U_{nm}\gamma_mU_{nm}^\dagger = \chi\gamma_n, \quad (4.60)$$

with $\chi = \pm 1$, as proved above. By setting $\chi = 1$, the unitary operator can be defined using the Majorana operators as

$$U_{nm} = \frac{1}{\sqrt{2}} (1 + \gamma_n \gamma_m) = \exp \left(\frac{\pi}{4} \gamma_n \gamma_m \right). \quad (4.61)$$

Indeed, one can insert (4.61) in the left-hand-side of (4.60) and, using the idempotent and anticommutation relations of the Majorana modes, will recover the correct right-hand-side. The exponential form is obtained in Appendix D. Furthermore, the inverse of U_{nm} , given by

$$U_{nm}^\dagger = U_{mn} = \frac{1}{\sqrt{2}} (1 + \gamma_m \gamma_n) = \exp \left(\frac{\pi}{4} \gamma_m \gamma_n \right), \quad (4.62)$$

also corresponds to an exchange of the two same MZMs but with a distinct outcome for the resulting wavefunction, an opposite phase than in (4.60) for the two modes. This is a key feature of low-dimensional space: there are many ways to exchange multiple particles associated to their respective outcome. A more visual sketch of this property for two anyons is shown in Figure 4.8. As a consequence, the exchange operators of three MZMs do not commute. Indeed, for $n \neq m \neq p \neq q$,

$$[U_{nm}, U_{mn}] = 0, \quad (4.63)$$

$$[U_{nm}, U_{pq}] = 0, \quad (4.64)$$

$$[U_{nm}, U_{mp}] = \gamma_n \gamma_p. \quad (4.65)$$

The non-Abelian aspect of the theory is encoded in the non-commutative nature of the two exchange operators sharing a single common particle (4.65). Moreover, we also observe that the exchange operators for a two-particle exchange always commute (4.63), and that the exchange of two particles do not affect the exchange of two others (4.64).

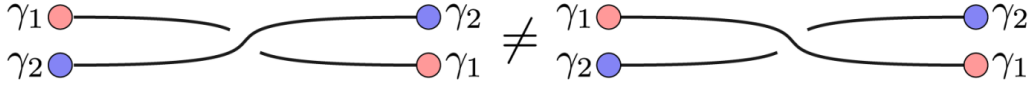


Figure 4.8: Sketch of the non-equivalence between the exchange operators U_{12} and U_{21} . (Figure taken from [31].)

Having shown the non-Abelian nature of the MZMs, here we define a qubit in a parity sector of the degenerate ground state subspace. Because of superselection rules¹⁷ [48, 49], one cannot define a physical fermionic state by superposing two modes of different parities. In a quantum computing framework, one requires quantum superposition to perform useful algorithms, and thus cannot use the degenerate ground state of only two MZMs to define a qubit. Indeed, recall that the two ground states show opposite parities. Thus, we need more than two MZMs. Let us consider four MZMs $\gamma_i : i = 1, \dots, 4$. From these, we can define two zero-energy fermionic modes, as usual, as

$$d_1 = (\gamma_1 + i\gamma_2)/2 \quad \text{and} \quad d_2 = (\gamma_3 + i\gamma_4)/2. \quad (4.66)$$

These two fermionic modes generate a 4-fold degenerate ground state with two states in each parity sector. The zero-energy states are $\{|00\rangle, d_1^\dagger |00\rangle = |10\rangle, d_2^\dagger |00\rangle = |01\rangle, d_1^\dagger d_2^\dagger |00\rangle = |11\rangle\}$ which are eigenstates of the parity operator $P = (1 - 2d_1^\dagger d_1)(1 - 2d_2^\dagger d_2)$ with

$$P |00\rangle = |00\rangle, \quad P |11\rangle = |11\rangle \quad \Rightarrow \text{even parity sector}, \quad (4.67)$$

$$P |10\rangle = -|10\rangle, \quad P |01\rangle = -|01\rangle \quad \Rightarrow \text{odd parity sector}. \quad (4.68)$$

¹⁷These superselection rules arise from the relativistic theory of electrons and the needed Lorentz invariance of the theory [48, 49].

Hence, we have two choices to define a logical qubit with a fixed parity:

$$|0\rangle \equiv |00\rangle \quad \text{and} \quad |1\rangle \equiv |11\rangle, \quad (4.69)$$

or

$$|\bar{0}\rangle \equiv |10\rangle \quad \text{and} \quad |\bar{1}\rangle \equiv |01\rangle. \quad (4.70)$$

Here, we have shown that, in order to define a qubit in a given parity sector, we need four MZMs, thus two zero-energy fermionic modes. In general, if one wants to define more than one qubit, one will require additional Kitaev chain to increase the size of the composite degenerate ground state [5, 44, 46].

Let us now define some 1-qubit gates that can be applied on the even parity qubit (4 MZMs) using the unitary operations for exchange of MZMs. One can prove that all exchange operations can be generated by

$$U_{12} = \exp\left(\frac{\pi}{4}\gamma_1\gamma_2\right) = \exp\left(i\frac{\pi}{4}\left(1 - 2d_1^\dagger d_1\right)\right), \quad (4.71)$$

$$U_{23} = \exp\left(\frac{\pi}{4}\gamma_2\gamma_3\right) = \frac{1}{\sqrt{2}}\left(1 + i\left(d_1^\dagger - d_1\right)\left(d_2^\dagger + d_2\right)\right), \quad (4.72)$$

$$U_{34} = \exp\left(\frac{\pi}{4}\gamma_3\gamma_4\right) = \exp\left(i\frac{\pi}{4}\left(1 - 2d_2^\dagger d_2\right)\right), \quad (4.73)$$

which actions on the even parity qubit basis¹⁸ are represented in matrix form, considering $|0\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix}^T$ and $|1\rangle = \begin{pmatrix} 0 & 1 \end{pmatrix}^T$, as

$$U_{12} = \begin{pmatrix} e^{i\pi/4} & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix}, \quad (4.74)$$

$$U_{23} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad (4.75)$$

$$U_{34} = \begin{pmatrix} e^{i\pi/4} & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix}. \quad (4.76)$$

From these matrices, we clearly see that we can build important unitary gates implementing logical operations such as

- The *NOT*-gate corresponding to a bit-flip:

$$X = -iU_{23}^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (4.77)$$

- The *Z*-gate corresponding to a phase shift of π :

$$Z = -i(U_{12})^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.78)$$

- The *Y*-gate corresponding to a bit-flip and π phase shift:

$$Y = -i(U_{12}U_{32}U_{21})^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (4.79)$$

¹⁸Recall that the braiding operations do not change the parity of the ground state, hence its matrix form on the whole subspace must be block-diagonal, each block corresponding to one parity sector. Thus, the 4×4 matrix acting on the 4-fold degenerate ground state can be reduced to a 2×2 matrix acting only on the even or odd sectors.

- The Hadamard gate that produces quantum superposition:

$$H = -iU_{12}U_{23}U_{21} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (4.80)$$

- The S -gate corresponding to a phase shift of $\pi/2$:

$$S = e^{i\pi/4}U_{21} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}. \quad (4.81)$$

One of the main advantages of topological quantum computing with anyons over other quantum computing platforms relies on the fact that the outcome of the exchange gates does not depend on the details of the anyons' trajectories. Indeed, the logical operations depending on the exchange of the particles, as long as no scattering event or perturbation alters the topology of the braids, the outcome remains unchanged. These gates are thus said to be 'topologically protected' [46] (see Figure 4.9).

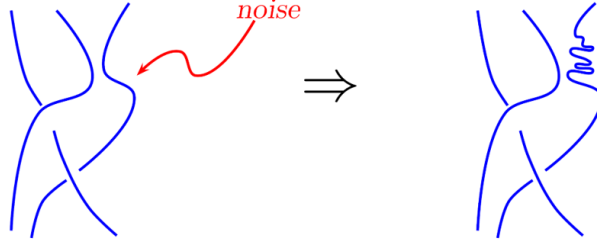


Figure 4.9: Naive representation of the 'topological protection' of the braiding gates. As long as a noise do not alter the anyons' trajectories, the outcome remains unchanged. (Figure taken from [46].)

In order to get quantum supremacy over classical computer, one would need to build a *universal quantum computer*, *i.e.*, a quantum computer able to perform any unitary operations on a set of qubits. This means that it must include a finite universal set of gates which can approximate any unitary evolution of the system to an arbitrary precision only by multiple combinations of them. An instance of this set of gates is $\mathcal{S} = \{H, T, cX\}$. The two last gates are defined as:

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \quad \text{and,} \quad (4.82)$$

$$cX = \left(\frac{\mathbf{1}}{\mathbf{0}} \middle| \frac{\mathbf{0}}{X} \right), \quad (4.83)$$

where T corresponds to a phase shift of $\pi/4$, and cX is a 2-qubit gate which applies a *NOT*-gate on the second qubit only if the first one is in state $|1\rangle$. Otherwise the second one is unchanged. While the H gate can be performed by braiding (4.80) and the cX -gate can be implemented through fermion-parity projective measurement and braiding operations [50], this is not possible to compose the T -gate through braiding operations. However, it is possible to build a T -gate in a topologically unprotected ways, which would then require error correction protocols [31].

Finally, since the qubit is encoded in the degenerate ground state of two Kitaev chains, it is protected from external excitations by the energy gap $2t$ from external excitations (see Fig. 4.6). Moreover, the qubit belongs to a definite parity sector of the combined ground state and cannot transition to the opposite sector since the Kitaev Hamiltonian conserves fermionic parity, *i.e.*, $[H, P] = 0$. This intrinsic noise resilience along with the topological protection of braiding gates makes topological quantum computing with MZMs a highly promising platform for the realization of scalable and fault-tolerant quantum computation.

4.5 Finite-size Kitaev chain and end-to-end correlations

The major issue encountered with the Kitaev model is that, in reality, the chain is always finite. Indeed, in a finite case, the zero-energy mode (4.51) is no longer an eigenmode of the Kitaev Hamiltonian (4.1), except for the perfect sweet spot $\mu = 0$ which is not tractable experimentally. This finite size effect comes from the boundary conditions (4.41), only met when $N \rightarrow \infty$. In fact, this mode corresponds to a non-zero energy E_M which Hamiltonian reads

$$H_M = \frac{i}{2} E_M \gamma_A \gamma_B = E_M \left(d_M^\dagger d_M - \frac{1}{2} \right). \quad (4.84)$$

As a result, for a finite number site, the latter degenerate ground state is no longer degenerate. Hence, the protection of the qubit vanishes since an external excitation of energy E_M could break the computational basis (the parity is altered). However, we can show that, in the topological phase, this energy decays exponentially as $E_M \propto e^{-N/\xi_M}$ [13]. This is shown in Figure 4.10. Hence, as long as $N \gg \xi_M$, the ground state can be considered degenerate, and the transitions between the two ground states¹⁹ are exponentially suppressed.

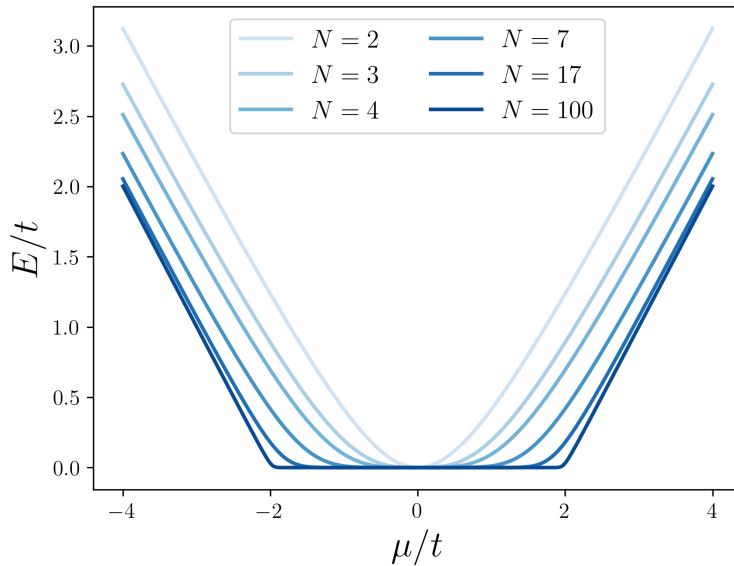


Figure 4.10: Energy of the lowest excitation mode of the Kitaev Hamiltonian for $N = 2, 3, 4, 7, 17, 100$. We clearly see that in the topological region $|\mu/t| < 2$, the energy decays with N until reaching a null value for sufficiently large chains.

Another consequence of this finite size is the impossibility to properly define a topological invariant for the chain. Indeed, the topology encoded in the band structure of the model is obtained when $N \rightarrow \infty$, which can be seen in the definition of the winding number W (4.24), requiring a continuous interval of values for the momentum k . However, as we will see now, we can still probe the topological nature of a state through the so-called *end-to-end correlations* [51]. The main idea behind this relies on the fact that, if the chain is sufficiently long, correlations between the edge modes, c_1 and c_N , could only appear if the chain is in a state where a fermion delocalizes at each of its edges. Let us try to build a function that quantifies these correlations.

If we consider the chain such that $\mu = 0$ and $\Delta = t$, the Kitaev Hamiltonian takes the form (4.32) from which the mode

$$d_M = \frac{1}{2} (\gamma_{B,N} - i\gamma_{A,1}) \quad (4.85)$$

¹⁹Note here that the term 'ground state' is improper for the occupation of mode d_M when $E_M \gg 0$.

is absent. Recall that this mode represents a perfectly delocalized fermion at each edge of the chain fully occupying the MZMs $\gamma_{A,1}$ and $\gamma_{B,N}$. From them, we can define the operator

$$Q_R = i\gamma_{A,1}\gamma_{B,N} = 2d_M^\dagger d_M - 1, \quad (4.86)$$

which eigenvalues are $+1$ if the mode d_M is filled, and -1 otherwise. However, for any of the degenerate ground states, $|GS\rangle_{\text{even}} = |0\rangle$ or $|GS\rangle_{\text{odd}} = |1\rangle = d_M^\dagger |0\rangle$, we notice that

$$|\langle GS| Q_R |GS\rangle| = 1. \quad (4.87)$$

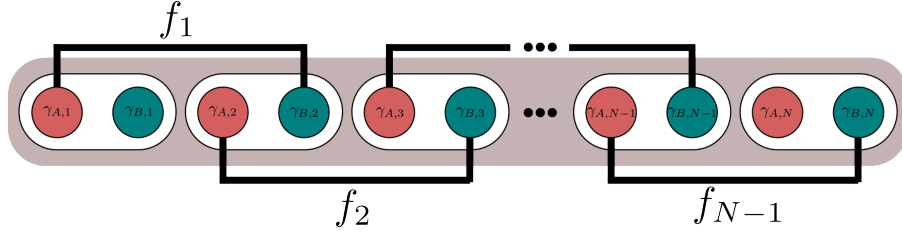


Figure 4.11: Alternative ‘perfect topological phase’ of the Kitaev chain with $\mu = 0$ and $t = -\Delta$. In this case the eigenexcitations of the system, $f_n = \frac{1}{2}(\gamma_{B,n+1} + i\gamma_{A,n})$, are still composed of two Majorana modes from neighboring physical sites, but with the complementary coupling of (4.31). Therefore, the uncoupled MZMs become $\gamma_{B,1}$ and $\gamma_{A,N}$.

Considering now, $\mu = 0$ and $t = -\Delta$, the Kitaev Hamiltonian reads,

$$H = -it \sum_{n=1}^{N-1} \gamma_{A,n} \gamma_{B,n+1}, \quad (4.88)$$

in which the missing Majorana operators are $\gamma_{B,1}$ and $\gamma_{A,N}$. This Hamiltonian corresponds to another phase of the Kitaev chain still containing two edge MZMs, as pictured in Figure 4.11. From these two, we define the new delocalized fermionic operator

$$f_M = \frac{1}{2}(\gamma_{B,1} - i\gamma_{A,N}), \quad (4.89)$$

such that we can define the operator

$$Q_L = i\gamma_{A,N}\gamma_{B,1} = 2f_M^\dagger f_M - 1, \quad (4.90)$$

which is the analog of (4.86), and shows the same eigenvalues. Thus, regardless of the choice of the parameter one can define the *end-to-end correlations*, or *Q-function*,

$$Q = |\langle Q_L + Q_R \rangle| = 2 \left| \langle c_N^\dagger c_1 + c_1^\dagger c_N \rangle \right|, \quad (4.91)$$

measuring the average end-to-end hopping between the two physical fermionic sites. The two extreme parameter regimes presented above give a value of 1 for the *Q-function* when the system is in its ground state (odd or even). However, as shown in Section 4.3, when $0 \neq |\mu| < 2t$, the MBS spreads over multiple fermionic sites. Consequently, the *Q-function* will be lower than 1 even if the system is in a topological phase. Furthermore, for the trivial phase $|\mu| > 2t$, as the size of the system increases, the values *Q* converge to zero when $N \rightarrow \infty$ [51]. This can be seen in Figure 4.12. Hence, this function is a relevant tool to assess the topological character of the system.

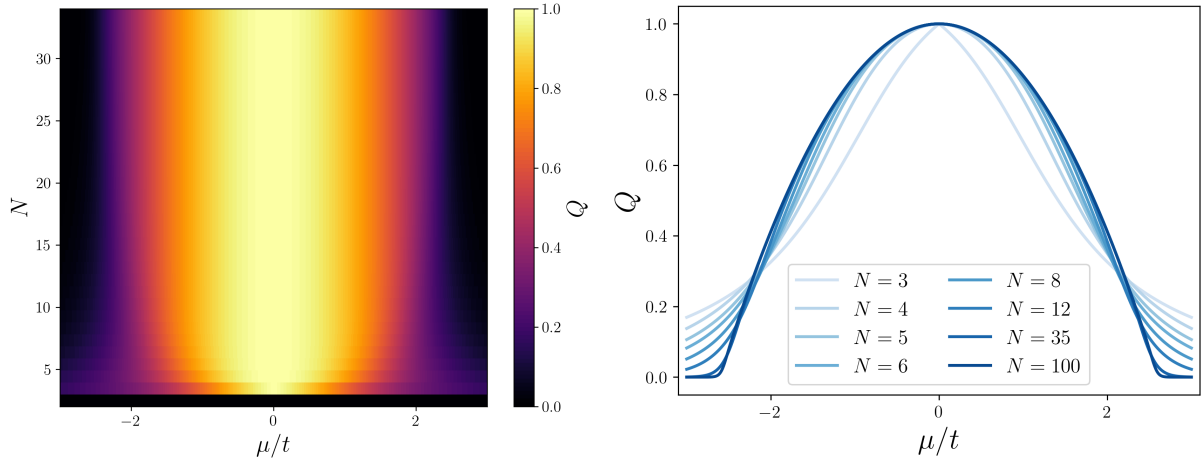


Figure 4.12: End-to-end correlations of the even ground state (the Bogoliubov vacuum) for increasing values of N with $\Delta = t$. Notice on the right plot that Q converges to zero when N increases for $|\mu| > 2t$. Moreover, the maximum value of Q happens for $\mu = 0$ and decreases when μ increases corresponding to a spreading wavefunction of the MBS over the bulk modes as depicted in Figure 4.7. Finally, the black horizontal line on the bottom corresponds to the correlations of the even ground state of the 2-site Kitaev chain. They are null for any chemical potential values, as we will see in Section 6.1. The computation of these correlations for the ground state is explained in Appendix C.

However, one should be careful when using this function as a sufficient condition to assess the presence of an MBS in a finite size Kitaev chain. Indeed, as we will show later, for very small chains, some eigenmodes of the system present a non-zero Q -function even though they are not associated to a null energy. This comes from the fact that, despite being well localized in the chain, these modes have a decay length longer than the chain size and spread over the edge modes c_1 and c_N .

To summarize the main results of the first part of this Master's thesis, we have emphasized the importance of the topological phase, ($|\mu| < 2t$), of the Kitaev chain for quantum computing. In this regime, a qubit can be encoded in the degenerate ground state of two Kitaev chains and is expected to exhibit intrinsic resilience to noise. This protection stems from the energy gap $2t$, which separates the degenerate ground states from the excited states. Furthermore, since the Kitaev Hamiltonian conserves fermionic parity, a computational basis defined within a given parity sector should remain stable under the system's intrinsic dynamics. In realistic experimental implementations [52, 53], however, the Kitaev chain is inevitably coupled to a fermionic environment. Such an environment can excite the system provided that a sufficient amount of energy is transferred ($E > 2t$). In addition, it can locally alter the parity of the chain while preserving the parity of the total chain-environment system [16]. Consequently, the parity of the chain alone is no longer necessarily conserved. In the second part of this work, we employ the GKSL master-equation framework to model the dissipative coupling between a finite-size Kitaev chain and a fermionic environment. This approach allows us to quantify the topological character of the system through the Q -function and to assess the impact of the environment on parity conservation and the population of excited states.

Part II

The Open Part

5 Open quantum systems

Before introducing the modeling of dissipation in a Kitaev chain coupled to a fermionic environment, we first present the theoretical tools required to describe open quantum systems within the GKSL framework.

5.1 Density operator

In quantum mechanics, the most complete description that can be given of an isolated system is provided by its wavefunction $|\psi(t)\rangle$, whose time evolution is deterministically dictated by the Schrödinger equation. However, when the system is no longer isolated and, instead, forms part of a larger composite system, a more general mathematical object is required to describe its state: the *density operator* ρ [25]. Indeed, when the system interacts with an environment, or when projective measurements are performed without complete knowledge of the outcomes, the wavefunction description is no longer sufficient. In such situations, the state of the system must incorporate a statistical aspect accounting for our uncertainty. The density operator precisely provides this generalized description, allowing both pure quantum states and statistical mixtures to be treated. Let us define it and give its most important properties relevant for this work.

If the state of the system $|\psi(t)\rangle$ is completely known, it is referred to as a *pure state*, and its density operator is given by

$$\rho = |\psi\rangle\langle\psi|. \quad (5.1)$$

However, for some of the reasons discussed above, it may no longer be possible to assign a pure state to the system. Instead, we may only know that the system can be found in a set of states $|\psi_k\rangle$, each occurring with probability $0 \leq p_k \leq 1$. In this case, its density operator is defined as

$$\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|, \quad (5.2)$$

with $\sum_k p_k = 1$. Such statistical state is called a *mixed state*.

Here are some properties of the density operator [22]:

- For any quantum state (pure or mixed), the trace of the density operator, represented in a given basis as the *density matrix* is always equal to 1. Indeed, considering an orthonormal basis $\{|b_i\rangle\}$ of the Hilbert space,

$$\text{Tr}(\rho) = \sum_i \langle b_i | \rho | b_i \rangle, \quad (5.3)$$

$$= \sum_{i,k} p_k |\langle b_i | \psi_k \rangle|^2, \quad (5.4)$$

$$= \sum_k p_k \sum_i |\langle b_i | \psi_k \rangle|^2 = 1. \quad (5.5)$$

The last equality follows from both the normalization of the probabilities, $\sum_k p_k = 1$, and the normalization of each state ψ_k . The proof for a pure state is straightforward since a pure state corresponds to a mixed state in which all probabilities vanish except one equal to 1.

- Only a pure state possesses a squared density operator with unit trace. Indeed,

$$\text{Tr}(\rho^2) = \sum_k p_k^2 \leq 1, \quad (5.6)$$

since $0 \leq p_k \leq 1$. The equality holds only for a pure state, *i.e.*, when one probability satisfies $p_k = 1$ while others vanish. The quantity $\text{Tr}(\rho^2)$ therefore provides a measure of the mixed character of the state ρ , and is called the *purity* of the state. Its value is bounded by, $\frac{1}{\dim(\mathcal{H}_S)} \leq \text{Tr}(\rho^2) \leq 1$, where $\mathcal{H}_S$ is the Hilbert space of the system. When the purity is equal to its minimal value, the state is said to be *maximally mixed*. In this case, the decomposition of the state in any basis of the Hilbert space is completely homogeneous, meaning that no particular state is statistically favored over another.

- The density operator is hermitian: $\rho = \rho^\dagger$. Hence, its matrix representation can always be diagonalized in a particular basis, which allows the identification of the pure states composing the statistical mixture. For this reason, the diagonal elements $\langle b_i | \rho | b_i \rangle$ of the density matrix are called the *populations*. They encode the probabilities associated with the different basis states $|b_i\rangle$ in the statistical mixture. By contrast, the off-diagonal elements are called the *coherences*. These terms quantify quantum superpositions between the populations and are non-zero only when the state ρ possesses superposed states.
- The time evolution of the density operator is determined through the *Liouville-von Neumann equation*:

$$\dot{\rho}(t) = -i[H, \rho(t)], \quad (5.7)$$

where H is the Hamiltonian of the system. This equation directly follows from the composite states in (5.2) obeying to the Schrödinger equation. Therefore, defining the *Liouvillian superoperator* $\mathcal{L}$ acting on the Hilbert-Schmidt vector space of operator $\mathcal{B}_2(\mathcal{H}_S)$ as

$$\mathcal{L} : \mathcal{B}_2(\mathcal{H}_S) \rightarrow \mathcal{B}_2(\mathcal{H}_S), \rho \mapsto -i[H, \rho], \quad (5.8)$$

we can rewrite the Liouville-von Neumann equation as

$$\dot{\rho}(t) = \mathcal{L}\rho(t). \quad (5.9)$$

Hence, the solution for a time-independent Liouvillian is given by

$$\rho(t) = e^{\mathcal{L}t} \rho(0), \quad (5.10)$$

where $\rho(0)$ is the initial state.

In the following, quantifying how close two quantum states are to each other will be relevant. For this, if the states are described by the density operators ρ and σ , we can use the *fidelity* $F(\rho, \sigma)$, defined as [54]

$$F(\rho, \sigma) = \left(\text{Tr} \left(\sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right) \right)^2. \quad (5.11)$$

This quantity is bounded by $0 \leq F(\rho, \sigma) \leq 1$. The value $F(\rho, \sigma) = 1$ is obtained when the two states are identical, *i.e.*, $\rho = \sigma$, while $F(\rho, \sigma) = 0$ corresponds to two perfectly distinguishable, orthogonal states²⁰. If one of the two states is pure, then the fidelity takes the simpler form

$$F(\rho, \sigma) = \text{Tr}(\rho\sigma). \quad (5.12)$$

Indeed, if ρ is pure, then $\sqrt{\rho} = \rho = |\psi^{(\rho)}\rangle\langle\psi^{(\rho)}|$, therefore

$$F(\rho, \sigma) = \left(\text{Tr} \left(\sqrt{|\psi^{(\rho)}\rangle\langle\psi^{(\rho)}| \sigma |\psi^{(\rho)}\rangle\langle\psi^{(\rho)}|} \right) \right)^2 = \langle\psi^{(\rho)}| \sigma |\psi^{(\rho)}\rangle = \text{Tr}(\rho\sigma). \quad (5.13)$$

²⁰Here, orthogonality means that the decompositions of the two density operators, as defined in (5.2), respectively involve states $|\psi_k^{(\rho)}\rangle$ and $|\psi_k^{(\sigma)}\rangle$ belonging to two orthogonal subspaces of the Hilbert space, making ρ and σ perfectly distinguishable.

A key result of the density-operator formalism is that the expectation value of an observable A can be expressed as

$$\langle A(t) \rangle = \text{Tr}(A\rho(t)). \quad (5.14)$$

Indeed, considering the statistical average over the different states composing ρ in (5.2), we obtain

$$\langle A(t) \rangle = \sum_k p_k \langle \psi_k(t) | A | \psi_k(t) \rangle = \text{Tr}(A\rho(t)). \quad (5.15)$$

Therefore, the expectation value at a given time t incorporates both the intrinsic quantum uncertainty associated with the measure, but also the statistical uncertainty arising from the fact that the system may be in different states with probabilities p_k .

Finally, a given a density operator ρ representing a composite system $S + B$ of corresponding Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$, we define the *partial trace* over B the operator [55]

$$\rho_S = \text{Tr}_B(\rho) : \mathcal{H}_S \rightarrow \mathcal{H}_S, \langle i | \rho_S | i' \rangle = \sum_k \langle i, k | \rho | i', k \rangle, \quad (5.16)$$

with $\{|i, k\rangle = |i\rangle \otimes |k\rangle\}$, the basis of $\mathcal{H}_S \otimes \mathcal{H}_B$. Similarly, the *partial trace* over S is the operator

$$\rho_B = \text{Tr}_S(\rho) : \mathcal{H}_B \rightarrow \mathcal{H}_B, \langle j | \rho_B | j' \rangle = \sum_k \langle k, j | \rho | k, j' \rangle. \quad (5.17)$$

These operators no longer act on the composite Hilbert space but instead on $\mathcal{H}_S$ and $\mathcal{H}_B$, respectively. The advantage of performing a partial trace is that it reduces the dimensionality of the density operator. Furthermore, the expectation value of an observable of the form $\hat{A} = A \otimes \mathbb{1}$, *i.e.*, an observable acting only on the subsystem S , is given by

$$\langle \hat{A} \rangle = \text{Tr}(\hat{A}\rho) = \text{Tr}(A\rho_S). \quad (5.18)$$

Therefore, once the partial trace has been performed, it is sufficient to compute the trace over the reduced density operator ρ_S to obtain the desired expectation value. An analogous result holds for observables acting only on the subsystem B .

5.2 Interaction picture

Quantum mechanics admits multiple equivalent representations. The most commonly used are the *Schrödinger picture* and the *Heisenberg picture*. In the Schrödinger picture, the state of the system is described by a time-dependent normalized wavefunction (or a density operator) whose evolution is governed by the Schrödinger equation (or Liouville-von Neumann equation). In this representation, observables are represented by operators that are non-intrinsically time dependent. By contrast, in the *Heisenberg picture*, the state of the system is time independent, while the observables become intrinsically time-dependent operators evolving according to the *Heisenberg equation* [22]. These two pictures are fully equivalent and are related to each other through unitary transformations acting on states and observables.

However, these two representations are not unique. Indeed, let us consider a system whose dynamics are governed by a Hamiltonian of the form

$$H(t) = H_0 + H_I(t), \quad (5.19)$$

where H_0 is the free Hamiltonian of the system and $H_I(t)$ corresponds to an interaction term. In this situation, instead of working in the Schrödinger or Heisenberg picture, we can introduce

the *interaction picture*, in which both the states and the observables become intrinsically time dependent. In the interaction picture, the time evolution of the states is governed by the interaction Hamiltonian $H_I(t)$, whereas the observables evolve according to the free Hamiltonian H_0 .

Let us now derive the interaction picture starting from the Schrödinger picture by considering a time-independent interaction H_I , such that the total Hamiltonian H is also time independent. Given an observable $A(t)$, which can be explicitly time dependent in the Schrödinger picture, and a state of the system $\rho(t)$, at all time the expectation value of the observable reads

$$\langle A(t) \rangle = \text{Tr} \left(A(t) U(t, t_0) \rho(t_0) U^\dagger(t, t_0) \right), \quad (5.20)$$

where we define the unitary time-evolution operator

$$U(t, t_0) = e^{-iH(t-t_0)}. \quad (5.21)$$

This latter maps the system at initial time t_0 on its state at time t . By introducing the time-evolution operators

$$U_0(t, t_0) = e^{-iH_0(t-t_0)}, \quad (5.22)$$

$$U_I(t, t_0) = U_0^\dagger(t, t_0) U(t, t_0) = e^{-iH_I(t-t_0)}, \quad (5.23)$$

the expectation value of the observable $A(t)$ can be rewritten as

$$\langle A(t) \rangle = \text{Tr} \left(U_0^\dagger(t, t_0) A(t) U_0(t, t_0) U_I(t, t_0) \rho(t_0) U_I^\dagger(t, t_0) \right) \quad (5.24)$$

$$= \text{Tr} (A_I(t) \rho_I(t)). \quad (5.25)$$

In the second line, we defined the representation of the observable in the interaction picture as

$$A_I(t) = U_0^\dagger(t, t_0) A(t) U_0(t, t_0), \quad (5.26)$$

in which we see that the intrinsic time dependence is indeed governed by the free Hamiltonian H_0 . The representation of the state of the system in the interaction picture is

$$\rho_I(t) = U_I(t, t_0) \rho(t_0) U_I^\dagger(t, t_0), \quad (5.27)$$

which evolution is governed by the interaction Hamiltonian H_I . The latter being an observable, it also has a representation following (5.26) as

$$H_I(t) = U_0^\dagger(t, t_0) H_I U_0(t, t_0). \quad (5.28)$$

Therefore, the Liouville-von Neumann equation becomes

$$\dot{\rho}_I(t) = -i[H_I(t), \rho_I(t)]. \quad (5.29)$$

5.3 Microscopic derivation of a GKSL master equation

While for simple closed quantum systems, the unitary dynamic is easily found by solving the Schrödinger (for a pure state) or the Liouville-von Neumann (for a mixed state) equations (5.29), in general, it is no longer possible to get a solution for complex open quantum systems. Indeed, by open quantum system, we refer to a system of interest S interacting with an environment B . Even though the global system composed of both systems $S + B$ evolves unitarily, finding a solution for its equation of motion becomes untractable. In general, the environment often presents a substantial number of degrees of freedom, resulting in a set of non-linear and coupled equations for the dynamics, from which no useful information can be extracted. However, one

can still get information on the system of interest by deriving an equation of motion containing only the degrees of freedom of this reduced system, but keeping track of the non-unitary effects arising from the $S + B$ interactions: *a master equation*. This section follows the microscopic derivation of [22].

In this framework, the global system $S + B$ is represented by a density operator ρ composed of states living in the Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$, where $\mathcal{H}_S$ and $\mathcal{H}_B$ are the Hilbert spaces of the isolated system of interest and the environment, respectively. The time evolution of this global state is unitary and is ruled by the global Hamiltonian

$$H(t) = H_S \otimes \mathbb{1}_B + \mathbb{1}_S \otimes H_B + H_I(t), \quad (5.30)$$

where H_S and H_B are the Hamiltonians of the isolated components, and $H_I(t)$ is the interaction Hamiltonian between them. A schematic representation is shown in Figure 5.1.

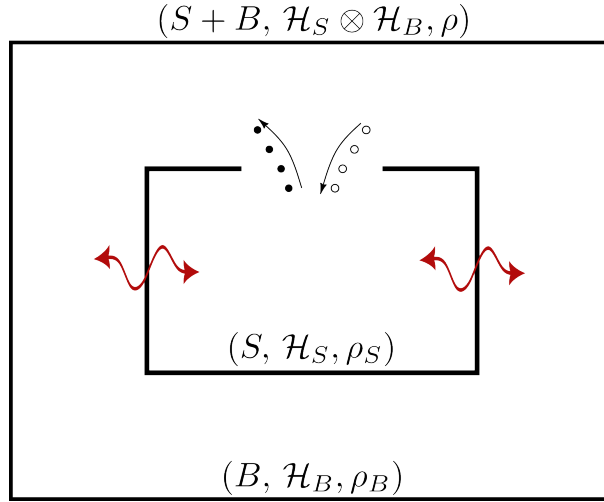


Figure 5.1: Schematic representation of an open quantum system S interacting with an environment B , together forming a globally closed system $S + B$. The interaction may involve the absorption or emission of particles, as well as other mechanisms of energy exchange, represented by the red wavy arrows.

As stated previously, we are interested in obtaining a reduced description for the open system. Thus, for all time, we want the form of the density operator for S given by

$$\rho_S = \text{Tr}_B(\rho), \quad (5.31)$$

which is the partial trace over all the degrees of freedom of the environment. Consequently, the time evolution of ρ_S is obtained by application of the unitary time-evolution operator (5.21) on the global state as

$$\rho_S(t) = \text{Tr}_B \left(U(t, t_0) \rho(t_0) U^\dagger(t, t_0) \right), \quad (5.32)$$

which gives the Liouville-von Neumann equation for the open system

$$\dot{\rho}_S(t) = -i \text{Tr}_B ([H(t), \rho(t)]). \quad (5.33)$$

Unfortunately, as stated before, this equation is often non-solvable. Thus, we are going to derive a master equation by performing few approximations.

For this purpose, it can be useful to start from the equation of motion of the global system and to switch to the interaction picture in which the operators and the density operator are given by (5.26) and (5.27). This being, the equation of motion for the global system reads²¹

$$\dot{\rho}(t) = -i [H_I(t), \rho(t)], \quad (5.34)$$

²¹In the following, we will say explicitly when we switch from a picture to another so that we do not need to index the variables.

where, now, the only appearing Hamiltonian is the $S + B$ interactions. Integrating (5.34), we obtain

$$\rho(t) = \rho(0) - i \int_0^t ds [H_I(s), \rho(s)] \quad (5.35)$$

which can be inserted back in (5.34) giving

$$\dot{\rho}_S(t) = - \int_0^t ds \text{Tr}_B ([H_I(t), [H_I(s), \rho(s)]]), \quad (5.36)$$

where we have applied the partial trace over B to get the reduced description for S , and supposed that $\text{Tr}_B([H_I(t), \rho(0)]) = 0$.

While the equation (5.36) is fully accurate, it is an integro-differential equation in which the global density operator still appears and is non-local in time. This means that the instantaneous variation of ρ_S depends on the past of the global system, *i.e.*, this involves memory effects. In order to get our master equation, we will perform two approximations to simplify the problem:

- the *Born approximation* which supposes a weak-coupling between the open system and the environment. This means that the state of the environment is negligibly affected and the global state of the system is given by

$$\rho(t) \approx \rho_S(t) \otimes \rho_B, \quad (5.37)$$

with ρ_B , the density operator of the environment. In (5.37), the global state is a product state which facilitates the partial trace over the degrees of freedom of B , and allows us to get rid of ρ .

- the *Markov approximation* which supposes that excitations that may appear in the environment will decay over time faster than the typical $S + B$ interaction dynamics. Hence, we can consider that ρ_S is local in time, *i.e.* there is no more memory effects of the environment over the system of interest.

Hence, given these two approximations, (5.36) becomes

$$\dot{\rho}_S(t) = - \int_0^t ds \text{Tr}_B ([H_I(t), [H_I(s), \rho_S(t) \otimes \rho_B]]), \quad (5.38)$$

which can be further simplified by performing the change of variable $s \rightarrow t - s$ and by taking the limit $t \rightarrow \infty$ for the integral upper bound as

$$\dot{\rho}_S(t) = - \int_0^\infty ds \text{Tr}_B ([H_I(t), [H_I(t - s), \rho_S(t) \otimes \rho_B]]). \quad (5.39)$$

This limit shows mere impacts as long as the memory of the bath, encoded in the decay time τ_B of the bath correlation functions (introduced later), is much smaller than the typical evolution time of the interacting open system τ_R , *i.e.*, $\tau_B \ll \tau_R$. Indeed, we can see that the integration variable s 'scans' the past of the interaction in the integrand. If the memory decays fast enough, then we can integrate over the infinite past with mere impact on the predictions accuracy. The next step is to develop the commutators.

In the Schödinger picture, the interaction Hamiltonian can always be decomposed as

$$H_I = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}, \quad (5.40)$$

where $A_\alpha = A_\alpha^\dagger$ and $B_\alpha = B_\alpha^\dagger$ are hermitian operators acting on $\mathcal{H}_S$ and $\mathcal{H}_B$, respectively. Considering a discrete spectrum for the open system Hamiltonian H_S which eigenvectors are noted $|\epsilon\rangle$, such that $H_S |\epsilon\rangle = \epsilon |\epsilon\rangle$, we define the operators

$$A_\alpha(\omega) = \sum_{\omega=\epsilon'-\epsilon} \langle \epsilon | A_\alpha | \epsilon' \rangle | \epsilon \rangle \langle \epsilon' |. \quad (5.41)$$

Since the set of operators $\{|\epsilon\rangle\langle\epsilon'|\}$ forms a complete basis of the Hilbert-Schmidt space $\mathcal{B}_2(\mathcal{H}_S)$, we have the completeness relations

$$\sum_{\omega} A_\alpha(\omega) = \sum_{\omega} A_\alpha^\dagger(\omega) = A_\alpha. \quad (5.42)$$

Therefore, the operators $A_\alpha(\omega)$ are simply the terms associated to the transition $\omega = \epsilon' - \epsilon$ of the system Hamiltonian spectrum in the $\{|\epsilon\rangle\langle\epsilon'|\}$ decomposition of A_α . Moreover, the operators (5.41) are *eigenoperators* of H_S , defined by the following properties:

$$[H_S, A_\alpha(\omega)] = -\omega A_\alpha(\omega), \quad (5.43)$$

$$[H_S, A_\alpha^\dagger(\omega)] = +\omega A_\alpha^\dagger(\omega). \quad (5.44)$$

Given (5.43) and (5.44), we can show by the use of the *Baker-Campbell-Hausdorff formula* [56] that

$$e^{iH_S t} A_\alpha(\omega) e^{-iH_S t} = e^{-i\omega t} A_\alpha(\omega), \quad (5.45)$$

$$e^{iH_S t} A_\alpha^\dagger(\omega) e^{-iH_S t} = e^{+i\omega t} A_\alpha^\dagger(\omega), \quad (5.46)$$

which allows us to easily switch back to the interaction picture where the interaction Hamiltonian now reads

$$H_I(t) = \sum_{\alpha, \omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha(t) = \sum_{\alpha, \omega} e^{i\omega t} A_\alpha^\dagger(\omega) \otimes B_\alpha^\dagger(t), \quad (5.47)$$

with $B_\alpha(t) = e^{iH_B t} B_\alpha e^{-iH_B t}$. Thus, by developing the commutators in (5.39), we get

$$\dot{\rho}_S(t) = \int_0^\infty \text{Tr} [H_I(t-s) \rho_S(t) \rho_B H_I(t) - H_I(t) H_I(t-s) \rho_S(t) \rho_B + \text{h.c.}] \quad (5.48)$$

$$= \sum_{\alpha, \beta} \sum_{\omega, \omega'} e^{i(\omega' - \omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S(t) A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_S(t) \right) + \text{h.c.}, \quad (5.49)$$

where we defined the one-sided Fourier transform

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds e^{i\omega s} \langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle, \quad (5.50)$$

with the *bath correlation functions* (BCFs)

$$\langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle \equiv \text{Tr}_B \left(B_\alpha^\dagger(t) B_\beta(t-s) \rho_B \right). \quad (5.51)$$

By considering a stationary bath, we simply have

$$\langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle = \langle B_\alpha^\dagger(s) B_\beta(0) \rangle \equiv \alpha_{\alpha\beta}(s). \quad (5.52)$$

These functions measure the time-correlations in the environment emerging from its interaction with the system of interest, *i.e.*, the memory of interaction events in the environment. In order to preserve the reliability of the Markov approximation, we want a decay time τ_B for these functions much smaller than the typical evolution time of the system due to its interaction,

τ_R . The equation of motion (5.49) obtained after applying the Born-Markov approximations is known as the *Redfield master equation*. A major limitation of this equation is that it does not, in general, generate a completely positive and trace-preserving dynamical map. Consequently, the density operator evolving according to the Redfield equation may develop negative populations at certain times, which is unphysical since populations represent probabilities and must therefore remain non-negative.

In order to solve this problem, a final approximation can be performed if the typical time scale of the isolated system $\tau_S \sim |\omega' - \omega|^{-1}$, for some transition frequencies $\omega \neq \omega'$ in the spectrum of H_S , is small compared to the evolution time due to the interaction with the environment τ_R . In such case, the terms with $\omega \neq \omega'$ in (5.49) can be neglected. Indeed, these terms are oscillating fast and average, then, to zero through time. This approximation, called the *secular approximation*, preserves the positivity of the density operator for all time. Therefore, (5.49) becomes

$$\dot{\rho}_S(t) = \sum_{\alpha,\beta} \sum_{\omega} \Gamma_{\alpha\beta}(\omega) \left(A_{\beta}(\omega) \rho_S(t) A_{\alpha}^{\dagger}(\omega) - A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega) \rho_S(t) \right) + \text{h.c.} \quad (5.53)$$

Finally, we can decompose the Fourier transforms of the BCFs as follows

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2} \gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega), \quad (5.54)$$

with

$$S_{\alpha\beta}(\omega) = \frac{1}{2i} (\Gamma_{\alpha\beta}(\omega) - \Gamma_{\beta\alpha}^*(\omega)), \quad (5.55)$$

and

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma_{\beta\alpha}^*(\omega) = \int_{-\infty}^{+\infty} ds e^{i\omega s} \langle B_{\alpha}^{\dagger}(s) B_{\beta}(0) \rangle, \quad (5.56)$$

Hence, by switching back to the Schrödinger picture, we finally obtain the *Gorini-Kossakowski-Sudarshan-Linblad (GKSL) master equation* governing the full dynamics of the open system interacting with its environment

$$\dot{\rho}_S(t) = -i[H_S + H_{LS}, \rho_S(t)] + \mathcal{D}(\rho_S(t)), \quad (5.57)$$

where we defined the *dissipator* as

$$\mathcal{D}(\rho_S(t)) = \sum_{\alpha,\beta} \sum_{\omega} \gamma_{\alpha\beta}(\omega) \left(A_{\beta}(\omega) \rho_S(t) A_{\alpha}^{\dagger}(\omega) - \frac{1}{2} \left\{ A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega), \rho_S(t) \right\} \right), \quad (5.58)$$

and the *Lamb-Shift Hamiltonian* as

$$H_{LS} = \sum_{\alpha,\beta} \sum_{\omega} S_{\alpha\beta}(\omega) A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega). \quad (5.59)$$

Therefore the system evolves through time as

$$\rho_S(t) = e^{\mathcal{L}t} \rho_S(0), \quad (5.60)$$

where the Liouvillian $\mathcal{L}$ now contains two contributions. The first one generates a unitary evolution, showing that the system evolves according to its free Hamiltonian, together with corrections induced by the $S + B$ coupling known as the *Lamb shifts*. The second contribution, resulting from the dissipator, describes a non-unitary evolution accounting for the dissipative dynamics of the system. The system therefore converges to a *steady state*

$$\rho_{ss} = \lim_{t \rightarrow \infty} \rho_S(t), \quad (5.61)$$

which is the kernel of the Liouvillian $\mathcal{L}$, *i.e.*, $\mathcal{L}\rho_{ss} = 0$. In the following sections, we will investigate this open-quantum-system framework in greater details by introducing the concept of thermal fermionic bath and spectral density.

5.4 Thermal fermionic bath

Let us consider a fermionic environment at thermal equilibrium, described by the density operator

$$\rho_B = \frac{e^{-H_B/T}}{\text{Tr}(e^{-H_B/T})}. \quad (5.62)$$

where T is the equilibrium temperature and

$$H_B = \sum_k \omega_k b_k^\dagger b_k. \quad (5.63)$$

is the Hamiltonian of this environment. This latter will be referred to as a *thermal fermionic bath*. The bath operators $b_k^\dagger$ and b_k satisfy the CAR

$$\{b_k, b_{k'}^\dagger\} = \delta_{kk'}, \quad (5.64)$$

$$\{b_k, b_{k'}\} = \{b_k, A_\alpha\} = \{b_k^\dagger, A_\alpha\} = 0, \quad (5.65)$$

in which the system operators A_α are also considered to be fermionic. Therefore, for a hopping-like interaction between the open system and the bath of the form

$$H_I = \sum_{\alpha, k} \lambda_k A_\alpha^\dagger b_k + \lambda_k^* b_k^\dagger A_\alpha, \quad (5.66)$$

the Hamiltonian can be rewritten in a form similar to (5.40) as

$$\sum_\alpha \left(A_0^{(\alpha)} B_0 + A_1^{(\alpha)} B_1 \right), \quad (5.67)$$

with

$$A_0^{(\alpha)} = A_\alpha^\dagger \quad \text{and} \quad A_1^{(\alpha)} = A_\alpha, \quad (5.68)$$

$$B_0 = \sum_k \lambda_k b_k \quad \text{and} \quad B_1 = - \sum_k \lambda_k^* b_k^\dagger. \quad (5.69)$$

Hence, the microscopic derivation of the master equation gives rise to different bath correlation functions corresponding to different combinations of the indices 0 and 1 with the bath operators (5.69). For distinct indices, the BCFs vanish,

$$\alpha_{01}(s) = \langle B_0^\dagger(s) B_1(0) \rangle = 0, \quad (5.70)$$

$$\alpha_{10}(s) = \langle B_1^\dagger(s) B_0(0) \rangle = 0, \quad (5.71)$$

as a direct consequence of the CAR. For identical indices, we obtain

$$\alpha_{00}(s) = \langle B_0^\dagger(s) B_0(0) \rangle = \sum_{k, k'} \lambda_k^* \lambda_{k'} e^{i\omega_k s} \langle b_k^\dagger b_{k'} \rangle \quad (5.72)$$

$$= \sum_k |\lambda_k|^2 e^{i\omega_k s} n(\omega_k), \quad (5.73)$$

$$\alpha_{11}(s) = \langle B_1^\dagger(s) B_1(0) \rangle = \sum_{k, k'} \lambda_k \lambda_{k'}^* e^{-i\omega_k s} \langle b_k b_{k'}^\dagger \rangle \quad (5.74)$$

$$= \sum_k |\lambda_k|^2 e^{-i\omega_k s} (1 - n(\omega_k)), \quad (5.75)$$

where we introduced the *Fermi-Dirac distribution*,

$$n(\omega) = \frac{1}{1 + e^{\omega/T}}, \quad (5.76)$$

which gives the average occupation number of fermions with frequency ω for a bath at thermal equilibrium with temperature T . The last equalities, (5.73) and (5.75), are obtained using the thermal-equilibrium identities

$$\langle b_k^\dagger b_{k'} \rangle = n(\omega_k) \delta_{kk'}, \quad (5.77)$$

$$\langle b_k b_{k'}^\dagger \rangle = (1 - n(\omega_k)) \delta_{kk'}. \quad (5.78)$$

Finally, if the bath possesses an infinite number of degrees of freedom, we can perform the continuum limit, leading to the two bath correlation functions

$$\alpha(s) \equiv \alpha_{00}(s) = \int_{-\infty}^{+\infty} d\omega J(\omega) e^{i\omega s} n(\omega), \quad (5.79)$$

$$\bar{\alpha}(s) \equiv \alpha_{11}(s) = \int_{-\infty}^{+\infty} d\omega J(\omega) e^{-i\omega s} (1 - n(\omega)), \quad (5.80)$$

where we have introduced the spectral density $J(\omega)$ discussed in details in the next section. The BCF $\alpha(s)$ quantifies the memory of the bath associated to bath-fermion absorption in the system, while the BCF $\bar{\alpha}(s)$ quantifies the memory associated to emission process from the system to the bath.

Hence, in the Redfield master equation (5.53), only the terms involving identical indices survive. The equation can be rewritten in the interaction picture as

$$\dot{\rho}_S(t) = \sum_{\alpha} [L_{\alpha} \rho(t), A_{\alpha}^{\dagger}] + [\bar{L}_{\alpha} \rho(t), A_{\alpha}] + \text{h.c.}, \quad (5.81)$$

where

$$L_{\alpha} = \int_0^{\infty} ds \alpha(s) e^{-iH_S s} A_{\alpha} e^{iH_S s}, \quad (5.82)$$

$$\bar{L}_{\alpha} = \int_0^{\infty} ds \bar{\alpha}(s) e^{-iH_S s} A_{\alpha}^{\dagger} e^{iH_S s}. \quad (5.83)$$

This equation will be our starting point in the derivation of a GKSL master equation for the Kitaev chain.

5.5 Spectral density

Let us now examine more carefully the continuum limit performed in (5.85) and (5.86). By defining the *spectral density* $J(\omega)$ of the bath as the weighted Dirac comb

$$J(\omega) = \sum_k |\lambda_k|^2 \delta(\omega - \omega_k), \quad (5.84)$$

then the BCFs can be rewritten exactly as

$$\alpha(s) = \sum_k |\lambda_k|^2 e^{i\omega_k s} n(\omega_k) = \int_{-\infty}^{+\infty} d\omega e^{i\omega s} J(\omega) n(\omega), \quad (5.85)$$

$$\bar{\alpha}(s) = \sum_k |\lambda_k|^2 e^{-i\omega_k s} (1 - n(\omega_k)) = \int_{-\infty}^{+\infty} d\omega e^{-i\omega s} J(\omega) (1 - n(\omega)). \quad (5.86)$$

At this stage, no continuum approximation has been performed yet, since $J(\omega)$ is still defined as a discrete weighted sum of Dirac delta functions. This spectral density quantifies the strength of the coupling between the system and the bath for each frequency ω , and therefore determines how efficiently energy can be exchanged with the bath at that frequency. For a bath with discrete spectrum, this naturally explains the Dirac-comb form of the spectral density. Then, if the bath eigenfrequencies ω_k are sufficiently close to one another, we can perform the continuum limit by assuming a continuous functional form for $J(\omega)$. By doing this, we effectively give a structure to the bath, meaning that the system-bath coupling will favor certain frequencies over others.

A commonly used choice is the Lorentzian spectral density

$$J(\omega) = \frac{\Gamma W^2}{\omega^2 + W^2}, \quad (5.87)$$

where Γ denotes the maximal coupling strength between the system and the bath, and W the full width at half maximum (FWHM) of the Lorentzian profile. This latter selects a specific window of bath frequencies, whose width is governed by the FWHM W . In reality, such a choice is only a rough approximation of the actual non-trivial bath structure, and many other spectral densities can be considered [57] depending on the interaction nature. However, the Lorentzian form shows two advantages. First, it has been proven that arbitrary spectral density profiles can be decomposed as sums of Lorentzian [58–60]. Then, this choice naturally allows bath memory effects to emerge in the non-unitary dynamics of the system. Indeed, if we consider the limit where the Lorentzian is centered infinitely far from the decay region of the Fermi-Dirac distribution, *i.e.*, a window of available coupling frequencies infinitely detuned from the bath chemical potential, the absorption BCF is approximately given by

$$\alpha(s) = \int_{-\infty}^{+\infty} d\omega \frac{\Gamma W^2}{\omega^2 + W^2} e^{i\omega s} = \pi \Gamma W e^{-W|s|} \quad (5.88)$$

showing that the BCF reduces to Fourier transform of the Lorentzian and therefore exhibits an exponential decay of the absorption memory with characteristic decay time $\tau_B \sim W^{-1}$. On the other hand, if we consider a structureless bath, *i.e.*, a bath with the same coupling strength for all frequencies such that $J(\omega) = \Gamma$ (a Lorentzian with an infinite width), then the absorption BCF becomes

$$\alpha(s) = \int_{-\infty}^{+\infty} d\omega \Gamma e^{i\omega s} = 2\pi \Gamma \delta(s), \quad (5.89)$$

describing an instantaneous decay of the bath memory. Physically, this behavior can be understood intuitively: when the system is coupled homogeneously to an infinite range of bath frequency, emitted or absorbed excitations can dissipate into the continuum of bath modes without restriction since there is no preferred coupling bath frequency. As a consequence, the bath instantaneously loses memory of its interaction with the system and is thus perfectly Markovian. By contrast, when the coupling is restricted to a thin frequency window, the excitations have fewer available decay channels within the bath. The information exchanged between the system and the environment is then kept for a longer time since the Lorentzian favors a range of bath frequencies, leading to memory effects in the dynamics.

6 The 2-site dissipative Kitaev chain

In this section, we derive a master equation for a 2-site Kitaev chain. We consider an on-site hopping interaction between the Kitaev chain and local thermal fermionic baths, and look at the effect of both the temperature and emerging structure in the baths through their spectral densities. Even if the topological phase of the 2-site Kitaev chain is not properly defined, it

is still relevant to study the effect of dissipation on the end-to-end correlations through this master equation formalism. Indeed, as we will see in the next sections, this formalism provides us interpretations that can be extrapolated for larger dissipative chains.

6.1 Spectrum and correlations for the isolated 2-site Kitaev chain

Let us consider a 2-site Kitaev chain which Hamiltonian reads

$$H_S = -\mu \left(\sum_{i=1}^2 c_i^\dagger c_i - \frac{1}{2} \right) - t (c_1^\dagger c_2 + c_2^\dagger c_1) + \Delta (c_1 c_2 + c_2^\dagger c_1^\dagger) \quad (6.1)$$

$$= \mathbf{c}^\dagger \mathbf{H}_S \mathbf{c}, \quad (6.2)$$

with the Nambu spinor and the BdG Hamiltonian

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ c_1^\dagger \\ c_2^\dagger \end{pmatrix} \quad \text{and} \quad \mathbf{H}_S = \frac{1}{2} \begin{pmatrix} -\mu & -t & 0 & -\Delta \\ -t & -\mu & \Delta & 0 \\ 0 & \Delta & \mu & t \\ -\Delta & 0 & t & \mu \end{pmatrix}, \quad (6.3)$$

respectively. In order to obtain the eigenexcitations of the chain and their associated energy, we can diagonalize the BdG Hamiltonian by finding the unitary matrix $\mathbf{U}$ which gives

$$\mathbf{d} = \mathbf{U}^\dagger \mathbf{c}, \quad (6.4)$$

the Nambu spinor containing the fermionic operators associated to the eigenexcitations of the system, *i.e.*, which is associated with a diagonal BdG Hamiltonian. Thus, the 2-site Kitaev Hamiltonian can be rewritten as

$$H_S = \mathbf{d}^\dagger \mathbf{H}_\Delta \mathbf{d} = \epsilon_1 \left(d_1^\dagger d_1 - \frac{1}{2} \right) + \epsilon_2 \left(d_2^\dagger d_2 - \frac{1}{2} \right), \quad (6.5)$$

with $\mathbf{H}_\Delta = \mathbf{U} \mathbf{H}_S \mathbf{U}^\dagger = \frac{1}{2} \text{diag}(\epsilon_1, \epsilon_2, -\epsilon_1, -\epsilon_2)$, the diagonal BdG Hamiltonian. If we consider that both t and Δ are positive, we get, for the diagonalization, the unitary matrix

$$\mathbf{U} = \frac{1}{2} \begin{pmatrix} -A & A & B & B \\ A & A & B & -B \\ B & B & -A & A \\ B & -B & A & A \end{pmatrix}, \quad (6.6)$$

with $A = \sqrt{1 - \frac{\mu}{\sqrt{\Delta^2 + \mu^2}}}$ and $B = \sqrt{1 + \frac{\mu}{\sqrt{\Delta^2 + \mu^2}}}$, and the eigenvalues

$$\epsilon_1 = t + \sqrt{\Delta^2 + \mu^2}, \quad (6.7)$$

$$\epsilon_2 = -t + \sqrt{\Delta^2 + \mu^2}, \quad (6.8)$$

which correspond to the eigenenergies of the fermionic modes d_1 and d_2 , respectively. Of course, this is only true when we rescale the Hamiltonian (6.5) to erase the $\frac{1}{2}$ terms. The energy being defined up to a constant, it has no physical consequences to perform this rescaling. Figure 6.1 shows the spectrum of the BdG Hamiltonian where the positive branches correspond to the particle energies, and the negative ones to the hole energies. The eigenmode d_2 , represented by the red line, is associated to a null energy when $\mu = 0$. Therefore, this mode converges to the MBS of the 2-site Kitaev chain when μ tends to zero. Then, we can notice, in accordance with Section 4.5, that in the topological region $|\mu| < 2t$, the energy of d_2 is non-zero everywhere else. This comes from the non-topological nature of this short finite-size Kitaev chain, the MZMs

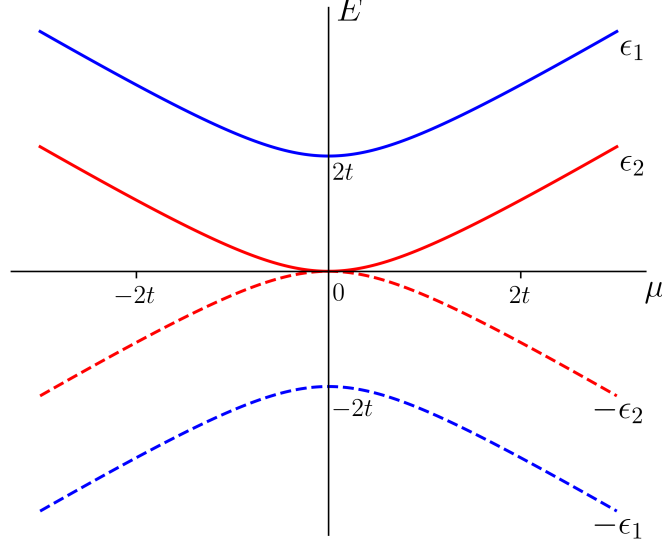


Figure 6.1: Dependence of the BdG Hamiltonian spectrum with respect to the chemical potential μ (we have set $t = \Delta$). The solid lines represent the particle energies, while the dashed ones correspond to the hole energies. We observe that at $\mu = 0$, the particle-hole gap closes meaning that the mode d_2 is the MBS in this sweet spot.

decay lengths are longer than the chain itself for any non-zero value of the chemical potential, resulting in a lifting of the ground state degeneracy.

Furthermore, these eigenmodes, d_1 and d_2 , are given in terms of the physical modes c_1 and c_2 following (6.4) and (6.6) as

$$d_1 = \frac{1}{2} \left[A(c_2 - c_1) + B(c_1^\dagger + c_2^\dagger) \right], \quad (6.9)$$

$$d_2 = \frac{1}{2} \left[A(c_1 + c_2) + B(c_1^\dagger - c_2^\dagger) \right], \quad (6.10)$$

in which we observe that the particle-hole nature of these modes is weighted by A and B , respectively. Indeed, recall that the BdG transformation (6.4) results in fermionic modes showing a mixed particle-hole character. The inverse transformation is given by

$$c_1 = \frac{1}{2} \left[A(d_2 - d_1) + B(d_1^\dagger + d_2^\dagger) \right], \quad (6.11)$$

$$c_2 = \frac{1}{2} \left[A(d_1 + d_2) + B(d_1^\dagger - d_2^\dagger) \right]. \quad (6.12)$$

Then, following the Majorana decomposition (4.25) for the physical modes, the eigenmodes are given in terms of the Majorana operators as

$$d_1 = \frac{B - A}{4}(\gamma_{A,1} - i\gamma_{B,2}) + \frac{A + B}{4}(\gamma_{A,2} - i\gamma_{B,1}), \quad (6.13)$$

$$d_2 = \frac{A + B}{4}(\gamma_{A,1} + i\gamma_{B,2}) + \frac{A - B}{4}(\gamma_{A,2} + i\gamma_{B,1}). \quad (6.14)$$

Once more, we observe that the fermionic mode d_2 corresponds to the MBS. Indeed, if $\mu = 0$, then $A = B = 1$ and $d_2 = (\gamma_{A,1} + i\gamma_{B,2})/2$, which is a fermion composed of the two edge MZMs. The weights of the modes d_1 and d_2 in their Majorana decomposition, *i.e.*, the factors $\frac{A+B}{4}$ and $\frac{A-B}{4}$, are schematically represented in Figure 6.2 for different values of μ . For $\mu = 0$, we observe that d_2 is perfectly localized at the edges of the chain, while the other fermion d_1 is entirely composed of the bulk Majorana modes. When the chemical potential increases, the weights of

both modes, d_1 and d_2 , spread over multiple Majorana modes, which is the expected behavior for a regime distinct from the 'perfect topological phase' $\mu = 0$ and $\Delta = t$ (see Figure 4.7). However, even for a small value of μ , the weights of the mode d_2 are non-zero in the bulk of the chain. Thus, the wavefunction of the two MZMs overlap and the degeneracy is lifted.

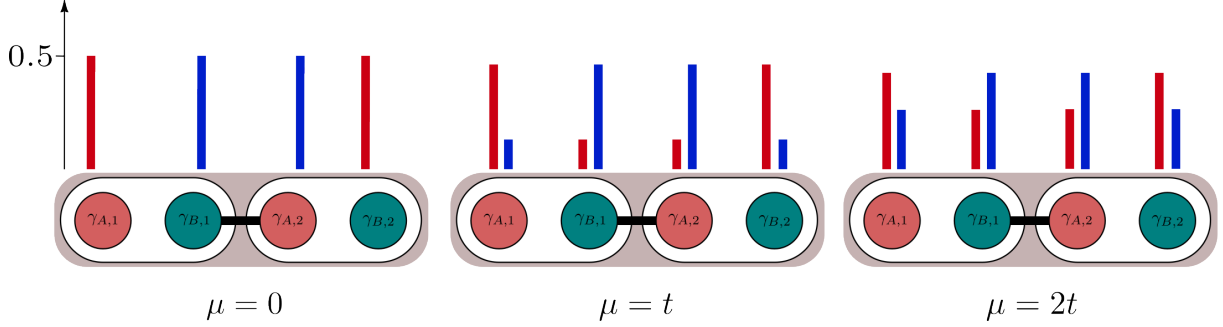


Figure 6.2: Norm of the weights in the decomposition of d_1 (blue) and d_2 (red) in terms of the Majorana operators for different values of μ (we have set $\Delta = t$). For the 'perfect' topological phase $\mu = 0$, the mode d_2 is delocalized at each edge of the chain while d_1 is in the bulk of the chain. Then, when μ increases, their weights start to spread over multiple Majorana operators (be aware that the weights are not normalized).

Let us now define the 2-mode Fock basis generated from the bare electron vacuum $|00\rangle$. As usual, the vacuum is defined as the state destroyed by all annihilation operators, *i.e.*, $c_1|00\rangle = c_2|00\rangle = 0$. Then, the other elements of the basis are generated by application of the creation operators as: $|10\rangle = c_1^\dagger|00\rangle$, $|01\rangle = c_2^\dagger|00\rangle$ and $|11\rangle = c_1^\dagger c_2^\dagger|00\rangle$. Of course, these states corresponding to the occupation of the physical modes c_1 and c_2 are not eigenstates of the Hamiltonian. In order to find the eigenstates, we need to derive the normalized basis generated by the fermionic modes $d_1^\dagger$ and $d_2^\dagger$. In Appendix E.1, we show that this eigenbasis is defined from the previous one as

$$|+\rangle_0 = \frac{1}{\sqrt{2}} (A|00\rangle + B|11\rangle), \quad (6.15)$$

$$|-\rangle_0 = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) = d_1^\dagger |+\rangle_0, \quad (6.16)$$

$$|-\rangle_1 = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) = d_2^\dagger |+\rangle_0, \quad (6.17)$$

$$|+\rangle_1 = \frac{1}{\sqrt{2}} (B|00\rangle - A|11\rangle) = d_1^\dagger d_2^\dagger |+\rangle_0, \quad (6.18)$$

where the ' $\pm$ ' signs refer to the parity of the states, and the '0' and '1' indices tell us whether the state is associated with a null energy or not when $\mu = 0$, respectively. Indeed, the state $|+\rangle_0$ is the Bogoliubov vacuum such that $d_1|+\rangle_0 = d_2|+\rangle_0 = 0$. Its parity is obviously even and the state is always associated with a null energy. The other ones are derived from this Bogoliubov vacuum as: $|-\rangle_1 = d_1^\dagger |+\rangle_0$, $|-\rangle_0 = d_2^\dagger |+\rangle_0$ and $|+\rangle_1 = d_1^\dagger d_2^\dagger |+\rangle_0$. The state $|-\rangle_0$ is of odd parity and associated with a null energy when $\mu = 0$. Therefore, this state corresponds to the MBS when the chain is in the 'perfect' topological phase, which is the wanted result since it is generated by $d_2^\dagger$.

Finally, since we are analyzing, in the next sections, the impact of dissipation on the end-to-end correlations described by the Q -function (4.12) which in the 2-site Kitaev chain reads

$$Q = 2 \left| \langle c_1^\dagger c_2 + c_2^\dagger c_1 \rangle \right|, \quad (6.19)$$

it will show relevant to compute these values for the eigenstates of the Kitaev chain. From the decomposition of these latter in terms of the first Fock basis (6.15-6.18), we easily obtain

$$Q_0^+ = 0, Q_0^- = 2, Q_1^- = 2, \text{ and } Q_1^+ = 0, \quad (6.20)$$

following the same notation. These results do not depend on the parameters of the Hamiltonian. As already stated in Section 4.5, end-to-end correlations appear for non-topological excited states. This obviously comes from the fact that the edge modes of the 2-site Kitaev chain are also the bulk modes, and all excitations are spreading over the two physical sites which leads to correlations between them. However, we expect these correlations to vanish for non-topological states when $N \rightarrow \infty$. Moreover, we notice the value $Q_0^+ = 0$ for all μ -values (even $\mu = 0$). This result is in accordance with the black horizontal line on the simulated left plot of Figure 4.12, corresponding to the end-to-end correlations of the vacuum state of the 2-site Kitaev chain.

6.2 Interacting 2-site Kitaev chain and GKSL master equation

Now that all relevant features of the isolated 2-site Kitaev chain have been surveyed, in this section we derive a GKSL master equation for the chain when interaction is added. For this, we consider an on-site hopping interaction with thermal fermionic baths, meaning that each physical fermionic site, c_1 and c_2 , interacts with its own bath. The Hamiltonian modeling the global system reads

$$H = H_S + H_{B,1} + H_{B,2} + H_I, \quad (6.21)$$

where the isolated Hamiltonians, H_S and H_B , represent the chain and the baths, respectively. The chain Hamiltonian H_S is given in (6.1) and the Hamiltonian for an isolated bath is

$$H_{B,l} = \sum_k (\omega_{l,k} + \mu_B) b_{l,k}^\dagger b_{l,k}, \quad (6.22)$$

where the index ' l ' refers to the chain site with which the bath interacts, μ_B is the shared chemical potential of the baths, chosen to be the same for both baths, and $b_{l,k}$ is the bath fermionic mode associated to the frequency $\omega_{l,k}$. These modes obey the CAR

$$\{b_{l,k}, b_{l',k'}^\dagger\} = \delta_{l,l'} \delta_{k,k'}, \quad (6.23)$$

$$\{b_{l,k}, b_{l',k'}\} = \{b_{l,k}^\dagger, b_{l',k'}^\dagger\} = \{c_n, b_{l,k}^\dagger\} = \{c_n, b_{l,k}\} = 0. \quad (6.24)$$

Finally, the interaction Hamiltonian reads

$$H_I = \sum_{l,k} t_{l,k} c_l^\dagger b_{l,k} + t_{l,k}^* b_{l,k}^\dagger c_l \quad (6.25)$$

which describes the coupling between the fermionic mode c_l and the bath modes $b_{l,k}$ associated with the same site l . In this model, the chain mode c_l interacts with all bath modes and the coupling strength to a given bath mode k is determined by the complex hopping amplitude $t_{l,k}$. Figure 6.3 displays a sketch of the global system.

As said previously, we will consider on-site thermal baths in thermal equilibrium which states are given by

$$\rho_{B,l} = \frac{e^{-H_{B,l}/T}}{\text{Tr}_{B,l}(e^{-H_{B,l}/T})}, \quad (6.26)$$

with T , their shared temperature. Therefore, we can derive the GKSL master equation describing the dissipative dynamics of the chain from the Redfield master equation (5.81) which in our case reads

$$\dot{\rho} = -i[H_S, \rho] + \sum_{l=1,2} \left([L_l \rho, c_l] + [c_l^\dagger, \rho L_l^\dagger] \right) + \sum_{l=1,2} \left([\bar{L}_l \rho, c_l^\dagger] + [c_l, \rho \bar{L}_l^\dagger] \right). \quad (6.27)$$

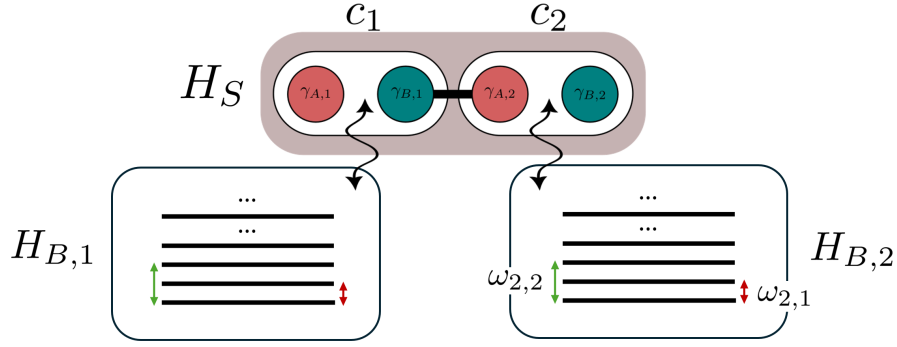


Figure 6.3: Sketch of the 2-site Kitaev chain with each site interacting with its own thermal fermionic bath.

By defining the functions

$$\zeta(\omega) = J(\omega - \mu_B)n(\omega - \mu_B) \quad \text{and} \quad \bar{\zeta}(\omega) = J(\omega - \mu_B)(1 - n(\omega - \mu_B)), \quad (6.28)$$

with $J(\omega)$ the shared bath spectral density and $n(\omega)$ the Fermi-Dirac distribution (5.76), the L -operators are given by

$$L_1 = \int_0^\infty \alpha(s) e^{-iH_S s} c_1^\dagger e^{iH_S s} ds \quad (6.29)$$

$$= \frac{\pi}{2} \left[B(\zeta(-\epsilon_1)d_1 + \zeta(-\epsilon_2)d_2) + A(\zeta(\epsilon_2)d_2^\dagger - \zeta(\epsilon_1)d_1^\dagger) \right], \quad (6.30)$$

$$\bar{L}_1 = \int_0^\infty \bar{\alpha}(s) e^{-iH_S s} c_1 e^{iH_S s} ds \quad (6.31)$$

$$= \frac{\pi}{2} \left[B(\bar{\zeta}(-\epsilon_1)d_1^\dagger + \bar{\zeta}(-\epsilon_2)d_2^\dagger) + A(\bar{\zeta}(\epsilon_2)d_2 - \bar{\zeta}(\epsilon_1)d_1) \right], \quad (6.32)$$

$$L_2 = \int_0^\infty \alpha(s) e^{-iH_S s} c_2^\dagger e^{iH_S s} ds \quad (6.33)$$

$$= \frac{\pi}{2} \left[B(\zeta(-\epsilon_1)d_1 - \zeta(-\epsilon_2)d_2) + A(\zeta(\epsilon_1)d_1^\dagger + \zeta(\epsilon_2)d_2^\dagger) \right], \quad (6.34)$$

$$\bar{L}_2 = \int_0^\infty \bar{\alpha}(s) e^{-iH_S s} c_2 e^{iH_S s} ds \quad (6.35)$$

$$= \frac{\pi}{2} \left[A(\bar{\zeta}(\epsilon_1)d_1 + \bar{\zeta}(\epsilon_2)d_2) + B(\bar{\zeta}(-\epsilon_1)d_1^\dagger - \bar{\zeta}(-\epsilon_2)d_2^\dagger) \right], \quad (6.36)$$

since the bath correlation functions are

$$\alpha(s) = \int_{-\infty}^{+\infty} d\omega e^{i(\omega + \mu_B)s} J(\omega) n(\omega), \quad (6.37)$$

$$\bar{\alpha}(s) = \int_{-\infty}^{+\infty} d\omega e^{-i(\omega + \mu_B)s} J(\omega) (1 - n(\omega)). \quad (6.38)$$

The computation of the L -operators is provided in Appendix E.2. Finally, after reordering and secularization of (6.27), we obtain the GKSL master equation for the 2-site Kitaev chain

$$\dot{\rho} = -i[H_S, \rho] + \underbrace{\kappa_1 \mathcal{D}[d_1^\dagger](\rho)}_{\text{I}} + \underbrace{\kappa_2 \mathcal{D}[d_2^\dagger](\rho)}_{\text{II}} + \underbrace{\bar{\kappa}_1 \mathcal{D}[d_1](\rho)}_{\text{III}} + \underbrace{\bar{\kappa}_2 \mathcal{D}[d_2](\rho)}_{\text{IV}} \quad (6.39)$$

with the dissipator $\mathcal{D}[O](\rho) = 2O\rho O^\dagger - \{O^\dagger O, \rho\}$. In this master equation, the first terms, I and II, describe the absorption of fermions d_1 and d_2 from the bath to the chain, with their associated

rates κ_1 and κ_2 . Analogously, the last terms, III and IV, describe the emission of fermions d_1 and d_2 from the chain to the bath, with their associated rates $\bar{\kappa}_1$ and $\bar{\kappa}_2$. Here, we observe that the fundamental dissipation channels describing the non-unitary dynamics of the chain are non-local, despite the fact that the system-bath couplings are local. More precisely, the dissipative processes induce the absorption and emission of the non-local fermionic excitations d_1 and d_2 , whereas the original interactions (6.25) act locally on the chain sites. This emergent non-locality can be understood by the presence of tunneling and pairing terms in the chain Hamiltonian (6.1) which allow the effects of the local baths to propagate throughout the chain.

Moreover, we have chosen not to take into account the Lamb-shifts in the master equation for simplicity, leaving the unitary dynamics of the system unchanged. This will facilitate the effects characterization of dissipation.

Let us now focus on the dissipation rates which expressions are given by

$$\kappa_1 = \frac{\pi}{2} (A^2 \zeta(\epsilon_1) + B^2 \bar{\zeta}(-\epsilon_1)), \quad (6.40)$$

$$\kappa_2 = \frac{\pi}{2} (A^2 \zeta(\epsilon_2) + B^2 \bar{\zeta}(-\epsilon_2)), \quad (6.41)$$

$$\bar{\kappa}_1 = \frac{\pi}{2} (A^2 \bar{\zeta}(\epsilon_1) + B^2 \zeta(-\epsilon_1)), \quad (6.42)$$

$$\bar{\kappa}_2 = \frac{\pi}{2} (A^2 \bar{\zeta}(\epsilon_2) + B^2 \zeta(-\epsilon_2)). \quad (6.43)$$

Each rate, which tells us the importance of its associated dissipation channel in the chain dynamics, presents both particle and hole contributions as

$$\kappa \sim A^2 * \text{particle} + B^2 * \text{hole}. \quad (6.44)$$

Indeed, each dissipation rate contains two contributions involving ζ -functions evaluated at the positive and negative eigenenergies of the dissipative fermionic mode. The presence of these two terms is expected since the fermionic modes d_1 and d_2 are obtained through a BdG transformation, and therefore possess a mixed particle-hole nature, weighted by the A and B factors, respectively. Recalling that, for pure²² fermionic modes of energy ϵ , absorption rates of particles (holes) are proportional to $n(\epsilon)$ ($1 - n(-\epsilon)$), and emission rates of particles (holes) are proportional to $1 - n(\epsilon)$ ($n(-\epsilon)$), we easily interpret the structure of these rates from the definition of the ζ -functions (E.26) as

$$\begin{aligned} \kappa_1 &\sim \text{abs. of particles with energy } \epsilon_1 + \text{abs. of holes with energy } -\epsilon_1, \\ \kappa_2 &\sim \text{abs. of particles with energy } \epsilon_2 + \text{abs. of holes with energy } -\epsilon_2, \\ \bar{\kappa}_1 &\sim \text{em. of particles with energy } \epsilon_1 + \text{em. of holes with energy } -\epsilon_1, \\ \bar{\kappa}_2 &\sim \text{em. of particles with energy } \epsilon_2 + \text{em. of holes with energy } -\epsilon_2. \end{aligned}$$

Furthermore, the chemical potential μ_B of the baths will favor one of the two dissipation natures (particle or hole) of these rates, since the Fermi-Dirac statistics is shifted from 0 by μ_B . If $\mu_B = 0$ at fixed A and B , the particle-hole contributions are perfectly symmetric, but if $\mu_B > 0$ the particle contribution will dominate the hole one for absorption, while the hole contribution will dominate for emission, as shown on Figure 6.4. The inverse is true for $\mu_B < 0$.

In addition to providing us a valuable understanding of the underlying physics behind the dissipative processes, the analysis of the rates is of particular importance because the steady state density matrix can be expressed, in the Fock basis (6.15-6.18), as

$$\rho_{ss} = \frac{1}{(\kappa_1 + \bar{\kappa}_1)(\kappa_2 + \bar{\kappa}_2)} \begin{pmatrix} \bar{\kappa}_1 \bar{\kappa}_2 & 0 & 0 & 0 \\ 0 & \kappa_1 \bar{\kappa}_2 & 0 & 0 \\ 0 & 0 & \bar{\kappa}_1 \kappa_2 & 0 \\ 0 & 0 & 0 & \kappa_1 \kappa_2 \end{pmatrix}. \quad (6.45)$$

²²Pure refers here to the absence of particle-hole mixed character, not the statistical purity of the state.

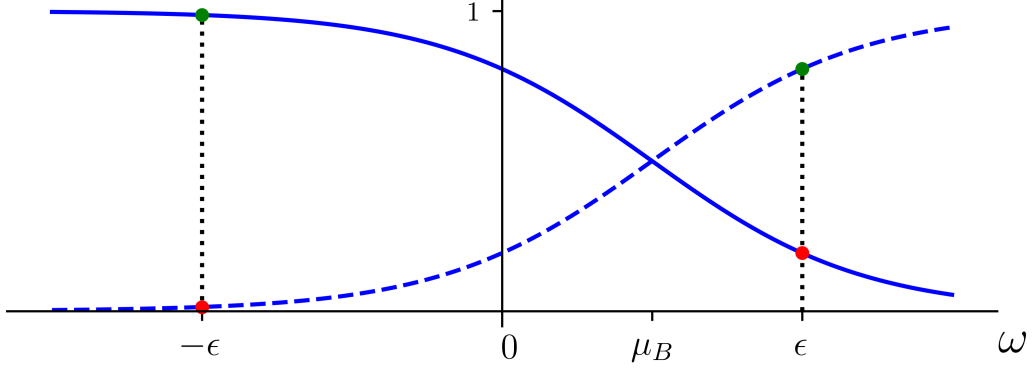


Figure 6.4: *Fermi-Dirac distribution $n(\omega)$ (solid line) and $1 - n(\omega)$ (dashed line) for a bath of chemical potential $\mu_B > 0$ and temperature $T \neq 0$. The red (green) dots represent the contributions for the absorption (emission) of a BdG fermion of energy ϵ . The particle contributions for both processes are found following the vertical black dotted lines from ϵ , and the hole contributions from $-\epsilon$. For $\mu_B > 0$, we clearly see that the particle (hole) contribution is favored compared to the hole (particle) one for absorption (emission).*

Hence, we observe that the steady-state corresponds to a mixed state of the eigenstates with no coherences. Furthermore, we can already notice that the populations follow expected behaviors:

- $p_0^+ = \langle + | \rho_{ss} | + \rangle_0 \propto \bar{\kappa}_1 \bar{\kappa}_2$, the population of the Bogoliubov vacuum, is enhanced by the emission rates of both fermions d_1 and d_2 ,
- $p_1^- = \langle - | \rho_{ss} | - \rangle_1 \propto \kappa_1 \bar{\kappa}_2$, the population of the excited fermions d_1 , is enhanced by the absorption rate of d_1 and the emission rate of d_2 ,
- $p_0^- = \langle - | \rho_{ss} | - \rangle_0 \propto \bar{\kappa}_1 \kappa_2$, the population of the excited fermions d_2 (the MBS at $\mu = 0$), is enhanced by the absorption rate of d_2 and the emission rate of d_1 ,
- $p_1^+ = \langle + | \rho_{ss} | + \rangle_1 \propto \kappa_1 \kappa_2$, the population of the occupation of both d_1 and d_2 , is enhanced by the absorption rates of both fermions d_1 and d_2 .

Given that these rates depend on the ζ -functions (E.26), both temperature and emerging structure in the baths through the spectral density will directly influence the steady state and the transient dynamics.

In the following analysis, we focus on two limiting cases for the BCFs:

1. A flat (constant) spectral density, $J(\omega) = \Gamma$, with varying temperature T . This case allows us to check the influence of the temperature on the correlations and the transient dynamics in the presence of structureless baths,
2. Zero-temperature baths, $T = 0$, with a Lorentzian spectral density of varying width W . This setting is used to examine the impact of emerging structure in the bath on the system.

6.3 Impact of the temperature T

In this section, we consider a flat spectral density of the form

$$J(\omega) = \Gamma, \quad \forall \omega \in \mathbb{R}, \quad (6.46)$$

corresponding to a structureless bath with frequency-independent coupling. In this case, the only nontrivial frequency dependence arises from the thermal equilibrium properties of the reservoir through the Fermi-Dirac distribution. As explained in Section 5.5, the decay time of the BCFs

vanishes as the chemical potential of the bath tends to infinity (5.89) since it would correspond to a perfectly flat spectral density. Therefore, the baths lose all memory effects and are purely Markovian.

In the previous section, we showed that the decay rates are determined by the ζ -functions, which now read

$$\zeta(\omega) = \Gamma n(\omega - \mu_B) \quad \text{and} \quad \bar{\zeta}(\omega) = \Gamma(1 - n(\omega - \mu_B)). \quad (6.47)$$

The frequency-dependence of these functions is now fully described by the Fermi-Dirac distribution

$$n(\omega) = \frac{1}{1 + e^{\omega/T}}, \quad (6.48)$$

and hence, show an explicit dependence on the bath temperature. Thence, given (6.45) and (6.39), both the steady-state and the transient dynamics will be affected by the temperature.

First, we investigate the influence of the temperature on the steady-state. Figure 6.5 shows multiple μ - μ_B phase diagrams for increasing values of T , in which the steady state populations are characterized for each pair of values (μ, μ_B) . In addition, we analyze the purity of the steady-state

$$\text{Purity} = \text{Tr}(\rho_{ss}^2) = (p_0^+)^2 + (p_1^-)^2 + (p_0^-)^2 + (p_1^+)^2, \quad (6.49)$$

where the second line follows from the diagonal form of steady-state density matrix in the considered basis.

First, let us describe these four phase diagrams²³ without giving the origin of their structure:

- a) $T = 0$: on this diagram, we see three dominant regions of almost pure populations p_0^+ (blue), p_0^- (green) and p_1^+ (yellow). Moreover, for $|\mu/t| \lesssim 1$, we see three other regions: mixtures with dominant populations (p_0^+, p_0^-) (teal), (p_0^-, p_1^+) (lime) and $(p_0^+, p_1^-, p_0^-, p_1^+)$ (grey). These pure and mixed states are confirmed by the purity phase diagram, where the three pure region appear as lighter areas, while the mixed states are contained in a darker region. Especially, at $\mu = 0$, for which the purity is minimal, namely $\text{Purity} = 1/4$ which therefore corresponds to a maximally mixed state. Note also that, for fixed $\mu/t \gg 0$ and increasing μ_B (vertical cut), the boundaries separating the pure-state regions are sharp in the sense that the system transitions directly from a pure state to another without passing through a mixed-state region.
- b) $T = 0.1t$: we see more or less the same regions than for $T = 0$ except that the pure regions are now fully separated by mixed regions. This is confirmed by the hyperbolic dark regions appearing on the purity phase diagram and separating the lighter ones.
- c) $T = t$: the mixed regions start to overlap, erasing totally the pure regions p_0^- . Indeed, we observe on the purity diagram that the dark boundaries are spreading.
- d) $T = 10t$: the fully mixed region $(p_0^+, p_1^-, p_0^-, p_1^+)$ spreads almost on the whole phase diagram. No more pure region is visible which is confirmed by the fully dark purity diagram.

From this, we conclude that increasing the temperature decreases the purity of the system. Therefore, the steady state converges to a maximally mixed state with the temperature for any pair of values (μ, μ_B) .

Let us interpret these results by examining the effect of temperature on the rates (6.40-6.43). For this, Figure 6.6 shows the dissipation rates for several temperatures along a vertical cut at $\mu/t = -2$ in the μ - μ_B phase diagram.

²³From now on, all results are obtained with $t = \Delta$.

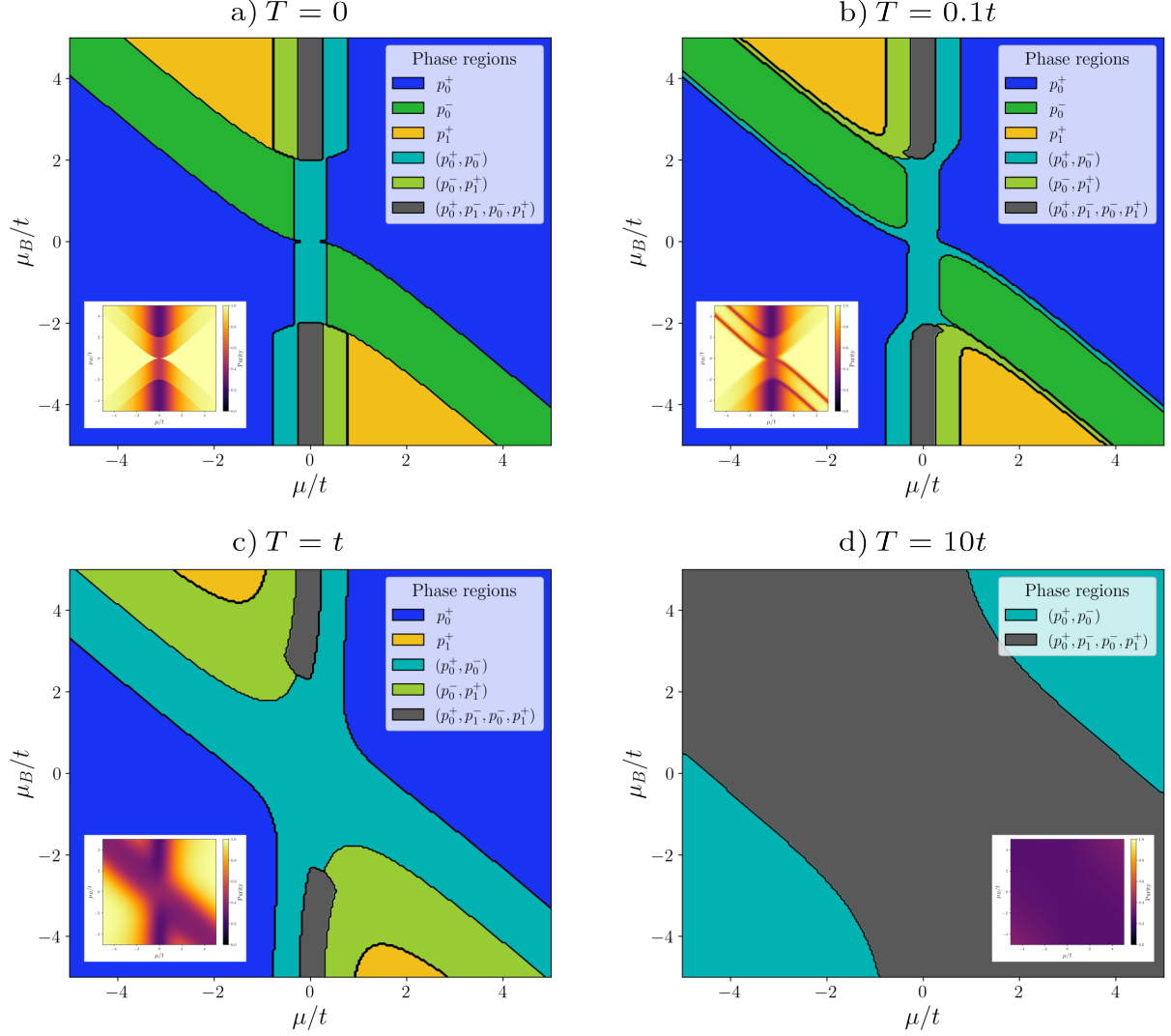


Figure 6.5: Population distribution in the μ - μ_B phase diagram. At $T = 0$, the distribution follows the structure of the energy spectrum of a 2-site Kitaev chain. As the temperature increases, this structure gradually blurs and the regions corresponding to mixed states expand. The color coding is based on the following criteria: a region is considered pure when one population exceeds 0.65. It is classified as a mixture of two populations when the difference between the two dominant populations is smaller than 0.15, otherwise, it is classified as a mixture of four populations. For clarity, regions corresponding to mixtures of three populations are not displayed separately. To assess the departure from purity within each region, the corresponding purity phase diagrams are also provided. The exact population distributions, together with the purity phase diagrams, can be found in Appendix E.3.

In order to understand these plots, we must recall that the populations of the steady states are rates-dependent (see (6.45)). The first observation we can make is that whenever a pair of rates strongly dominates over the other combinations, the steady-state purity is significantly enhanced. However, when no dominant pair exists for a given value of μ_B , the steady state becomes mixed. Indeed, in Fig. 6.6(a)-(b), one pair of rates almost always dominates the others. For instance, around $\mu_B = 0$, one finds $\bar{\kappa}_1, \bar{\kappa}_2 \gg \kappa_1, \kappa_2$, which leads to the pure population p_0^+ . By contrast, Fig. 6.6(c)-(d) show regions where no pair clearly dominates. In these regimes, the competition between several comparable rates results in a mixed steady state. This behavior is visible in the blurred regions of the plots, where no single color (blue, green, yellow) clearly dominates over the others.

Furthermore at $T = 0$, the rates vary sharply as functions of μ_B . As the temperature

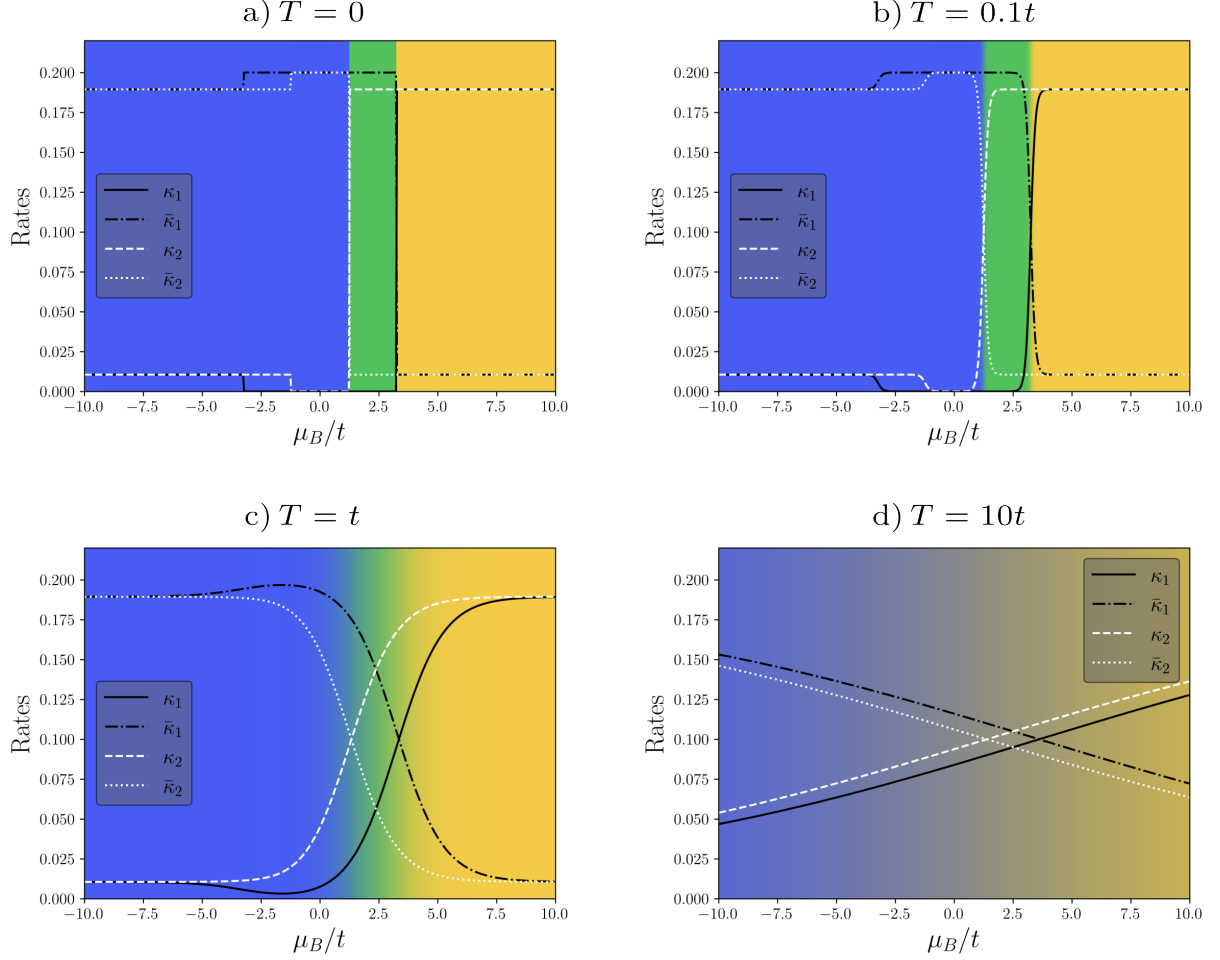


Figure 6.6: Temperature dependence of the dissipation rates as a function of μ_B for $\mu = -2$. According to the population enhancement mechanism discussed in Section 6.2, whenever a pair of dissipation rates dominates over the others, the corresponding population is favored in the steady state. As the temperature increases, however, the rates become progressively modulated by the broadening of the Fermi-Dirac distribution, making the distinction between competing pairs of rates increasingly difficult. As a consequence, no single population can be preferentially stabilized, and the steady state becomes progressively more mixed. This behavior is also reflected in the background color map, where the actual steady-state populations (now displayed without thresholding) exhibit an increasing degree of mixing, resulting in progressively blurred boundaries between regions. The color code is identical to that used previously: blue corresponds to the Bogoliubov vacuum population p_0^+ , green to p_0^- , corresponding to the occupation of the mode d_2 (the MBS at $\mu = 0$), and yellow to p_1^+ , corresponding to the simultaneous occupation of the modes d_1 and d_2 .

increases, however, these variations become progressively smoother. As a consequence, broader regions with comparable rates appear and, as discussed above, these regions are associated with mixed steady states. This smoothing of the rate variations with increasing temperature follows directly from their definition in (6.40-6.43), since the rates depend on the ζ -functions, which are fully determined by the Fermi-Dirac distribution. Therefore this progressive smoothing comes from the thermal broadening of the Fermi-Dirac profile: as the temperature increases, the average fermionic occupation number at a given frequency becomes less sharply defined due to thermal fluctuations. This smoothing of the Fermi-Dirac distribution is illustrated on Figure 6.7.

A last observation we can make from Figure 6.5 is that the population seems to follow borders given by the spectrum (see Fig. 6.1) of the Kitaev Hamiltonian. This can be physically understood as follows:

- for a fixed negative value of $\mu/t < -3/4$, we have $A > 2B$, meaning that the particle

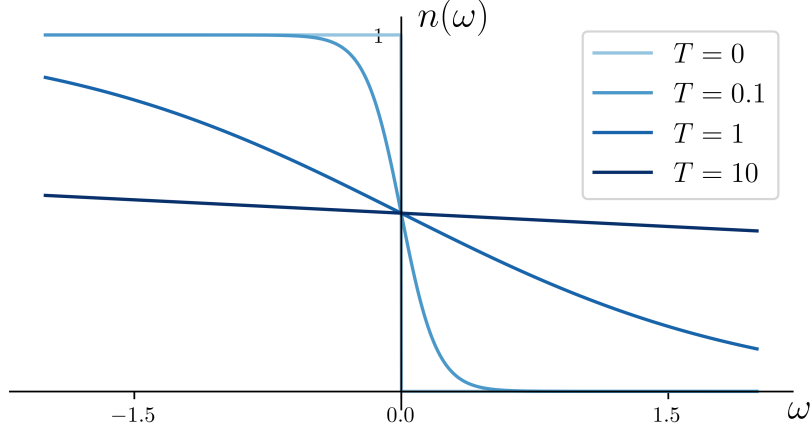


Figure 6.7: *Temperature broadening of the Fermi-Dirac distribution for a zero chemical potential.*

character of the eigenexcitations d_1 and d_2 largely dominates over the hole one (see Eq. (6.9) and (6.10)). Hence, when the bath chemical potential μ_B increases, fermionic excitations of the bath with particle nature find it energetically favorable to populate the chain, which leads to steady states with occupied fermionic mode. More precisely, if $\mu_B < \epsilon_2$, the bath fermions do not possess enough energy to populate the chain, so that the chain remains the Bogoliubov vacuum p_0^+ (blue). For $\epsilon_2 < \mu_B < \epsilon_1$, the population of bath fermions with energy above ϵ_2 becomes significant, allowing the mode d_2 to be populated, while the energy remains insufficient to excite the mode d_1 . In this regime, the steady state is therefore dominated by p_0^- (green). Finally, when $\mu_B > \epsilon_1$, the most energetic bath fermions are able to populate both modes d_1 and d_2 , leading to the occupation of both fermionic modes and thus, to the steady state p_1^+ (yellow).

- for a fixed positive value of $\mu/t > 3/4$, we have $B > 2A$ which means that the hole component is dominating over the particle one in the decomposition of chain eigenmodes (6.9-6.10). Therefore, the above interpretation is reversed: instead of particle-like excitations populating the chain as μ_B increases, it is now hole-like excitations with negative energy that effectively hop from the bath into the chain as μ_B decreases. This naturally explains the invariance of the phase diagram under a π -rotation.
- for a value $|\mu/t| < 3/4$, both particle and hole components show a comparable value which explains why the states in this interval are mixed. The bath hops both particles and holes in the chain.

Figure 6.8 shows the weights of the particle component A and hole component B of the mode d_1 and d_2 in terms of μ . The graph highlights the threshold $|\mu/t| = 3/4$ that we consider to be the boundary between the particle ($A > 2B$) and hole ($B > 2A$) characters and the mixed character ($|\mu/t| < 3/4$).

Now that the underlying physics governing the effect of temperature on the steady state is well understood, together with the different purity regimes and their associated populations in terms of (μ, μ_B) , we are in a position to address our original goal: the characterization of the steady-state end-to-end correlations. The latter can be obtained analytically from the steady state (6.45) and reads

$$Q_{ss} = 2 \left| \frac{\kappa_1}{\kappa_1 + \bar{\kappa}_1} - \frac{\kappa_2}{\kappa_2 + \bar{\kappa}_2} \right|. \quad (6.50)$$

As for the populations, the effects of temperature on the end-to-end correlations Q can be visualized on μ - μ_B phase diagrams, as the ones displayed in Figure 6.9. From this figure, we

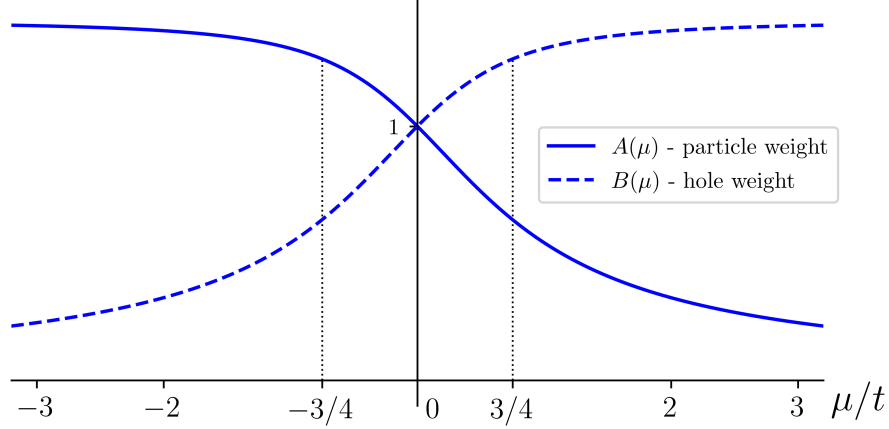


Figure 6.8: Particle weight A and hole weight B as functions of the normalized chemical potential μ/t . By introducing the arbitrary thresholds $A = 2B$ and $B = 2A$ to identify fermionic states with a clearly dominant particle or hole character, respectively, we obtain the conditions $\mu/t < -3/4$ and $\mu/t > 3/4$. In contrast, for $|\mu/t| < 3/4$, the fermionic states exhibit a significant particle-hole mixed character. This latter explains the population mixtures observed in Figure 6.5 within the corresponding range of μ/t .

clearly observe that correlations appear only in the regions where the population p_0^- is present. In particular, the correlations reach the value 2 when this population is pure, while they vanish in the regions associated with pure populations p_0^+ and p_1^+ (see Fig. 6.5). This behavior is fully consistent with the values of the Q -function computed in Eq. (6.20) for each eigenstate of the chain. Moreover, when the steady state becomes mixed, the correlations are reduced, since the corresponding expectation values are averaged over statistical mixture of populations with different contributions to the correlations.

A notable result is that non-vanishing correlations persist in the steady state of the chain. Moreover, these correlations are associated with the population p_0^- . Strictly speaking, this state is topological only at $\mu = 0$, where it corresponds to a fully delocalized zero-energy mode. Nevertheless, significant correlations are also observed for a broad range of positive values $\mu > 0$, for which p_0^- is no longer fully delocalized and acquires a finite energy. As will be shown in the final section, this observation can be generalized to longer chains, where topological states may exist away from this special 'sweet spot' value of μ . Once more, one must be cautious when using end-to-end correlations alone as a diagnostic of the topological nature of an open Kitaev chain.

The steady-state properties being fully characterized, let us now describe the effects of temperature on the transient dynamics of the 'perfect topological' state at $\mu = 0$. In this 'sweet spot', we initialize the dynamics with the odd-parity zero-energy pure state (the MBS),

$$\rho(0) = |-\rangle\langle -|_0 \quad (\text{MBS}) \quad (6.51)$$

Since the Liouvillian superoperator $\mathcal{L}$ is time-independent, the Linblad master equation (6.39) can be written as

$$\dot{\rho} = \mathcal{L}\rho, \quad (6.52)$$

whose solution yields the transient state at an arbitrary time $\tilde{\tau}$ as

$$\rho(\tilde{\tau}) = e^{\mathcal{L}\tilde{\tau}}\rho(0). \quad (6.53)$$

In order to quantify the lifetime of the zero-energy state and its persistence against thermal effects, in Figure 6.10 we compare the fidelities between the transient state and the initial pure MBS, defined as

$$F(\rho(\tilde{\tau}), \rho(0)) = \text{Tr}(\rho(\tilde{\tau})\rho(0)) = \langle - | \rho(\tilde{\tau}) | - \rangle_0, \quad (6.54)$$

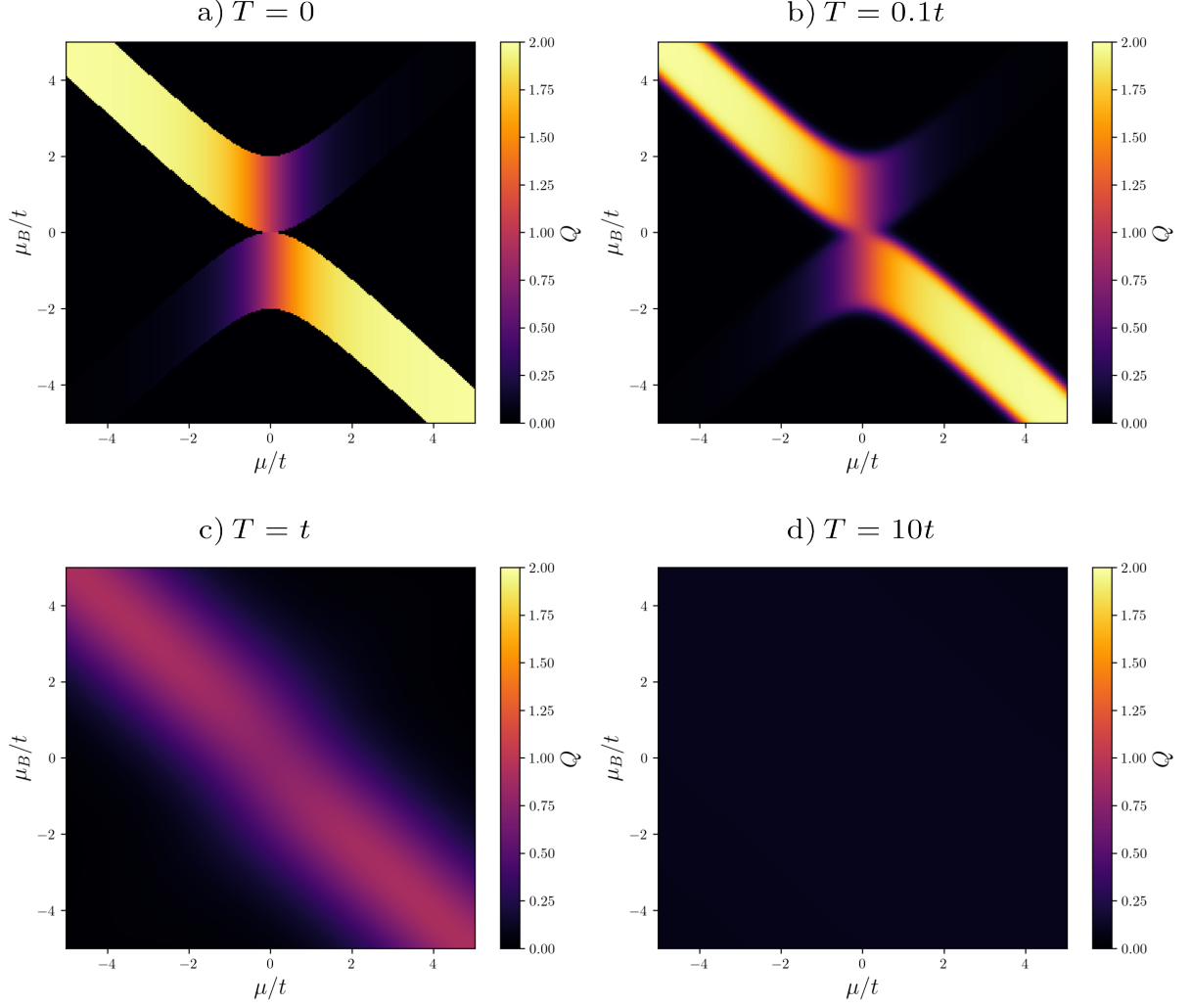


Figure 6.9: Temperature dependence of the steady-state end-to-end correlations Q_{ss} in the μ - μ_B phase diagram. At $T = 0$, the only region exhibiting nonzero correlations coincides with the region where the population p_0^- is dominant (see Figure 6.5). This result is in accordance with the Q -functions values (6.20). However, as the temperature increases, p_0^- becomes progressively mixed with the other populations, leading to a gradual attenuation of the correlations.

for different temperatures. Recall that the fidelity measures the degree of similarity of the two states.

Figure 6.10(a), corresponding to $T = 0$, shows two distinct dynamical regimes. In the central region, delimited by $|\mu_B| < 2t$, the fidelity decays comparatively slowly before saturating at the value $1/2$. In comparison, in the outer region $|\mu_B| > 2t$, the fidelity decreases faster towards the value $1/4$. The final fidelity values directly reflect the nature of the corresponding steady states: for $|\mu_B| < 2t$, the chain converges toward the mixed steady state characterized by the populations (p_0^+, p_0^-) , whereas for $|\mu_B| > 2t$ it converges toward the maximally mixed state. This behavior is in perfect accordance with the vertical cut at $\mu = 0$ in Fig. 6.5(a). As the temperature increases, the sharp boundary between these two regions is progressively smoothened. At sufficiently high temperature ($T = 10t$), the $|\mu_B| < 2t$ region no longer exhibits distinct behaviors compared to $|\mu_B| > 2t$. In this regime, the fidelity uniformly decays toward the maximally mixed-state value, in accordance with Fig. 6.5(d). Once again, this thermal smoothing originates for the dependence of the dissipative rates on the ζ -functions, and therefore on the Fermi-Dirac distribution. This effect is pictured in Figure 6.11. On these plots, we also observe that, in the region $|\mu_B| < 2t$, the absorption rate associated with the fermionic mode d_1 , namely $\bar{\kappa}_1$ is much smaller

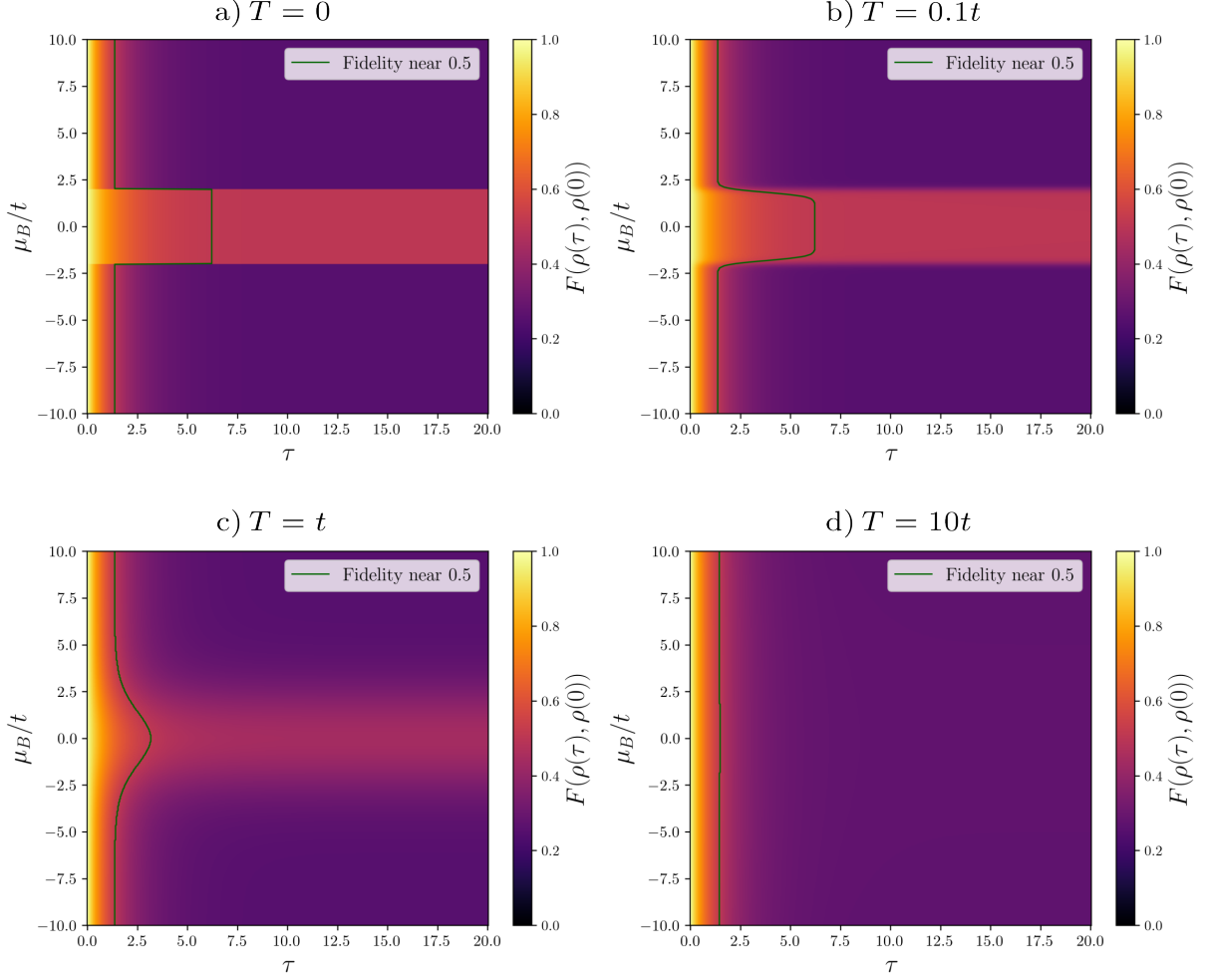


Figure 6.10: Time evolution of the fidelity of the MBS with respect to μ_B/t at $\mu = 0$ for different temperatures with the adimensional time $\tau = t\tilde{\tau}$. The green curve marks the threshold $F = 0.51$, which is used to define a characteristic decay time of the MBS. At $T = 0$, two distinct regions can be identified. In the central region, the fidelity converges towards 0.5 (mixture of p_0^+ and p_0^-) and is associated with longer decay times, whereas in the outer regions it converges towards 0.25, corresponding to a maximally mixed state and shorter decay times. These regions are consistent with the vertical cut at $\mu = 0$ shown in Figure 6.5. As the temperature increases, the sharp distinction between these regions progressively fades due to the thermal broadening of the Fermi-Dirac distribution.

than corresponding emission rate κ_1 . This property, together with the relation $\bar{\kappa}_2 = \kappa_2$, explains the mixed (p_0^+, p_0^-) character of the steady state (teal region) at $\mu = 0$. Indeed, excitations in the d_1 mode are emitted more efficiently than they are absorbed, while the d_2 corresponding processes are balanced. However, when $|\mu_B| > 2t$, all the dissipative rates show comparable values, leading to a maximally mixed state (brownish gray). Increasing the temperature smoothens the Fermi-Dirac distribution entering the rates, therefore reducing their dependence in μ_B . More specifically, the thermal effects flatten the profile of κ_1 while lifting $\bar{\kappa}_1$, eventually making the emission and absorption processes similar in magnitude. The difference in decay times observed between the two regions $|\mu_B| \gtrless 2t$ can therefore be traced back to the slowest decaying rate $\bar{\kappa}_1$ which remains small in the central region (at small temperature). Physically, this behavior can be understood from the occupation properties of the baths as follows: when $|\mu_B| > 2t = \epsilon_1$, the baths contain a significant population of fermions (holes) capable of interacting with the modes d_1 of energy ϵ_1 . In contrast, if $\mu_B < 2t = \epsilon_1$, this population is suppressed (depending on the temperature) and the only chain states that can host the baths fermions are $|+\rangle_0$ and $|-\rangle_0$ of zero-energy. This behavior illustrates the effectiveness of the energy-gap protection against exci-

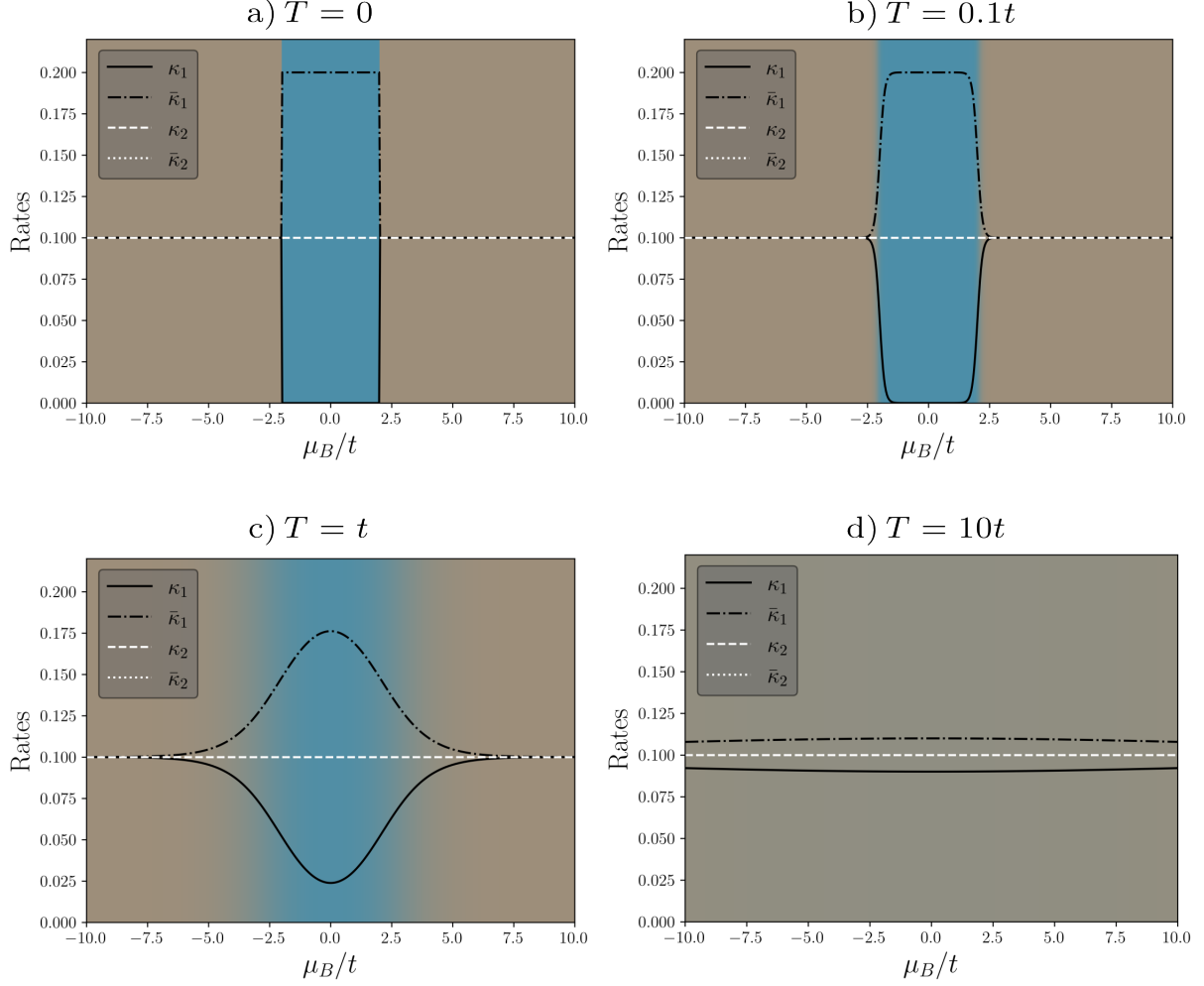


Figure 6.11: Temperature dependence of the dissipation rates at $\mu = 0$ as a function of μ_B/t . At $T = 0$, a sharp central region is observed for $|\mu_B/t| < 2$. In this region, the emission rate of the mode d_1 , $\bar{\kappa}_1$, is finite, whereas the corresponding absorption rate κ_1 vanishes. This asymmetry explains the steady-state mixture (p_0^+, p_0^-) and the longer decay times observed in the central region. In contrast, in the outer regions, all rates become comparable, leading to a maximally mixed steady state and consequently to shorter decay times. As the temperature increases, the dissipation rates are progressively modified by the thermal broadening of the Fermi-Dirac distribution. In particular, the distinction between κ_1 and $\bar{\kappa}_1$ in the central region becomes less pronounced, and their values gradually approach those of the other rates. As a result, the preferential stabilization of the (p_0^+, p_0^-) mixture is altered, driving the steady state towards a maximally mixed configuration even within the central region.

tations while simultaneously providing clear evidence of parity breaking. Indeed, in this central region, the Kitaev chain converges to a mixed steady state composed of $|+\rangle_0$ and $|-\rangle_0$, which belong to different parity sectors. Consequently, even for a zero-temperature bath and a low bath chemical potential μ_B , the encoded qubit is inevitably degraded, as its computational basis is no longer protected by parity conservation.

6.4 Impact of emerging baths structure

In this section, we investigate the impact of emerging bath structure by considering a Lorentzian spectral density of the form,

$$J(\omega) = \frac{\Gamma W^2}{\omega^2 + W^2}, \quad (6.55)$$

where we remind that W is the FWHM of the Lorentzian and Γ characterizes the maximum strength of the system-bath coupling. Recall from Section 5.5 that introducing a non-flat spectral density consists in selectively favoring bath frequencies in the system-bath interaction. In this case, the bath is no longer perfectly Markovian anymore. Indeed, the finite FWHM W induces a non-vanishing decay time in the BCFs, which now decay exponentially rather than instantaneously. Physically, this behavior originates from the restricted range of bath frequencies effectively available to absorb excitations (de-excitations) emitted (absorbed) by the system resulting in memory effects.

In order to characterize the impact of this emerging structure, in this section we consider a constant null bath temperature $T = 0$ leading to a Fermi-Dirac distribution,

$$n(\omega) = 1 - \Theta(\omega), \quad (6.56)$$

where the *Heaviside function* $\Theta(\omega)$ is defined as

$$\Theta(\omega) = \begin{cases} 0 & \text{if } \omega \leq 0, \\ 1 & \text{if } \omega > 0. \end{cases} \quad (6.57)$$

Therefore the ζ -functions now read,

$$\zeta(\omega) = \frac{\Gamma W^2}{(\omega - \mu_B)^2 + W^2} (1 - \Theta(\omega - \mu_B)) \quad \text{and} \quad \bar{\zeta}(\omega) = \frac{\Gamma W^2}{(\omega - \mu_B)^2 + W^2} \Theta(\omega - \mu_B), \quad (6.58)$$

and are modulated by the Lorentzian spectral density. We already see from these equations that the rates, given by the ζ -functions, will mostly be enhanced for eigenenergies ϵ_1 and ϵ_2 around the bath chemical potential μ_B .

Similarly to the previous section, we investigate, first, the effects of the bath structure on the steady-state properties by varying the FWHM W . The corresponding μ - μ_B phase diagrams for different values of W are pictured in Figure 6.12.

Let us describe these plots:

- a) $W = \infty$: since the FWHM is infinite, the spectral density reduces to the flat form $J(\omega) = \Gamma$. Consequently, this phase diagram is exactly identical to Fig. 6.5(a) corresponding to the $T = 0$ case.
- b) $W = 10$: when the spectral width remains large compared to the gap $|\epsilon_1 - \epsilon_2| = 2t$, the populations are still essentially unchanged. However, in comparison to the flat spectral density case, non-negligible populations p_1^- begin to appear in mixtures (p_0^+, p_1^-) (violet) and (p_1^+, p_1^-) (salmon).
- c) $W = 1$: once W is comparable to the gap $2t$, the mixed regions (p_0^+, p_1^-) (violet) and (p_1^+, p_1^-) (salmon) spread over high (low) bath chemical potential region for $\mu > 0$ ($\mu < 0$). Furthermore, new mixed regions (p_0^+, p_0^-) (teal) emerge in the intervals $-\epsilon_1 < \mu_B < -\epsilon_2$ for $\mu < 0$ and $\epsilon_2 < \mu_B < \epsilon_1$ for $\mu < 0$. We also observe an enhancement of the purity for the regions corresponding to the nearly pure steady states p_0^+ , p_0^- and p_1^+ .
- d) $W = 0.1$: the FWHM is now much smaller than the gap but taken at the limit of validity of the Markov approximation such that $\tau_B \sim \tau_R$. The regions containing populations p_1^- spread even further, resulting in regions of almost pure steady state p_1^- . Similarly, the new regions (p_0^+, p_0^-) continue to expand and also develop regions dominated by an almost pure population p_0^- .

From this, we can conclude that decreasing the FWHM W favors the emission of certain population for given values (μ, μ_B) , while enhancing the absorption of others. This selective filtering

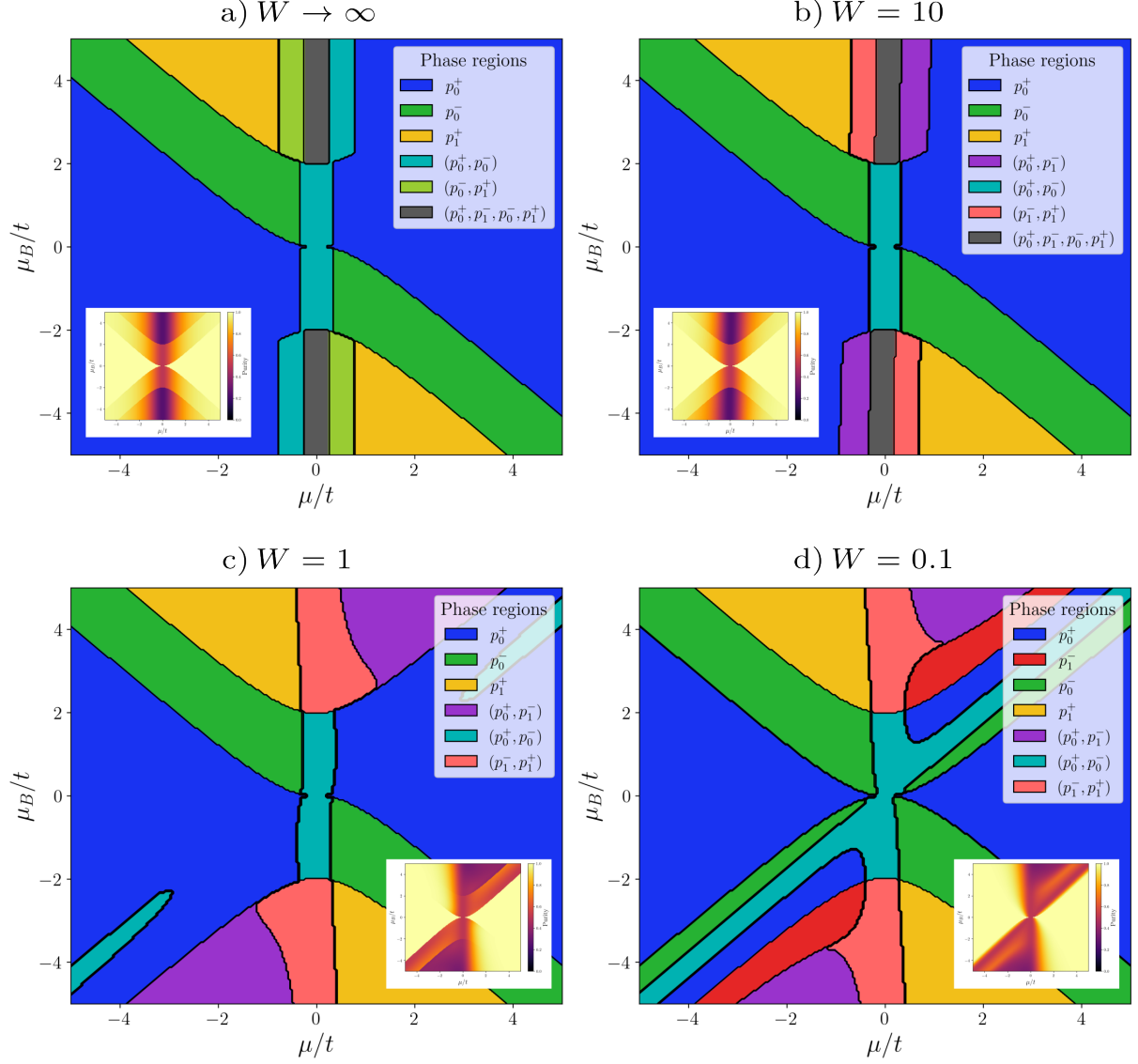


Figure 6.12: Population distribution in the μ - μ_B phase diagram. For large values of the W , the population structure is identical to that obtained for the flat spectral density at $T = 0$ (see Figure 6.5). As W decreases, however, new regions characterized by a population p_1^- emerge, together with additional regions of p_0^- . Furthermore, the purity of the initially 'pure' regions is progressively enhanced as the FWHM is reduced. The color-legend thresholds are identical to those used in Figure 6.5. The exact population distributions, as well as the corresponding purity phase diagrams, are provided in Appendix E.3.

effect induced by the structured bath leads to an increase in purity, together with the emergence of new mixed and nearly pure steady-state regions.

Once again, we are going to interpret the results by analyzing the behavior of the dissipation rates as functions of μ_B , for a fixed value of the chemical potential $\mu = -2$ (a vertical cut of the phase diagram), which is displayed in Figure 6.13.

It is clear that the dissipative rates are modulated not only by the Heaviside function, but also by the Lorentzian profile of the spectral density. As the FWHM W decreases, the Lorentzian increasingly suppresses or enhances rates relative to one another. This selective enhancement modulation creates regions in which the rates favoring a given population become dominant over their competing counterparts. In particular, this behavior enhances the population p_1^- (red), associated to larger absorption processes governed by the rate κ_1 (solid black line). Furthermore, the purity of the nearly pure regions, p_0^+ , p_0^- and p_1^+ , is also enhanced. Indeed, the Lorentzian

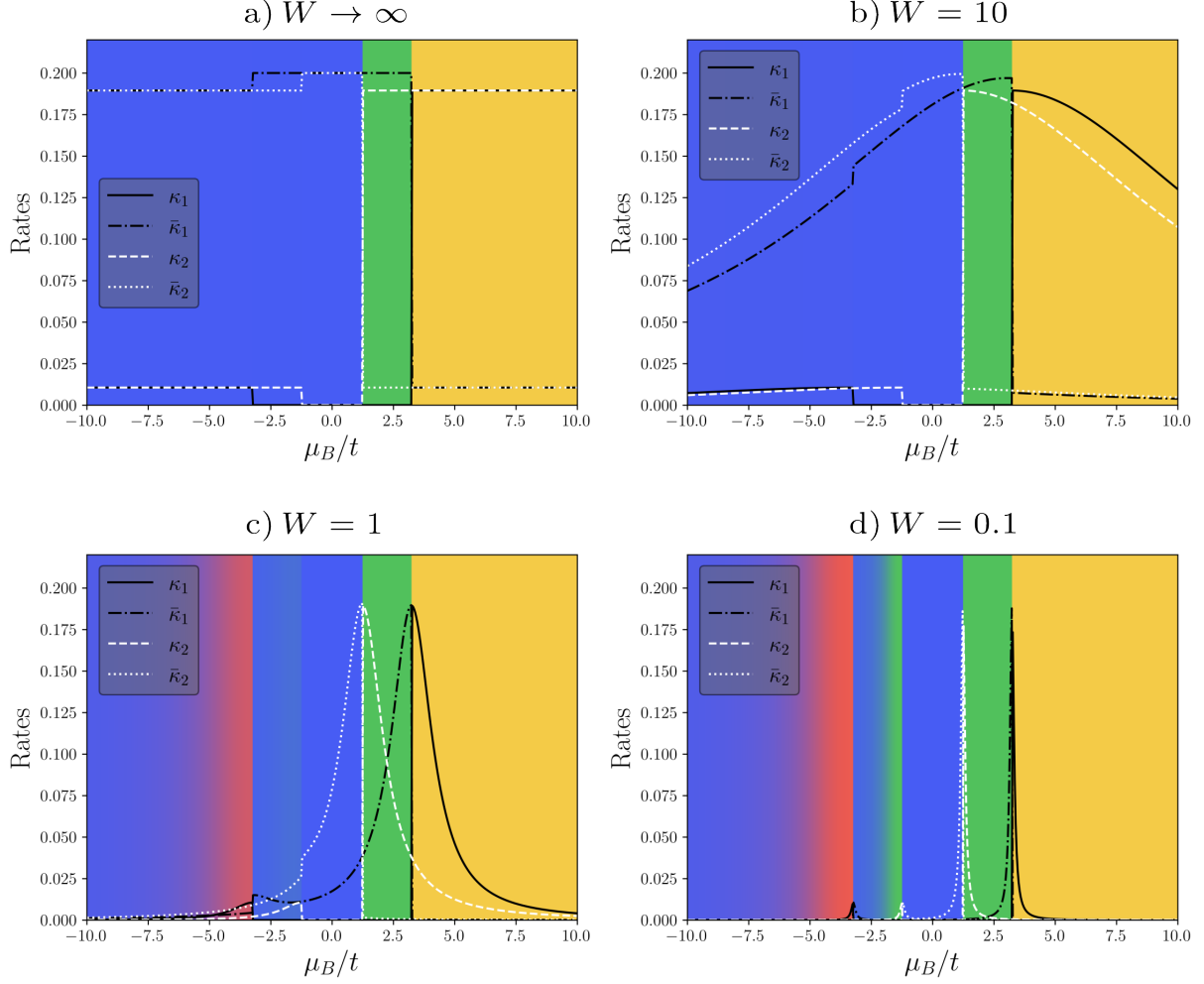


Figure 6.13: Width dependence of the dissipation rates as a function of μ_B for $\mu/t = -2$. As in the previous cases, the steady-state populations, represented by the background colors (with p_1^- shown in red), are determined by the dominance of specific pairs of dissipation rates over the others. As the FWHM W decreases, the rates become increasingly modulated by the Lorentzian spectral profile. This modulation gives rise to new regions in which the rate pairs associated with p_1^- or p_0^- become dominant, thereby explaining the emergence of the additional steady-state regions observed in Figure 6.12. Moreover, in the regions that were already classified as pure for large W , the Lorentzian modulation further suppresses the competing rates whenever no additional population becomes dominant. As a consequence, the purity of the corresponding steady states is enhanced as the FWHM is reduced.

modulation suppresses the competing rates responsible for mixing these states, while preserving the dominant dissipative rates driving the system toward a specific population. As a result, the steady states in these regions approach perfectly pure states more closely than in the flat-spectrum case. Physically, these enhancement mechanisms for purity and population selection can be understood as follows: as the spectral density gets narrower, the range of bath frequencies involved in the system-bath interaction decreases. Therefore, the Lorentzian spectral density acts as an effective band-pass filter for the bath, allowing only fermionic excitations within a specific energy window to be absorbed or emitted by the system. This filtering explains the preferential enhancement or suppression of specific populations, as well as the increased purity observed in certain steady-state regions.

As in the previous section, we see in Figure 6.14 that the steady-state end-to-end correlations given by (6.50) acquire non-zero values in the regions containing populations p_0^- and p_1^- . Consequently, decreasing W generates new regions in the phase diagram where correlations emerge, while simultaneously enhancing the correlations already present in the initial pure p_0^- region.

These emerging and enhanced correlations are therefore directly associated with the emergence and spreading of the new regions characterized by p_0^- and p_1^- . Once more this behavior of the end-to-end correlations can be generalized for larger Kitaev chains.

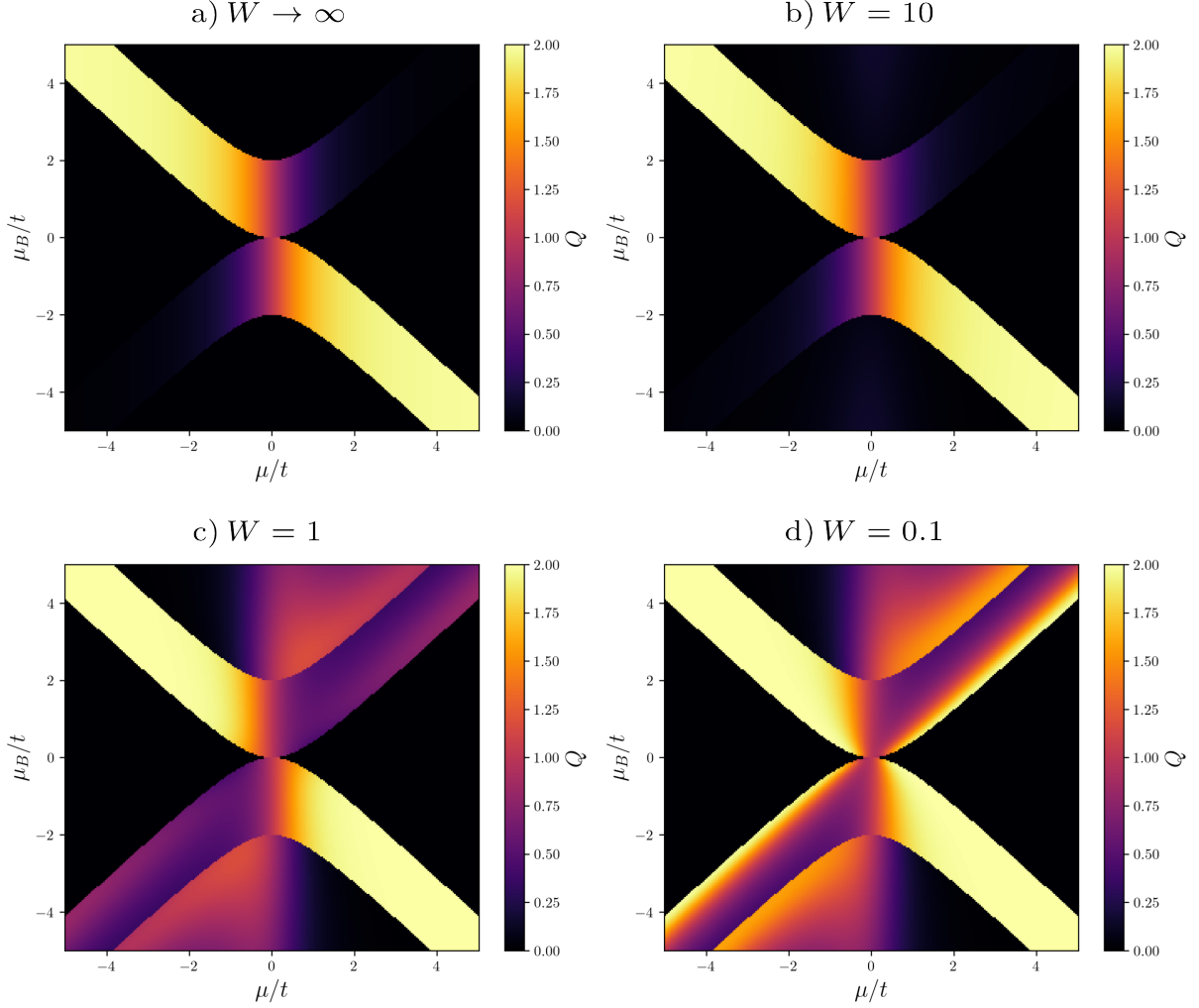


Figure 6.14: *FWHM dependence of the steady-state end-to-end correlations. For a flat spectral density ($W = \infty$), the correlations follow the distribution of p_0^- , as observed previously. As the FWHM W decreases, however, new regions dominated by p_0^- and p_1^- emerge, giving rise to additional regions with nonzero end-to-end correlations. Moreover, since the purity of the initially ‘pure’ regions is enhanced as the width is reduced, the corresponding correlations become increasingly pronounced.*

Now that the impact of the emerging bath structure on the steady-state properties has been investigated, we turn to the transient dynamics, following the same procedure as in the previous section. More precisely, we initialize the system in the MBS $\rho(0) = |-\rangle\langle -|_0$ and let it evolve dissipatively in time. The persistence of the initial state is then quantified through the fidelity between the evolved state and the initial one. The resulting dynamics are shown in Figure 6.15.

As the FWHM W decreases, the fidelity becomes significantly more robust over time. In particular, in the outer region $|\mu_B| > 2t$, the typical fidelity-decay time (green curve) increases and progressively bends toward the inner region, from the highest value of μ_B toward $\mu_B = 2t$. Furthermore, while the fidelity was decaying towards a $1/4$ -value for the flat spectral density case, the fidelity now goes to zero when W increases. This stems from the population p_1^- starting to dominate over p_0^- when the spectral density becomes narrower. Indeed, for $\mu_B > 0$ and $\mu = 0$, the previously maximally-mixed steady state becomes a mixture (p_1^-, p_1^+) , these populations being the only states that the baths can couple to due to the thin frequency window available. Additionally, in the inner region $|\mu_B| < 2t$, we observe the emergence of two spikes of

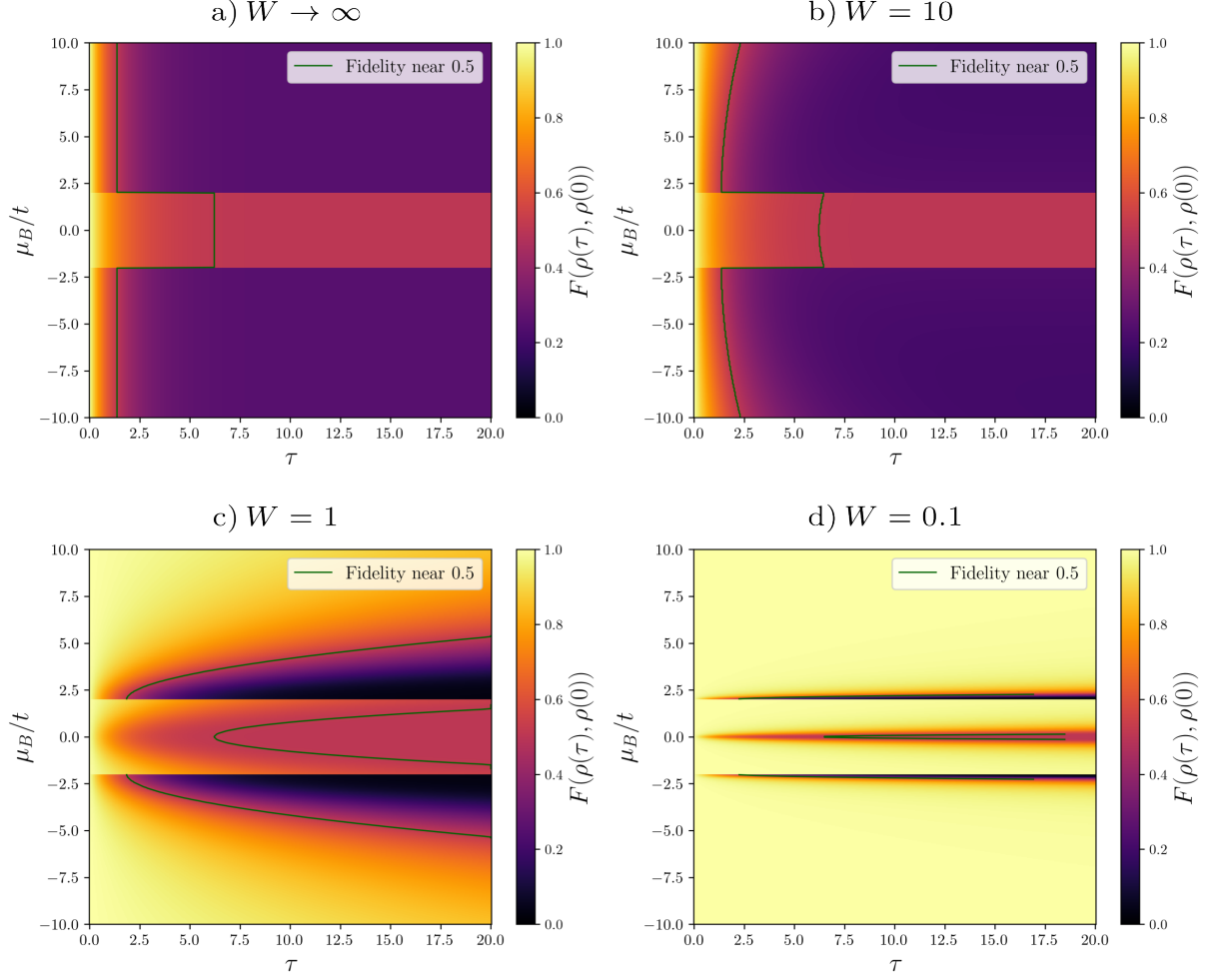


Figure 6.15: Time evolution of the fidelity of the MBS at $\mu = 0$ with respect to μ_B/t for different values of the FWHM W , plotted as a function of the dimensionless time $\tau = t\tilde{\tau}$. As the width decreases, the characteristic decay time of the MBS, defined by the threshold $F = 0.51$ (green curve), increases significantly. Short decay times remain only for bath chemical potentials near the eigenenergies of the BdG Hamiltonian of the Kitaev chain. This behavior originates from the frequency selectivity introduced by the Lorentzian spectral density. Indeed, as the spectral profile becomes narrower, only bath modes with chemical potentials resonant with the system energies contribute significantly to the dissipative dynamics. Consequently, dissipation is strongly suppressed away from these resonances, leading to a substantial enhancement of the MBS lifetime.

long fidelity lifetimes, which also spread progressively as W increases. In order to understand this behavior physically, it is relevant to analyze once more the dissipation rates for $\mu = 0$ as a function of μ_B , as shown in Figure 6.16. Once again, this behavior can be understood from the modulation of the dissipative rates by the Lorentzian profile of the spectral density. In the outer region, as the bath chemical potential μ_B increases, the frequency window selected by the band-pass filter becomes progressively detuned from the system eigenenergies. As a consequence, the rates decrease, leading to longer decay time. Indeed, in the definition of the rates (6.40-6.43), the ζ -functions are evaluated at the eigenenergies of the system. For $\mu = 0$, these energies are $\pm\epsilon_1 = \pm 2t$ and $\epsilon_2 = 0$. Therefore, when the Lorentzian FWHM becomes sufficiently narrow, the corresponding ζ -functions vanishes unless the chemical potential aligns with these energies. In the inner region, the emission rate $\bar{\kappa}_1$ becomes progressively localized around $\mu_B = \pm\epsilon_1 = \pm 2t$, while the rates κ_2 and $\bar{\kappa}_2$ are squeezed around $\mu_B = \epsilon_2 = 0$. This is the expected behavior for a sharply peaked spectral density: only dissipation channel allowed are the ones associated to the eigenenergies of the system. All other channels are suppressed.

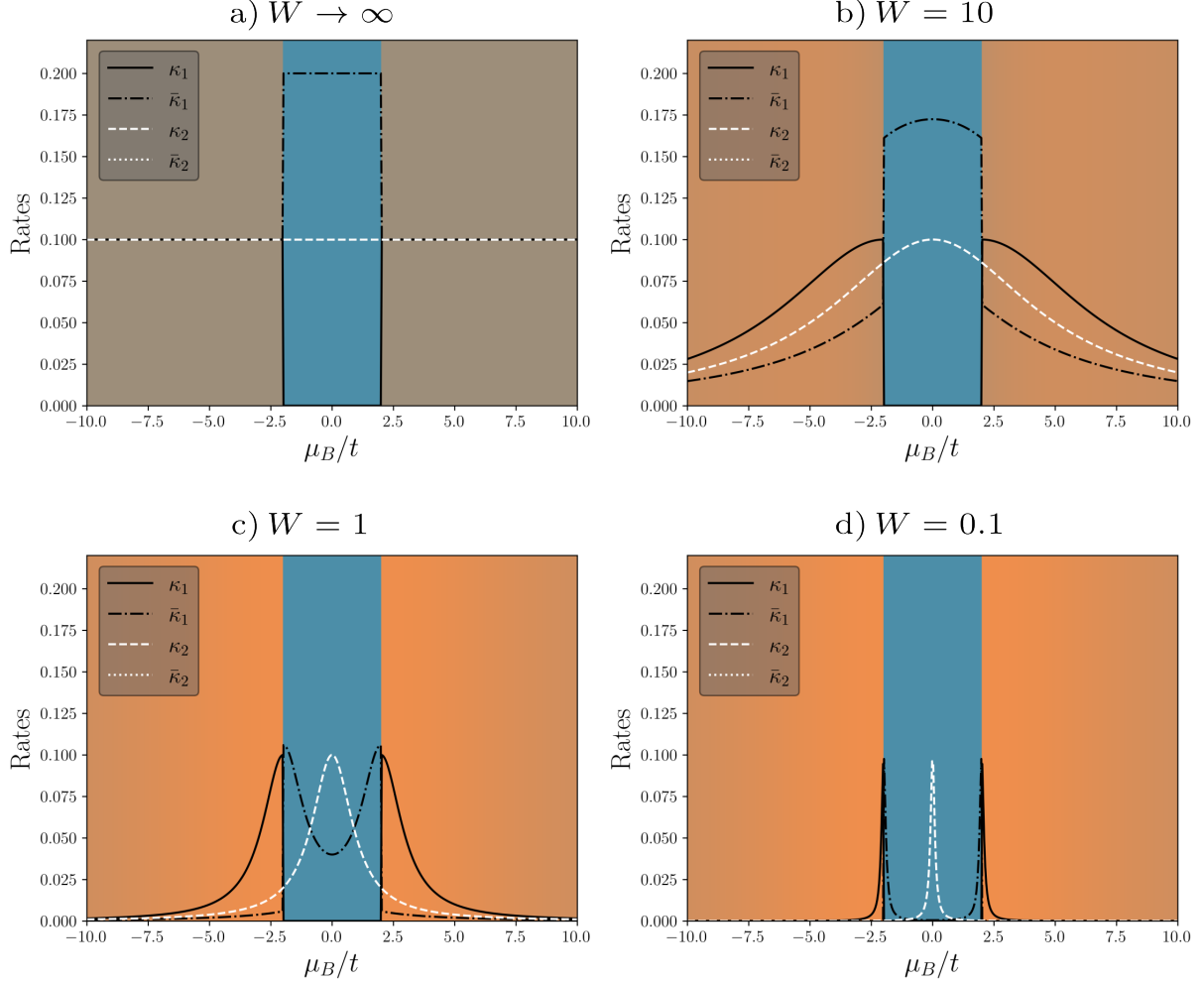


Figure 6.16: FWHM dependence of the dissipation rates at $\mu = 0$ as a function of μ_B/t . The influence of the Lorentzian spectral density is clearly visible through the progressive modulation of the dissipation rates around the eigenenergies of the two-site Kitaev chain. As the FWHM W decreases, the rates become increasingly squeezed near these resonant energies, while dissipation away from resonance is strongly suppressed. This enhanced frequency selectivity is responsible for the increase in the MBS lifetime observed in Figure 6.15.

To conclude this section on the dissipative 2-site Kitaev chain, we find that the MBS is not absolutely protected when coupled to a thermal fermionic bath. Indeed, the only regions of the steady-state population phase diagram exhibiting an almost pure p_0^- population do not overlap with the sweet spot $\mu = 0$. Furthermore, at $\mu = 0$, the MBS dynamics either converges towards a mixed state containing excited non-topological states for $\mu_B > 2t$, or towards an equal mixture of the MBS and the Bogoliubov vacuum for $\mu_B < 2t$ at $T = 0$. In both cases, the parity of an encoded qubit would be lost. Moreover, temperature has a detrimental effect on the MBS lifetime. Indeed, the central region, where the MBS initially only converges towards an equal mixture with the Bogoliubov vacuum due to the gap protection, evolves towards increasingly mixed steady states as the temperature increases with lower decay time. Nevertheless, these effects can be mitigated by coupling the chain to a structured bath with a Lorentzian spectral density. The FWHM W then acts as a frequency window, selecting the bath chemical potentials that efficiently contribute to the dissipative dynamics. Consequently, preserving the MBS over long times requires low temperatures together with a structured bath characterized by a narrow spectral density and a chemical potential detuned from the eigenfrequencies of the chain. Finally,

one may argue that a 2-site Kitaev chain supports an MBS only at the sweet spot $\mu = 0$, a situation that is difficult to realize experimentally. Nevertheless, understanding the dissipative dynamics of the 2-site case remains relevant, both as a minimal model for the dynamics of larger finite-size chains and because recent experiments have successfully realized a 2-site Kitaev chain [23].

7 The N -site dissipative Kitaev chain

7.1 Interacting N -site Kitaev chain and secularized master equation

Recall that our main goal is to investigate the impact of dissipation on the topological phase $|\mu| < 2t$ of the Kitaev chain by analyzing the end-to-end correlations (4.12). However, this phase is not properly defined for the 2-site Kitaev chain. Indeed, since the chain is too short, for $0 < |\mu| < 2t$, both MZMs spread over the whole chain and overlap strongly, which lifts the ground state degeneracy. Nevertheless, the results obtained in the previous sections for the correlations can be extrapolated to larger finite chains.

Therefore, we consider an N -site Kitaev chain coupled through on-site hopping interactions with N fermionic baths at thermal equilibrium, all characterized by the same temperature T and chemical potential μ_B . The Hamiltonian of the global system, sketched in Figure 7.1, reads

$$H = H_S + \sum_{l=1}^N H_{B,l} + H_I \quad (7.1)$$

where H_S is the Kitaev Hamiltonian given by (4.1), $H_{B,l}$ the Hamiltonian for the l^{th} bath given by (6.22) and the interaction Hamiltonian H_I is given by (6.25). Since the interaction Hamilto-

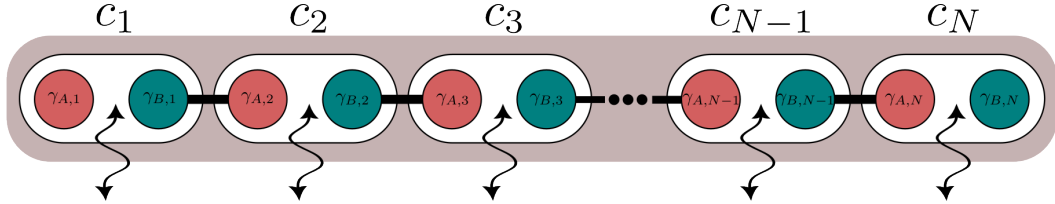


Figure 7.1: Sketch of the N -site Kitaev chain with on-site hopping interaction.

nian is identical to that considered in the 2-site dissipative case, the BCFs remain unchanged. Consequently, the derivation of the master equation follows the same procedure, starting from the Redfield master equation,

$$\dot{\rho} = -i[H_S, \rho] + \sum_{l=1}^N \left([L_l \rho, c_l] + [c_l^\dagger, \rho L_l^\dagger] \right) + \sum_{l=1}^N \left([\bar{L}_l \rho, c_l^\dagger] + [c_l, \rho \bar{L}_l^\dagger] \right). \quad (7.2)$$

However, recall that the dynamical map generated by this Redfield master equation is not, in general, completely positive and trace-preserving. As we observed non-physical states (i.e., non-positive states) in some parameter regimes here, we secularized the master equation by erasing the terms in (7.2) that do not obey some secularization conditions. This can be done as follows: suppose we have found the orthonormal eigenbasis $\{|k\rangle\} : k = 1, \dots, 2^N$ of the Kitaev Hamiltonian. This latter can therefore be decomposed as

$$H_S = \sum_{k=1}^{2^N} \epsilon_k |k\rangle \langle k|, \quad (7.3)$$

where ϵ_k is the eigenenergy associated to $|k\rangle$. Since $\{|k\rangle\}$ is a basis of the Hilbert space of the system $\mathcal{H}_S$, the set of operators $\{|i\rangle\langle j|\} : i, j = 1, \dots, 2^N$ forms a basis of the Hilbert-Schmidt space $\mathcal{B}_2(\mathcal{H}_S)$, *i.e.*, the vector space of operators acting on $\mathcal{H}_S$. These operators are the eigenoperators of H_S following

$$[H_S, |i\rangle\langle j|] = (\epsilon_i - \epsilon_j) |i\rangle\langle j|. \quad (7.4)$$

Using this, we can decompose the fermionic operators of one site (dropping the site index for readability) in this basis as

$$c = \sum_{i,j} c_{i,j} |i\rangle\langle j|, \quad (7.5)$$

$$c^\dagger = \sum_{i,j} (c^\dagger)_{i,j} |i\rangle\langle j| = \sum_{i,j} c_{i,j}^* |j\rangle\langle i|, \quad (7.6)$$

where we have defined the matrix elements $c_{i,j} = \langle i|c|j\rangle$ and $(c^\dagger)_{i,j} = \langle i|c^\dagger|j\rangle$. Therefore, these decompositions allow us to compute the operators L and $\bar{L}$ as

$$L = \int_0^\infty \alpha(s) e^{-iH_S s} c^\dagger e^{iH_S s} ds = \pi \sum_{i,j} (c^\dagger)_{i,j} \zeta(\epsilon_i - \epsilon_j) |i\rangle\langle j|, \quad (7.7)$$

$$\bar{L} = \int_0^\infty \bar{\alpha}(s) e^{-iH_S s} c e^{iH_S s} ds = \pi \sum_{i,j} c_{i,j} \bar{\zeta}(\epsilon_j - \epsilon_i) |i\rangle\langle j|, \quad (7.8)$$

where the BCFs, $\alpha(s)$ and $\bar{\alpha}(s)$ are given by (6.37-6.38) and the ζ -functions by (E.26). Finally, we decompose each terms of the non-unitary part of the Redfield master equation (7.2) as

$$[L\rho, c] + [c^\dagger, \rho L^\dagger] = \pi \sum_{i,j,k,l} \zeta(\epsilon_i - \epsilon_j) \left((c^\dagger)_{i,j} c_{k,l} (|i\rangle\langle j| \rho |k\rangle\langle l| - |k\rangle\langle l| i\rangle\langle j| \rho \right. \\ \left. + c_{j,i} (c^\dagger)_{l,k} (|l\rangle\langle k| \rho |j\rangle\langle i| - \rho |j\rangle\langle i| l\rangle\langle k|) \right), \quad (7.9)$$

$$[\bar{L}\rho, c^\dagger] + [c, \rho \bar{L}^\dagger] = \pi \sum_{i,j,k,l} \bar{\zeta}(\epsilon_j - \epsilon_i) \left(c_{i,j} (c^\dagger)_{l,k} (|i\rangle\langle j| \rho |l\rangle\langle k| - |l\rangle\langle k| i\rangle\langle j| \rho \right. \\ \left. + (c^\dagger)_{j,i} c_{k,l} (|k\rangle\langle l| \rho |j\rangle\langle i| - \rho |j\rangle\langle i| k\rangle\langle l|) \right). \quad (7.10)$$

We know that the secular approximation amounts to removing all the oscillating terms when we switch to the interaction picture. For the terms of the form (7.9), the interaction picture generates oscillating factors of the form $\exp(-i(\epsilon_i - \epsilon_j + \epsilon_k - \epsilon_l)t)$ which leads to the secularization condition $\epsilon_i - \epsilon_j = \epsilon_l - \epsilon_k$. Similarly, for the terms of the form (7.10), the interaction picture produces factors $\exp(-i(\epsilon_i - \epsilon_j + \epsilon_l - \epsilon_k)t)$ yielding the secularization condition $\epsilon_i - \epsilon_j = \epsilon_k - \epsilon_l$. These conditions are then implemented numerically in the simulations to yield effective GKSL master equation dynamics.

7.2 Steady state and end-to-end correlations

Similarly as the 2-site Kitaev, we numerically obtain the steady-state end-to-end correlations by computing the Q -function as

$$Q_{ss} = 2 \left| \text{Tr} \left(\rho_{ss} (c_N^\dagger c_1 + c_1^\dagger c_N) \right) \right|, \quad (7.11)$$

where ρ_{ss} is the steady-state density operator. Let us observe the structure of Q_{ss} in the (μ, μ_B) phase diagram pictured in Figure 7.2. The structure of these Q_{ss} phase diagrams is similar to that obtained for the 2-site Kitaev chain. Indeed, in the 2-site case, the end-to-end correlations

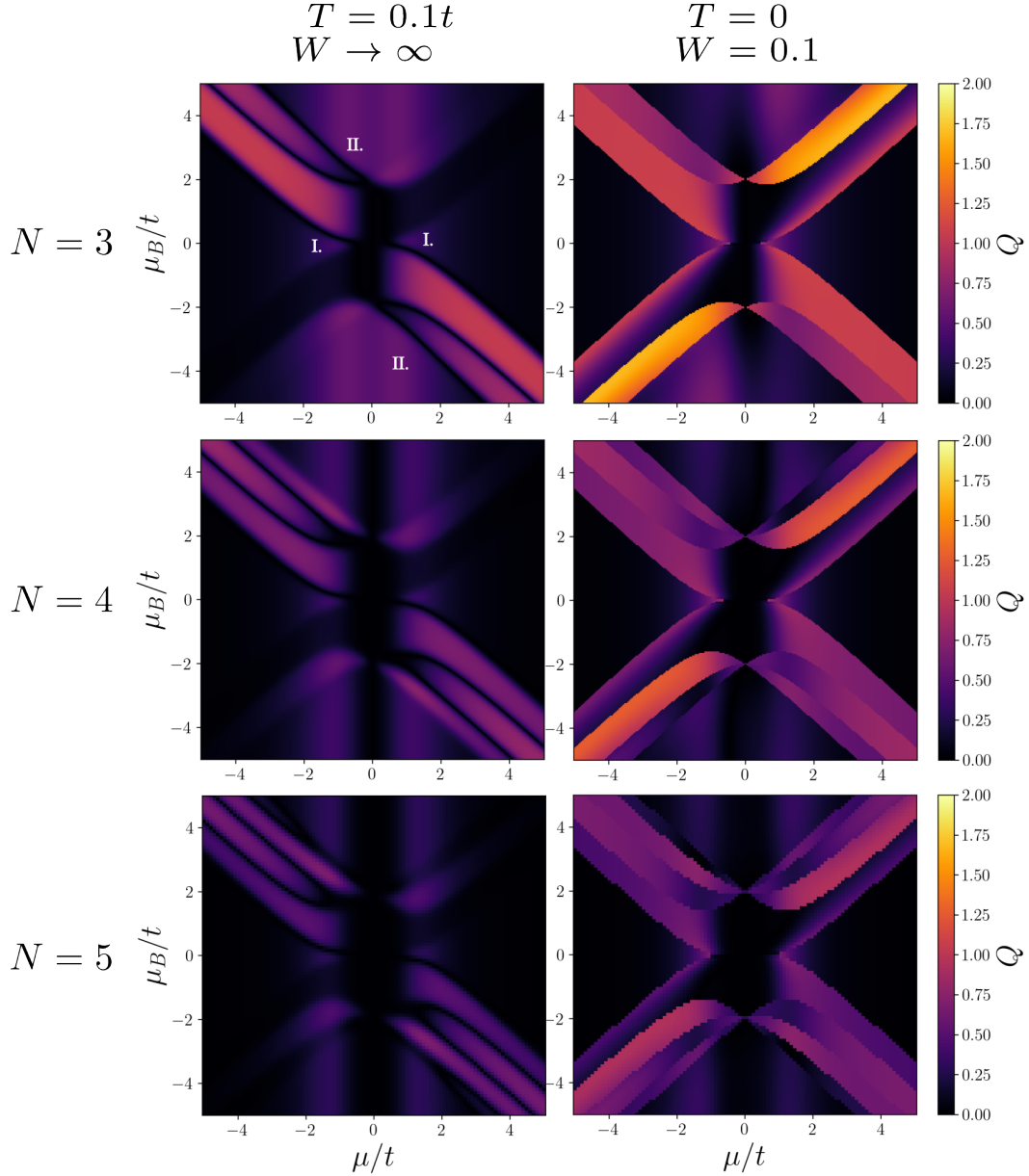


Figure 7.2: End-to-end correlations in the μ - μ_B phase diagram for finite Kitaev chains of length $N = 3, 4$, and 5 , shown for different temperatures and spectral widths W . The same qualitative effects observed for the 2-site chain are observed: thermal broadening of the Fermi-Dirac distribution progressively suppresses the correlations and blurs the boundaries between correlated regions, while the finite FWHM of the Lorentzian spectral density introduces a frequency selectivity that can enhance and reshape the correlation pattern. In all cases, the structure of the correlations closely follows the energy spectrum of the corresponding Kitaev chain. Furthermore, we observe new correlation areas in the 'topological region' $|\mu/t| < 2$ coming from the non-zero correlation of the Bogoliubov vacuum (I-II) and the 'MBS' (II) for a Kitaev chain of length $N > 2$.

were enhanced or suppressed depending on the dominant steady-state populations for a given pair of values (μ, μ_B) . The distribution of the population was itself determined by the relative value of the bath chemical potential with respect of the eigenenergies of the chain. More precisely, when the baths possess a sufficiently large chemical potential μ_B , they contain a significant population of fermions with energies high enough to populate the excited states of the chain. This leads to the correlation patterns reflecting the structure of the energy spectrum of the Kitaev Hamiltonian. In Figure 7.3, we indeed observe that the spectra of the Kitaev

chain for $N = 3, 4$ and 5 sites perfectly fit the structures appearing in the corresponding phase diagrams. Therefore, the origin of these structures can be understood for an arbitrary number of sites. On the phase diagrams, new regions, labeled I and II exhibiting non zero-correlations,

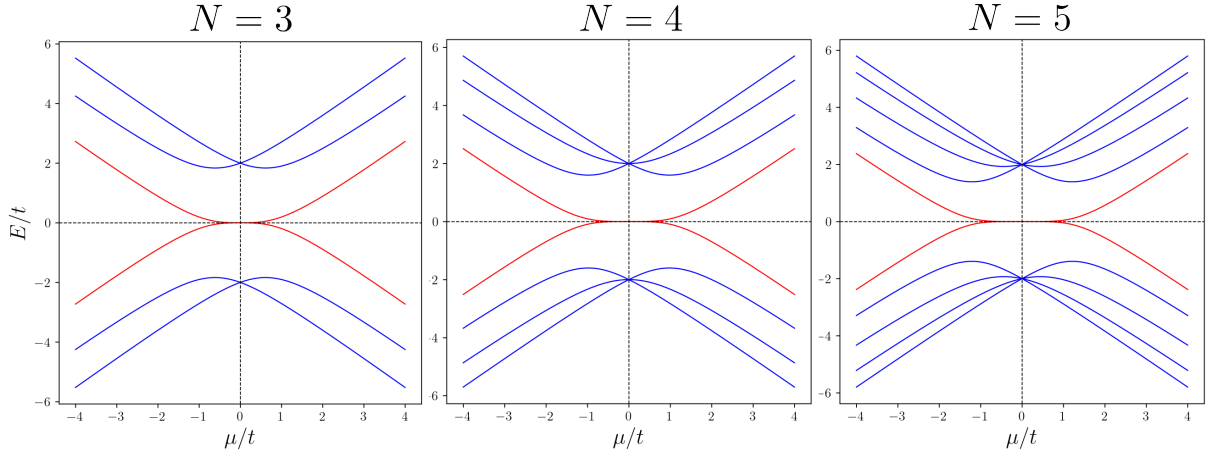


Figure 7.3: BdG spectra of finite Kitaev chains with $N = 3, 4$, and 5 sites. The red branches correspond to the Majorana bound state (MBS), which approaches zero energy for sufficiently small values of $|\mu/t|$, while the blue branches correspond to excited states that remain separated from zero energy by a finite gap. As already illustrated in Figure 4.10, the range of μ/t over which the lowest-energy mode remains close to zero energy increases with the chain length.

appear for $|\mu| < 2t$, *i.e.*, inside the topological region, whereas this was not observed in the 2-site case. Indeed, extrapolating the results of the 2-site Kitaev chain suggests that the dominant population in region I corresponds to the Bogoliubov vacuum which, for $N > 2$, shows non-zero end-to-end correlations whenever the chain is in its topological phase (see Figure 4.12). In region II, the purity phase diagrams (see Appendix F) show that the steady state is highly mixed. Thus, the correlations in this region likely originate from several contributing populations, such as the Bogoliubov vacuum and the MBS, the latter already being present in the corresponding region of the 2-site Kitaev chain. Hence, for larger chains, the end-to-end correlations associated with the topological states are preserved, either through nearly pure topological steady states, either through mixed steady states. However, non-zero correlations also appear outside the topological region $|\mu| < 2t$. This comes from the fact that the Kitaev chain for $N = 3, 4$ and 5 sites remains relatively short compared to the decay length of the eigenexcitations, spreading over the whole chain and therefore generating finite end-to-end correlations. Nevertheless, as N increases, the correlations in these non-topological regions of nearly pure population (see Appendix F) decrease, which is the expected behavior (as mentioned in Section 4.5).

Finally, we notice that the effects of the temperature T and the Lorentzian width W are also qualitatively similar to those of the 2-site case. Indeed, for $T = 0$, the regions corresponding to nearly pure populations with finite correlations are sharply separated. This behavior comes from the exact same modulation of the dissipative rates by the Fermi-Dirac distribution, which reduces to a Heaviside shape at zero temperature. This modulation arises from the presence of the ζ -functions in (7.9) and (7.10). As T increases, the Fermi-Dirac distribution becomes smoother, implying that the differences between the competing rates favoring a given population become less pronounced over certain parameter regimes, *e.g.*, $\mu_B = \epsilon_k$ for some k . Consequently, this results in a mixed steady-state with weaker end-to-end correlations. Then, for the case $W = 0.1$, new correlation regions emerge together with an enhancement of the purity of the initially nearly pure regions. This behavior stems from the Lorentzian modulation of the dissipative rates. Once again, the Lorentzian spectral density acts as an effective band-pass filter for the bath frequencies coupled to the system, allowing only dissipative processes associated with energies

lying inside the narrow Lorentzian window. As a result, specific populations of the Kitaev chain are selectively favored whenever their energies resonate with the restricted frequency range imposed by the structured bath.

7.3 Transient dynamics

Let us first examine the time evolution of an initial state corresponding to the lowest-energy state of the N -site Kitaev Hamiltonian at $\mu = 0$, and therefore corresponding to the MBS. In a similar fashion as in the 2-site case, we let this state evolve dissipatively in time and compute the fidelity of this evolved state with the initial MBS. The results are represented in Figure 7.4. We clearly observe the same qualitative dynamics as in the 2-site case. In the inner region

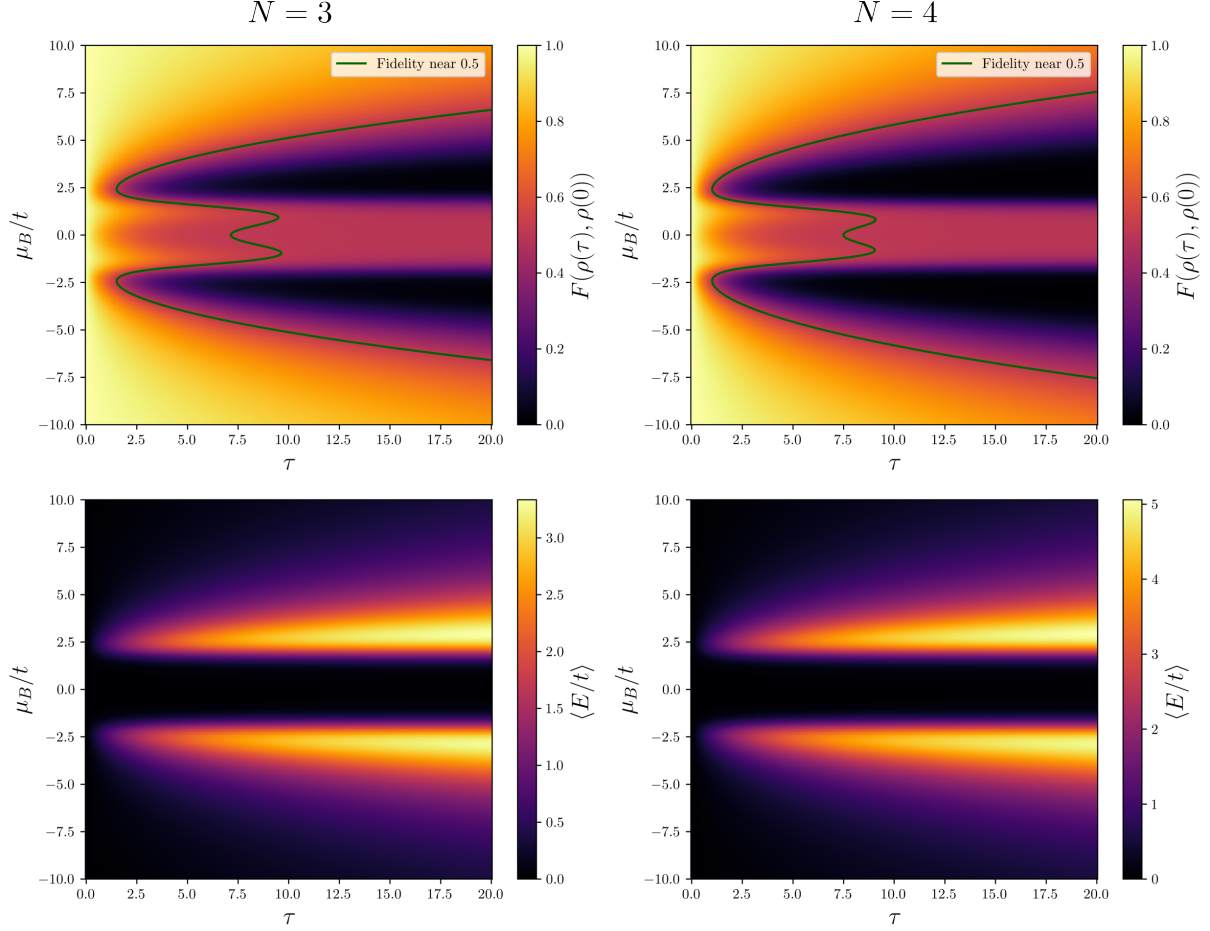


Figure 7.4: Time evolution of the fidelity of the MBS at $\mu = 0$ as a function of μ_B/t , together with the evolution of the normalized mean energy $\langle E/t \rangle$, for Kitaev chains of length $N = 3$ and $N = 4$. The parameters are fixed to $T = 0.1t$ and $W = 1$. The same qualitative behavior observed for the $N = 2$ case is recovered: the thermal broadening of the Fermi-Dirac distribution smooths the boundaries between regions, while the finite spectral width acts as a pass-band filter, concentrating the shortest decay times (represented by the green curve $F = 0.51$) around the eigenenergies of the chain. The evolution of the mean energy provides additional insight into the nature of the asymptotic states. In the central region, the system converges towards a zero-energy mixed state, corresponding to an equal mixture of the two topological ground states. In contrast, the outer regions evolve towards states with finite mean energy, indicating the presence of non-topological excited-state contributions in the steady state.

$|\mu_B| < 2t$, the fidelity decays toward a $1/2$ -value. This time, we do not have access to the population phase diagram allowing us to directly identify the composition of the steady-state mixture toward which the system evolves. However, we observe that the energy remains zero in this region, indicating that the steady state is composed of a mixture of the Bogoliubov vac-

uum and the MBS, *i.e.*, the two degenerate ground state. Once again, this behavior originates from the gap protection of the Kitaev degenerate ground state. Indeed, provided that the bath temperature is not too large, the baths do not contain a significant population of high-energy fermions in this region of chemical potential. Consequently, the non-zero energy excited states of the chain cannot be efficiently populated by the dissipative dynamics. Hence, the evolution of the system is restricted to the Bogoliubov vacuum and the MBS. In the outer region $|\mu_B| > 2t$, the fidelity eventually decays towards zero, which finds its explanation from the suppression of the MBS population by the higher-energy fermionic excitations. Because of the narrow spectral width ($W = 1$), the Lorentzian spectral density selectively enhances dissipative processes associated with energies close to μ_B , thereby favoring the occupation of excited states coupled to the baths. Furthermore, we recover the same dependence on temperature and spectral width as in the 2-site case. In particular, the blurred boundary $|\mu_B| = 2t$ at $T \neq 0$, and the decrease of the FWHM producing pronounced spikes of long decay time appearing in the inner region near the boundary and increasing the decay time as the bath chemical potential grows. These behaviors once again stems from the combined Fermi-Dirac and spectral modulations of the ζ -functions. A final observation we can make is the growth of the decay time towards a fidelity near 0.5 with the number of sites in the chain in the inner region. However, in the outer region the inverse phenomenon happens.

While, for the 2-site Kitaev chain, the only spot supporting a zero-energy MBS is $\mu = 0$, for an N -site Kitaev chain with $N > 2$, finite values of μ can still support a lowest-energy mode with an energy near zero. In this case, we must choose μ carefully in order to limit finite-size effects and avoid an excessive lifting of the ground-state degeneracy. Indeed, this degeneracy lifting arises from the overlap between the two MZM wavefunctions. To minimize this effect, we impose a condition on the chemical potential such that the typical MZM localization length ξ_M , given in (4.53), remains significantly smaller than the chain size. More precisely, we arbitrarily require ξ_M to be four times smaller than the system size, leading to the condition $\mu < e^{-4/N}$. In the following, we choose $\mu = -0.25$, which satisfies our arbitrary condition for $N = 3, 4$, and investigate the dissipative dynamics of the corresponding MBS through the time evolution of its fidelity.

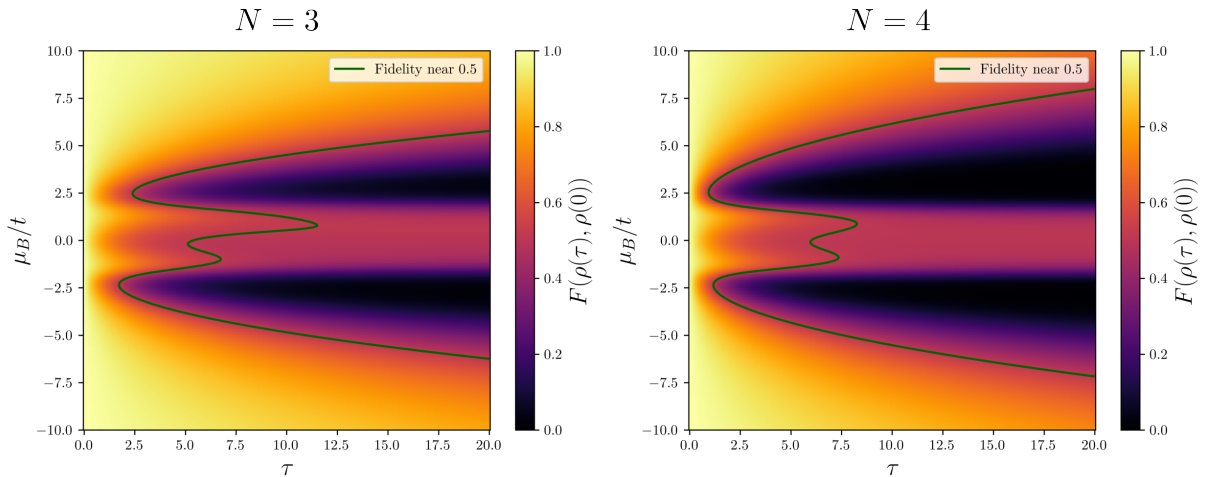


Figure 7.5: Time evolution of the fidelity of the MBS at $\mu = -0.25$ as a function of μ_B/t , for Kitaev chains of length $N = 3$ and $N = 4$. An asymmetry in the characteristic decay time is observed, originating from the dominant particle character of the imperfect MBS. Consequently, the MBS is more strongly affected by the Pauli exclusion principle when coupled to a bath with positive chemical potential than to one with negative chemical potential. As the chain length increases, this asymmetry becomes less pronounced, reflecting the convergence of the imperfect finite-size MBS towards an ideal one with increasingly balanced particle and hole components.

In Figure 7.5, we observe essentially the same qualitative structure as in the $\mu = 0$ case, except that the decay time now exhibits a clear asymmetry with respect to $\mu_B = 0$. This behavior can be easily understood. Since the chain is finite, choosing a nonzero chemical potential μ lifts the energy of the MBS, thereby introducing three resonant frequencies in the central region. Furthermore, generalizing the results obtained for the two-site Kitaev chain, when $\mu < 0$ the particle character of the MBS dominates over its hole character (see Fig. 6.8). Consequently, for a positive bath chemical potential ($\mu_B > 0$, corresponding to a particle-filled bath), the Pauli exclusion principle can partially inhibit transitions, thus slowing down the decay of the MBS compared to the case of a negative bath chemical potential ($\mu_B < 0$, corresponding to a hole-filled bath). This mechanism explains the asymmetry of the green curves associated with the characteristic fidelity threshold ($F = 0.51$), which show a larger peak for positive values of μ_B than for negative ones. Moreover, this interpretation is supported by the fact that the asymmetry becomes less pronounced as N increases for a fixed value of μ . Indeed, comparing the cases $N = 3$ and $N = 4$, the asymmetry is clearly reduced for $N = 4$. This behavior originates from the convergence of the imperfect finite-size MBS towards an ideal one, for which the particle and hole components become increasingly balanced towards the topological phase, $|\mu| < 2t$.

We can conclude this section on the N -site Kitaev chain by emphasizing that the underlying physics remains qualitatively similar to that of the 2-site case. The steady-state phase diagrams display the same spectral structure, with end-to-end correlations persisting for certain non-topological states. However, additional correlated regions emerge within the topological phase, $|\mu| < 2t$, due to the correlations of the Bogoliubov vacuum. Regarding the transient dynamics, for sufficiently low temperatures, the degenerate ground-state manifold remains protected against transitions to non-topological excited states when $|\mu_B| < 2t$, owing to the energy gap. Nevertheless, parity breaking still occurs within this region. As in the 2-site case, increasing the temperature has a detrimental effect on the MBS lifetime. These effects can, however, be mitigated by coupling the chain to a structured bath with a narrow spectral density. In this situation, choosing a bath chemical potential μ_B detuned from the eigenfrequencies of the chain significantly increases, once again, the characteristic decay time of the MBS. Finally, for $N > 2$, an imperfect MBS with energy close to zero can exist at nonzero values of the chemical potential μ , provided that the localization length of the edge Majorana modes remains much smaller than the chain length. In this regime, selecting a bath chemical potential within the protecting gap $|\mu_B| < 2t$ and with a sign opposite to that of μ can further increase the characteristic decay time of the MBS. Although this asymmetry becomes less pronounced at fixed μ as the chain length increases, due to the convergence of the imperfect MBS towards an ideal one, the range of chemical potentials supporting near-zero-energy Majorana modes expands with increasing N . Consequently, larger values of $|\mu|$ can be considered while remaining in the topological regime. Since the observed asymmetry appears to originate from the Pauli exclusion principle, one may expect this mechanism to remain effective at larger chain lengths by appropriately increasing $|\mu|$, thereby extending the lifetime of imperfect Majorana bound states.

8 Conclusion

Let us first summarize the main results obtained in this Master's thesis. After the introduction of fermionic tools and of the BCS theory of superconductivity in Sections 2 and 3, respectively, in Section 4, we began by introducing the Kitaev chain model and highlighting the importance of its topological phase, $|\mu| < 2t$, which hosts a Majorana bound state in the thermodynamic limit $N \rightarrow \infty$. Since the occupation of the MBS is associated with a zero-energy mode, the system exhibits a degenerate ground state separated from the excited states by an energy gap $2t$. This degenerate ground state forms the basis for the definition of a qubit. Indeed, a qubit can be encoded within a given parity sector of the composite ground state of two Kitaev chains. Furthermore, the MBS is composed of two Majorana zero modes exhibiting non-Abelian exchange statistics, allowing logical gates to be implemented through braiding operations. Consequently, quantum computing based on the Kitaev chain is expected to be intrinsically resilient to noise due to the energy gap protecting the ground state from excitations, the conservation of parity preserving the computational basis, and the topological protection of braiding operations.

However, physical systems realizing Kitaev-chain dynamics are typically coupled to thermal fermionic environments, which induce dissipation. This constitutes the central problem addressed in this work. To investigate these effects, after introducing the open-quantum-system framework in Section 5, we derived GKSL master equations describing the dissipative dynamics of first a 2-site Kitaev chain and then finite N -site chains in Sections 6 and 7, respectively. In order to characterize the topological properties of these finite-size systems, we employed the end-to-end correlation function Q (4.12) and computed its steady-state value.

For the 2-site Kitaev chain, we identified regions of nonzero steady-state correlations in the μ - μ_B phase diagram. These correlations can be understood from the corresponding steady-state population distributions, which follow the structure of the BdG spectrum of the system. Their behavior can be interpreted in terms of fermionic hopping processes between the bath and the chain, governed by the particle and hole characters of the system eigenexcitations. We showed that increasing the temperature T has a detrimental effect on these correlations, driving the system towards increasingly mixed steady states as a consequence of the thermal broadening of the Fermi-Dirac distribution. In contrast, reducing the FWHM W of the Lorentzian spectral density enhances the purity of the steady-state populations by increasing the frequency effective selectivity of the bath coupling, while also generating new population regions in the μ - μ_B phase diagram. Although a 2-site Kitaev chain hosts an MBS only at the sweet spot $\mu = 0$, these results remain relevant both because of the recent experimental realization of such system [23] and because they provide a foundation for understanding larger finite-size chains.

Indeed, extending the analysis to longer chains in Section 7, we found that the main features observed in the 2-site case persist. The steady-state correlations continue to reflect the structure of the BdG spectrum, while temperature and bath engineering retain their respective detrimental and beneficial effects, respectively. However, additional correlated regions emerge within the topological phase $|\mu| < 2t$. These correlations originate from the nonzero end-to-end correlations of the Bogoliubov vacuum in finite Kitaev chains with $N > 2$, leading to a richer structure of the steady-state phase diagrams. However, the correlations associated with the excited modes of the BdG spectrum are observed to decrease as the chain length increases. This behavior is expected, since the localization length of the corresponding excited modes becomes progressively smaller compared to the chain size, thereby reducing their contribution to end-to-end correlations.

The transient dynamics of the two-site Kitaev chain was also investigated by comparing the time-evolved MBS at $\mu = 0$ with its initial state as a function of μ_B through their corresponding fidelity. Two distinct regions were identified. A central region, $|\mu_B| < 2t$, characterized by longer decay times, in which the MBS evolves towards an equal mixture of the MBS and the Bogoliubov vacuum, and an outer region, $|\mu_B| > 2t$, where the MBS decays towards a maximally mixed state containing finite-energy excited states. Once again, this structure can be understood through a simple resonant hopping picture of the chain-bath coupling. In the central region, bath fermions

do not possess sufficient energy to populate the excited modes of the chain, which originates from the protecting gap $2t$, whereas in the outer region such processes become energetically allowed. However, in both regions the parity is broken and, consequently, so is the computational basis. In addition, the outer region allows for the excitation of non-topological states which is, of course, detrimental for a qubit.

As in the steady-state analysis, temperature has a detrimental effect on the transient dynamics. The central region progressively shrinks as the temperature increases due to the thermal broadening of the Fermi-Dirac distribution. Conversely, reducing the width of the Lorentzian spectral density increases the decay time for bath chemical potentials μ_B that are non-resonant with the eigenenergies of the system.

The transient dynamics of the $N > 2$ -site chains exhibits the same qualitative behavior. Furthermore, for larger chains, one may choose nonzero values of the chemical potential μ , provided that the localization length of the associated Majorana zero modes remains significantly smaller than the chain length. In this regime, the characteristic decay time of the MBS exhibits an asymmetry with respect to $\mu_B = 0$, with longer lifetimes obtained for bath chemical potentials having a sign opposite to that of the chain chemical potential. This effect originates from the imperfect particle-hole balance of finite-size MBSs and could be exploited to further enhance their lifetime.

As potential perspectives, one may first consider deriving an analytical generalization of the GKSL master equation (6.39) for an arbitrary number of sites. Such a result would enable us to confirm the interpretation extrapolated from the numerical simulations by providing direct access to the population distribution in the μ - μ_B phase diagram. This objective could potentially be achieved by applying the analytical framework developed in Ref. [61]. Furthermore, the system-bath interaction could be refined by including the Lamb-shift contributions in the analysis. In the present work, these terms were neglected in order to isolate and understand the effects of purely dissipative processes. However, Lamb shifts modify the unitary dynamics and may have non-negligible consequences, for instance on the protecting gap $2t$. Finally, we have assumed a Lorentzian spectral density throughout this work. Other realistic descriptions of dissipation could be obtained by considering spectral densities tailored to specific experimental environments. Such an approach would provide a more accurate modeling of open-system dynamics in realistic setups, for example in the presence of a thermal superconducting fermionic bath [52, 53]. Finally, it has recently been shown that coupling a Kitaev chain to a bosonic mode in a cavity-QED setup can affect its topological phase in a nontrivial manner. In particular, such a coupling can either destroy or induce MBSs in parameter regimes where they would, respectively, be expected to exist or not exist in the absence of the cavity field [62]. Furthermore, a local coupling between the chain and the cavity mode can be engineered, providing a possible way towards the implementation of braiding operations [63, 64]. However, these analyses have so far been performed within a closed-system framework. Extending them to an open-quantum-system description that incorporates the coupling to bosonic mode therefore constitutes an interesting perspective. Moreover, in these studies, the cavity-QED systems are assumed to be ideal, *i.e.*, lossless and perfectly isolated from their environment. In practice, however, cavities are subject to photon losses and other dissipative processes. Such imperfections can naturally be incorporated within the open-quantum-system framework through decaying bath correlation functions associated with the cavity bosonic mode [65].

A Continuous model Hamiltonian for BCS superconductivity

Let us show that the expressions (4.5-4.6) lead to the continuous model Hamiltonian (4.7). Recall that we have performed the continuum limit $\frac{1}{V} \sum_k \rightarrow \int \frac{dk}{2\pi}$ giving

$$H_0 = \sum_{\sigma} \iiint \frac{dk}{2\pi} dx dx' e^{ik(x-x')} \psi_{\sigma}^{\dagger}(x) \left(\frac{k^2}{2m} - \mu \right) \psi_{\sigma}(x'), \quad (\text{A.1})$$

$$H_1 = - \iiint \frac{dk}{2\pi} dx dx' e^{ik(x-x')} \left(\Delta \psi_{\uparrow}^{\dagger}(x) \psi_{\downarrow}^{\dagger}(x') + \Delta^* \psi_{\downarrow}(x) \psi_{\uparrow}^{\dagger}(x') \right). \quad (\text{A.2})$$

Therefore, the model Hamiltonian $H_M = H_0 + H_1$ is directly found given the Fourier identities [66]

$$\int \frac{dk}{2\pi} e^{-ik(x-x')} = \delta(x-x'), \quad (\text{A.3})$$

$$\int \frac{dk}{2\pi} k^2 e^{-ik(x-x')} = -\partial_x^2 \delta(x-x'). \quad (\text{A.4})$$

B Typical localization length of the MZMs

We have found that that

$$\gamma_A = \sum_n \phi_n \gamma_{A,n} \quad \text{and} \quad \gamma_B = \sum_n \phi_{N+1-n} \gamma_{B,n}, \quad (\text{B.1})$$

with the wavefunction

$$\phi_n = \frac{1}{Z} (z_+^n - z_-^n) \quad (\text{B.2})$$

where $|z_{\pm}| < 1$ and Z is the normalization constant. We can rewrite ϕ_n as

$$\phi_n = \frac{1}{Z} (e^{-\lambda_+ n} - e^{-\lambda_- n}), \quad (\text{B.3})$$

where we introduce $\lambda_{\pm} = -\ln(z_{\pm}) = -\ln|z_{\pm}| - i \arg(z_{\pm})$ (if $-\pi < \arg(z) < \pi$). From this, it is straightforward to see that the MZMs wavefunction decay exponentially as $|\phi_n| \propto e^{-n/\xi_M}$ with the typical localization length of the MZMs are given by

$$\xi_M = \max \left(\frac{1}{|\ln|z_+||}, \frac{1}{|\ln|z_-||} \right). \quad (\text{B.4})$$

C Fermionic Gaussian states and end-to-end correlations

We define a *fermionic Gaussian state* (FGS) as

$$\rho = \frac{e^{-H}}{Z} = \frac{e^{-\mathbf{c}^{\dagger} \mathbf{H} \mathbf{c}}}{Z}, \quad (\text{C.1})$$

where H is a fermionic quadratic Hamiltonian called the *parent Hamiltonian* of ρ , and Z is a normalization constant. Note that H is not necessarily the Hamiltonian ruling the dynamics of the system, but any quadratic Hermitian operator. The net advantage of such states is that all information about the FGS is contained in the so-called *correlation matrix* that we define later [30]. First, let us consider a single mode Gaussian state

$$\rho = \frac{e^{-H_1}}{Z}, \quad (\text{C.2})$$

where $H_1 = \epsilon(a^\dagger a - aa^\dagger)$. The basis of the single mode Fock space is $\{|0\rangle, |1\rangle = a^\dagger|0\rangle\}$, in which the states have the matrix form

$$\rho = \begin{pmatrix} 1-f & 0 \\ 0 & f \end{pmatrix}, \quad (\text{C.3})$$

with $f = \langle 1|\rho|1\rangle$ the average population of the state $|1\rangle$. Then, from the polynomial expansion of ρ , we can show that $f = \text{Tr}(\rho a^\dagger a) = \langle a^\dagger a \rangle$ [30]. Hence, a single-mode state is entirely described by the occupation of the fermionic mode $\langle a^\dagger a \rangle$. Let us generalize this result for an N -mode FGS defined as (C.2). Since H is quadratic, by finding the relevant unitary matrix, we can rewrite ρ in (C.2) as²⁴

$$\rho = \frac{e^{-\mathbf{a}^\dagger \mathbf{H}_\Delta \mathbf{a}}}{Z} = \frac{e^{-\sum_{k=1}^N \epsilon_k (a_k^\dagger a_k - a_k a_k^\dagger)}}{Z}. \quad (\text{C.5})$$

Having diagonalized the parent Hamiltonian, we can rewrite the density operator as a product of single-mode operator ρ_k each associated with its own eigenenergy ϵ_k as

$$\rho = \frac{1}{Z} \bigotimes_{k=1}^N \rho_k = \frac{1}{Z} \bigotimes_{k=1}^N e^{-\epsilon_k (a_k^\dagger a_k - a_k a_k^\dagger)} = \bigotimes_{k=1}^N \frac{e^{-\epsilon_k (a_k^\dagger a_k - a_k a_k^\dagger)}}{Z_k}, \quad (\text{C.6})$$

with $Z_k = \text{Tr}(e^{-\epsilon_k (a_k^\dagger a_k - a_k a_k^\dagger)})$. Therefore, we get that an N -mode FGS is entirely described by the set of the N single-mode occupations $\{\langle a_k^\dagger a_k \rangle\}$. All these occupation numbers are collected in the $2N \times 2N$ diagonal matrix

$$\mathbf{D} = \langle \mathbf{a} \mathbf{a}^\dagger \rangle, \quad (\text{C.7})$$

which is the *correlation matrix* in the eigenbasis of the parent Hamiltonian. To obtain the correlation matrix in terms of the original fermionic operators, correlation matrix that we note $\mathbf{C}$, we simply perform the inverse transformation (2.17) on $\mathbf{D}$

$$\mathbf{C} = \mathbf{U}^\dagger \mathbf{D} \mathbf{U}, \quad (\text{C.8})$$

$$= \mathbf{U}^\dagger \langle \mathbf{a} \mathbf{a}^\dagger \rangle \mathbf{U}, \quad (\text{C.9})$$

$$= \langle \mathbf{U}^\dagger \mathbf{a} \mathbf{a}^\dagger \mathbf{U} \rangle, \quad (\text{C.10})$$

$$= \langle \mathbf{c} \mathbf{c}^\dagger \rangle. \quad (\text{C.11})$$

This matrix is no longer diagonal and contains all two-point correlators $\langle c_i c_j^\dagger \rangle$ and $\langle c_i^\dagger c_j \rangle$. Finally, using Wick's theorem [30], all the information about the FGS is contained in this $2N \times 2N$ correlation matrix $\mathbf{C}$ which will prove useful in simulations since it scales as N^2 , compared to the density operator which dimension scales as 2^{2N} .

Furthermore, we can show that the ground state of a quadratic Hamiltonian is itself a Gaussian state [67], the ground state being the state of lowest energy, in the diagonal basis, its covariance matrix reads

$$\mathbf{D}_0 = \begin{pmatrix} \mathbb{1}_{N \times N} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}. \quad (\text{C.12})$$

²⁴If $A \in \mathcal{B}_2(\mathcal{H}_N)$, the Hilbert-Schmidt space of operators acting on the N -particle Hilbert space $\mathcal{H}_N$, can be written as $A = \sum_k \mathbb{1} \otimes \cdots \otimes A_k \otimes \cdots \otimes \mathbb{1}$ with $A_k \in \mathcal{B}_2(\mathcal{H}_1)$. Then [56],

$$e^A = \bigotimes_k e^{A_k}. \quad (\text{C.4})$$

Hence, we simply find the ground-state covariance matrix in the original basis as

$$\mathbf{C}_0 = \mathbf{U}^\dagger \mathbf{D}_0 \mathbf{U}. \quad (\text{C.13})$$

Therefore, the Kitaev Hamiltonian 4.1 being quadratic, the end-to-end correlations in Figure 4.12 are simply obtained by selecting the correlations $\langle c_1^\dagger c_N \rangle$ and $\langle c_N^\dagger c_1 \rangle$ in its associated ground-state covariant matrix (C.13).

D Braiding operator

Let us show that

$$U_{nm} = \frac{1}{\sqrt{2}}(1 + \gamma_n \gamma_m) = \exp\left(\frac{\pi}{4} \gamma_n \gamma_m\right). \quad (\text{D.1})$$

For this purpose, using the Taylor expansion of the exponential and the identity $(\gamma_n \gamma_m)^2 = -1$ [31], we start by computing:

$$\exp(\alpha \gamma_n \gamma_m) = \sum_{k=0}^{\infty} \frac{\alpha^k}{k!} (\gamma_n \gamma_m)^k \quad (\text{D.2})$$

$$= \sum_{k=0}^{\infty} (-1)^k \frac{\alpha^{2k}}{2k!} + \sum_{k=0}^{\infty} (-1)^k \frac{\alpha^{2k+1}}{(2k+1)!} \gamma_n \gamma_m \quad (\text{D.3})$$

$$= \cos(\alpha) + \sin(\alpha) \gamma_n \gamma_m, \quad (\text{D.4})$$

where we recognize the Taylor expansion of the cosine and sine functions in (D.3). Finally, by setting $\alpha = \frac{\pi}{4}$, we find the wanted relation:

$$\exp\left(\frac{\pi}{4} \gamma_n \gamma_m\right) = \frac{1}{\sqrt{2}}(1 + \gamma_n \gamma_m). \quad (\text{D.5})$$

E 2-site Kitav chain

E.1 Eigenbasis

First, let us find the normalized Bogoliubov vacuum $|+\rangle_0$ from the basis $\{|00\rangle, |10\rangle, |01\rangle, |11\rangle\}$ associated to the original fermionic operators c_1 and c_2 . Therefore, the Bogoliubov vacuum, defined as the state annihilated by both operators d_1 and d_2 , can be found by finding α , β , γ and δ such that

$$d_1 (\alpha |00\rangle + \beta |10\rangle + \gamma |01\rangle + \delta |11\rangle) = 0, \quad (\text{E.1})$$

$$d_2 (\alpha |00\rangle + \beta |10\rangle + \gamma |01\rangle + \delta |11\rangle) = 0. \quad (\text{E.2})$$

Given the decompositions (6.9-6.10), we find that

$$\beta = \gamma, \quad (\text{E.3})$$

$$\beta = -\gamma, \quad (\text{E.4})$$

$$B\alpha = A\delta. \quad (\text{E.5})$$

The first two equations enforce $\beta = \gamma = 0$ leaving us with a single equation to find the two unknowns α and δ . However, we impose the normalization of the Bogoliubov vacuum as $|\alpha|^2 + |\delta|^2 = 1$ which gives, together with (E.5),

$$\alpha = \frac{A}{\sqrt{2}} \quad \text{and} \quad \delta = \frac{B}{\sqrt{2}}, \quad (\text{E.6})$$

up to a complex phase. Therefore, the Bogoliubov vacuum is given in terms of the original basis as

$$|+\rangle_0 = \frac{1}{\sqrt{2}} (A|00\rangle + B|11\rangle). \quad (\text{E.7})$$

The rest of the eigenbasis is generated by the creation operators $d_1^\dagger$ and $d_2^\dagger$ from the Bogoliubov vacuum. Indeed, we directly obtain

$$|-\rangle_0 \equiv d_2^\dagger |+\rangle_0 = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle), \quad (\text{E.8})$$

$$|-\rangle_1 \equiv d_1^\dagger |+\rangle_0 = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle), \quad (\text{E.9})$$

$$|+\rangle_1 \equiv d_1^\dagger d_2^\dagger |+\rangle_0 = \frac{1}{\sqrt{2}} (B|00\rangle - A|11\rangle). \quad (\text{E.10})$$

E.2 L -operators

Given the general form of the L -operators:

$$L_l = \int_0^\infty ds \alpha(s) e^{-iH_S s} c_l^\dagger e^{iH_S s} \quad \text{and} \quad \bar{L}_l = \int_0^\infty ds \bar{\alpha}(s) e^{-iH_S s} c_l e^{iH_S s}, \quad (\text{E.11})$$

with the BCFs

$$\alpha(s) = \int_{-\infty}^{+\infty} d\omega e^{i(\omega + \mu_B)s} J(\omega) n(\omega) \quad \text{and} \quad \bar{\alpha}(s) = \int_{-\infty}^{+\infty} d\omega e^{i(\omega + \mu_B)s} J(\omega) n(\omega), \quad (\text{E.12})$$

let us compute the form of the L -operators in terms of the eigenmode d_1 and d_2 . Following the *Baker-Campbell-Hausdorff formula*, we can show that for two operators S and A [56], we have

$$e^S A e^{-S} = \sum_n \frac{A^{(n)}}{n!}, \quad (\text{E.13})$$

with

$$A^{(n)} = [S, A^{(n-1)}] \quad \text{and} \quad A^{(0)} = A. \quad (\text{E.14})$$

Therefore, we obtain the following identities:

$$e^{-iH_S s} d_1^\dagger e^{iH_S s} = e^{-i\epsilon_1 s} d_1^\dagger, \quad (\text{E.15})$$

$$e^{-iH_S s} d_2^\dagger e^{iH_S s} = e^{-i\epsilon_2 s} d_2^\dagger, \quad (\text{E.16})$$

$$e^{-iH_S s} d_1 e^{iH_S s} = e^{i\epsilon_1 s} d_1, \quad (\text{E.17})$$

$$e^{-iH_S s} d_2 e^{iH_S s} = e^{i\epsilon_2 s} d_2, \quad (\text{E.18})$$

with the BdG eigenenergies ϵ_1 and ϵ_2 . Now, let us show how to compute the operators L_1 using these previous identities and the decomposition

$$c_1^\dagger = \frac{1}{2} [A(d_2^\dagger - d_1^\dagger) + B(d_1 + d_2)], \quad (\text{E.19})$$

found from (6.9). Hence, this L_1 -operator reads

$$L_1 = \int_0^\infty \alpha(s) e^{-iH_S s} c_1^\dagger e^{iH_S s} = \frac{1}{2} \int_0^\infty \alpha(s) e^{-iH_S s} [A(d_2^\dagger - d_1^\dagger) + B(d_1 + d_2)] e^{iH_S s}. \quad (\text{E.20})$$

Each term in the last integral is computed using the identities (E.15-E.18) as follows:

$$\int_0^\infty ds \alpha(s) e^{-iH_S s} d_1 e^{iH_S s} = \int_0^\infty ds \left(\int_{-\infty}^{+\infty} d\omega e^{i(\omega+\mu_B)s} J(\omega) n(\omega) \right) e^{i\epsilon_1 s} d_1, \quad (\text{E.21})$$

$$= \int_{-\infty}^{+\infty} d\omega J(\omega) n(\omega) \left(\int_0^\infty ds e^{i(\omega+\mu_B+\epsilon_1)s} \right) d_1. \quad (\text{E.22})$$

The integral over the time s gives [66]

$$\int_0^\infty ds e^{i(\omega+\mu_B+\epsilon_1)s} = \pi \delta(\omega + \mu_B + \epsilon_1) + iP \left(\frac{1}{\omega + \mu_B + \epsilon_1} \right), \quad (\text{E.23})$$

where P denotes the Cauchy principal values. In the following, we decide to ignore these latter because they will only introduce *Lamb-shifts* in the chain dynamics [22]. Therefore, the integral E.22 becomes

$$\int_0^\infty ds \alpha(s) e^{-iH_S s} d_1 e^{iH_S s} = \pi d_1 \int_{-\infty}^{+\infty} d\omega J(\omega) n(\omega) \delta(\omega + \mu_B + \epsilon_1), \quad (\text{E.24})$$

$$= \pi J(-\epsilon_1 - \mu_B) n(-\epsilon_1 - \mu_B) d_1. \quad (\text{E.25})$$

By proceeding similarly for the last terms of the integral and by defining the ζ -functions

$$\zeta(\omega) = J(\omega - \mu_B) n(\omega - \mu_B) \quad \text{and} \quad \bar{\zeta}(\omega) = J(\omega - \mu_B) (1 - n(\omega - \mu_B)), \quad (\text{E.26})$$

we obtain the final form

$$L_1 = \frac{\pi}{2} \left[B (\zeta(-\epsilon_1) d_1 + \zeta(-\epsilon_2) d_2) + A \left(\zeta(\epsilon_2) d_2^\dagger - \zeta(\epsilon_1) d_1^\dagger \right) \right]. \quad (\text{E.27})$$

The other L -operators are found following the exact same procedure.

E.3 Additional figures

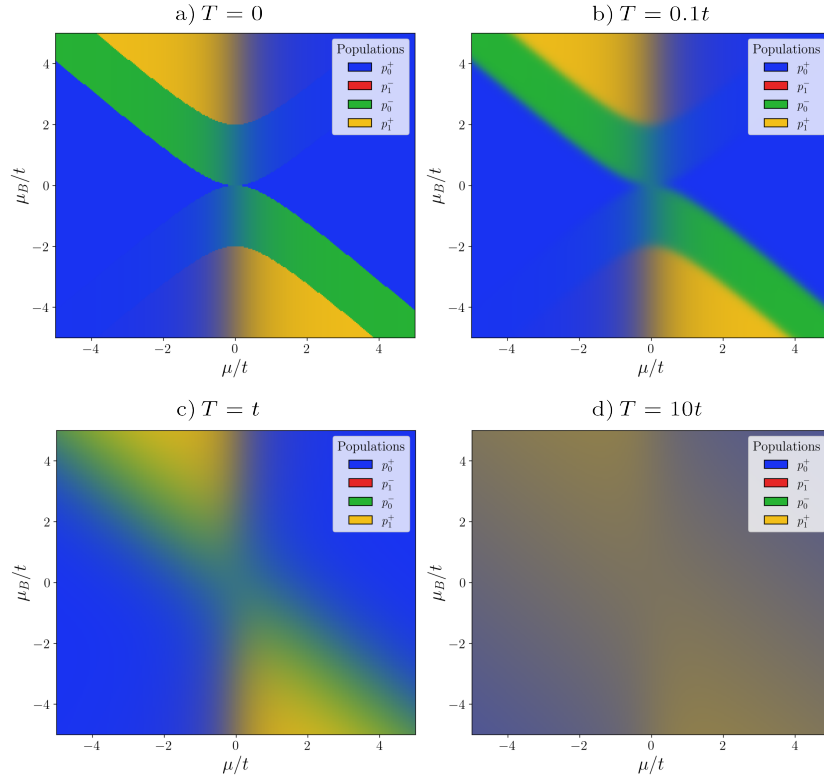


Figure E.1: Temperature dependence of the real steady-state population distribution (without arbitrary threshold) in the μ - μ_B phase diagram for a structureless bath, i.e., $J(\omega) = \Gamma$.

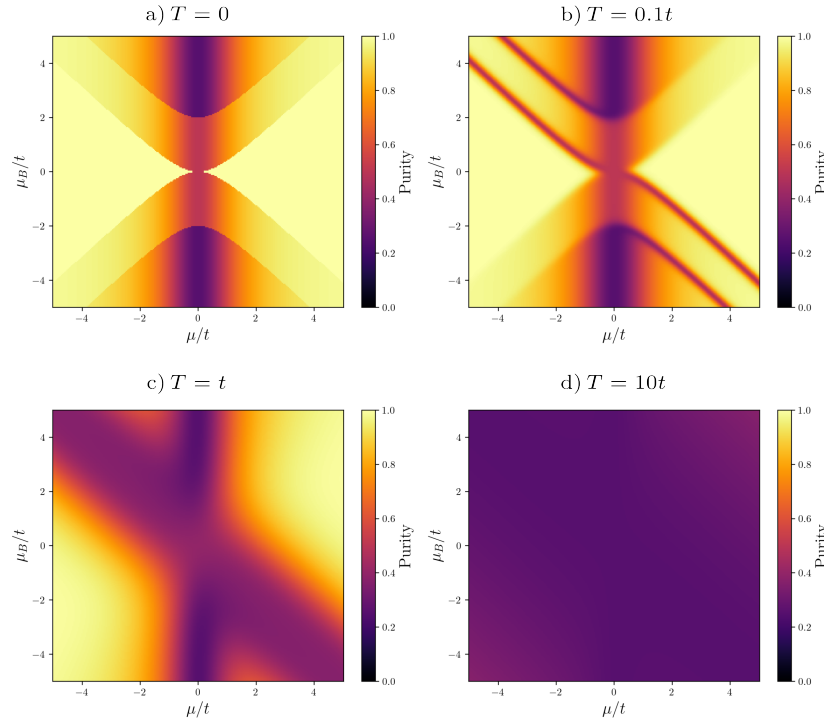


Figure E.2: Temperature dependence of the steady-state purity displayed in the μ - μ_B phase diagram for a structureless bath, i.e., $J(\omega) = \Gamma$.

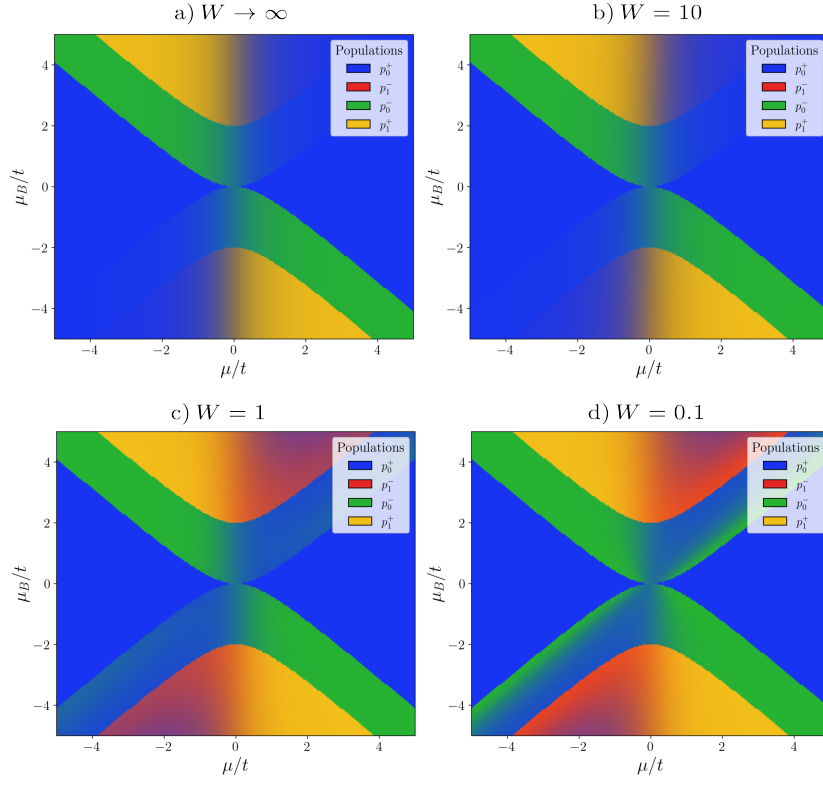


Figure E.3: *FWHM dependence of the real steady-state population distribution (without arbitrary threshold) in the μ - μ_B at temperature $T = 0$.*

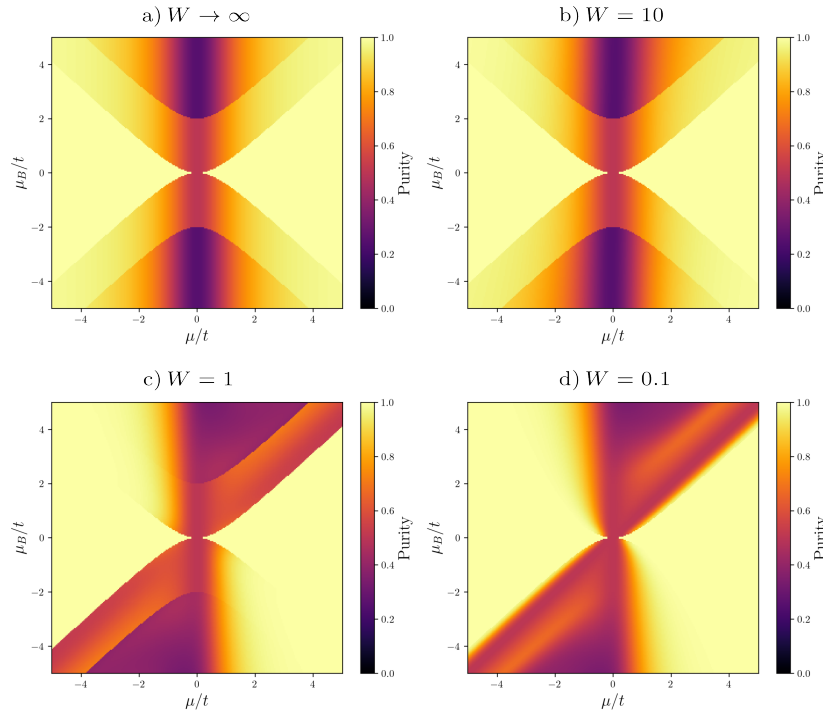


Figure E.4: *FWHM dependence of the steady-state purity displayed in the μ - μ_B phase diagram at temperature $T = 0$.*

F Additional figure – N -site chains

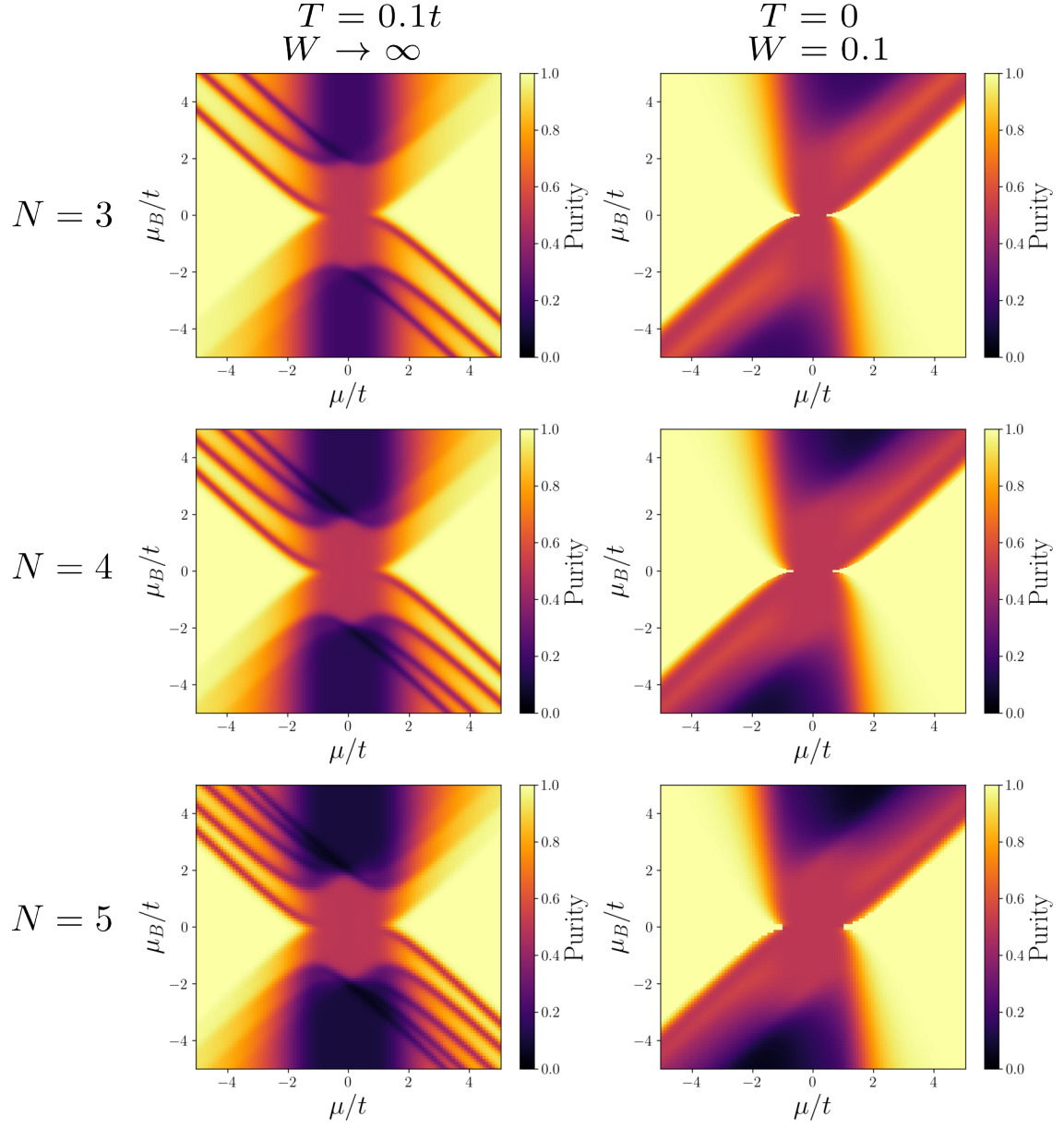


Figure F.1: Corresponding purities of Figure 7.2.

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