Methods and Characterization of Topological and Disordered-induced Protection of Coherence in Quantum Systems

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METHODS AND CHARACTERIZATION OF TOPOLOGICAL AND DISORDERED-INDUCED PROTECTION OF COHERENCE IN QUANTUM SYSTEMS

by

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A dissertation submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy in the Department of Physics in the College of Science at the University of Central Florida Orlando, Florida

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Quantum computers can efficiently simulate natural processes and solve certain types of mathematical problems. Two of the key issues preventing the development of platforms to realize a scalable quantum machine are the decoherence of the qubits due to the interaction with the environment and the existence of a large overhead to correct errors. Although there already exist noisy intermediate-scale quantum machines, we still need to improve much to be able to solve problems faster than the already existing classical computers. In this dissertation, we explore two approaches to tackle both issues. We propose a scheme where, using quasi-Majorana zero modes located at the edges of nanowires, we construct a logical Majorana zero mode on a network of nanowires. We show that just by modulating the voltage on the nanowires, it is possible to manipulate the position of the logical Majorana zero mode. This could be a significant step towards performing a braiding operation in two dimensions, which is a necessary part of making a fault-tolerant topological quantum computer. In addition to this, we study how disorder in an interacting quantum many-body system can help protect coherence on a given basis. We also employ an experimentally-accessible measurement-based protocol to study local coherence in such systems.
I dedicate this dissertation to my parents, whose incredible sacrifice has enabled my journey.
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P.W. Anderson, in his article "More Is Different"[1] described the hierarchical nature of the laws of physics. He explained how symmetry plays an important role in the emergence of the collective behavior of many particles. According to Landau’s theory [2], any phase transition happens with a spontaneously broken local symmetry. However, later systems were discovered where phase transitions would occur without symmetry breaking. In the absence of interactions, when such systems are gapped, the resulting phases can be characterized by a topological integer number such as the Chern number [3] in the case of integer quantum Hall state [4]. If the system is strongly interacting, then such collective exotic behavior of the interacting electrons creates topological order and the phases are denoted as topologically ordered phases. The fractional quantum Hall effect is such an example [5, 6]. In the last few decades, a lot about both the non-interacting and strongly interacting topological quantum phases has been studied, and as a result, a whole new world of quantum phases has been discovered. Among them, the topological superconductors and the emergent Majorana zero modes [7] in them have been considered to be able to encode quantum information in their decoherence-free subspace of the ground state manifold. Although topology can protect the non-local states from decoherence, they do not survive finite temperatures due to thermal fluctuation [8].

Another form of exotic quantum phases occurs in disordered interacting systems of electrons, where localization prevents the system to go to thermal equilibrium. Such a state, which is protected by the phenomenon of many-body localization (MBL) [9, 10], retains the memory of the initial state. Therefore, for the topological systems in finite temperatures, many-body localization can help protect the edge modes by localization of the bulk degrees of freedom [11]. Here, in this dissertation, we study the possible realization of an emergent topological zero mode inside the vortex core of a Kekulé modulated nanowire network, where each nanowire is Majorana zero
mode carrying. We show the specific need for a 5-wire junction to maintain the time-reversal symmetry in the network. The advantage of this hierarchical construction, as mentioned first by Yang et al. [12] is that the emergent logical Majorana zero modes are movable among the lattice sites. Next, we study the effect of many-body localization on the quantum coherence of an individual eigenstate with finite energy density in the computational basis. We also show that it is possible to distinguish the eigenstates in thermalized [13] and many-body localized [9, 10] phases by calculating quantum coherence in a particular basis.

Organization of the dissertation

This dissertation is organized as the following. In chapter 2, we review the effect of the Berry phase in Bloch Hamiltonians and discuss how symmetry and topology characterize these bulk-gapped systems. We then proceed by how Majorana zero modes appear in a toy model of a one-dimensional p-wave superconductor as introduced by Kitaev [14]. We also discuss the realistic nanowire model [15, 16] for the realization of such zero modes in experiments. Next, in chapter 3 we have described a protocol to construct a Majorana nanowire network in two dimensions. Such a network can accept a Majorana zero mode inside the vortex core while in the presence of the Kekule modulation of chemical potential. We have numerically shown that these vortices can be moved around the network just by manipulating the voltages, which can be an essential step for the realization of braiding protocol in 2D. In chapter 4 we have described the process of equilibration, thermalization, and MBL in isolated quantum many-body systems. Next in chapter 5, we have shown how coherence on the computational basis can be used as a tool to detect phase transition between ergodic and MBL phases. We then used quantum quench studies to show that the MBL protects the quantum coherence of an initial state on the computational basis. We have also used matrix product state (MPS)-based methods [17, 18] to calculate numerically the coherence-based
correlation in both an ergodic and a many-body localized phase.
In 1982, Richard Feynman [19] first proposed the idea of a computer that runs according to the rules of quantum mechanics. His idea was to simulate quantum mechanical processes with the help of quantum machines which perhaps could be more advantageous than classical computers. In the past two decades, there has been a lot of progress in the field of quantum computation and information. In the year 2000 David Divincenzo proposed the required criteria [20] for building a quantum computer which includes the following:

1. Availability of well-characterized and scalable qubits.

2. The ability to initialize all the qubits to a particular state repeatedly within an acceptable error margin.

3. Long coherence time to perform enough quantum operations.

4. The ability to perform arbitrary operations and therefore needing the universal set of gates.

5. The ability to accurately measure the qubits after the operation.

Since then, many different physical platforms have been proposed as effective routes toward building a quantum computer, which includes photonic devices [21], ion traps [22], neutral atoms [23] such as the Rydberg atom [24], superconducting qubits [25, 26], and topological platforms [27]. There has been a plethora of experimental and theoretical progress in each of these platforms. As a result, what we have today is a NISQ (Noisy Intermediate Scale Quantum) device [28] in each of the platforms except the topological platform.
The reason why topological platforms are interesting is that they are the only ones where the inherent quantum mechanical property of the exotic quasiparticles (Majorana fermions [7] or other Non-abelian anyons [27, 29]) help to store information non-locally and therefore makes them inherently resistant to local perturbations. One can construct such systems with gapped Hamiltonians whose ground state is formed by the degenerate and decoherence-free subspace of these exotic quasiparticles. These can then be moved around each other adiabatically to perform a braiding operation which is essential to construct quantum gates. In all the other platforms there is a need for quantum error correction and, therefore, to construct logical qubits, one might need hundreds or thousands of physical qubits, which results in a huge overhead in scalability. In topological platforms, the error correction is already being dealt with from the hardware level and thus it provides a way to realize fault-tolerant quantum computation.

Topology in quantum mechanics

In general, Topology is a branch of mathematics that classifies objects according to their geometry and shapes. One can also classify the quantum mechanical wavefunctions according to the way they change to different wavefunctions if the system Hamiltonian is adiabatically evolved in parameter space.

_Berry Phase and Berry curvature_

According to Bloch’s theorem [30], the eigenstates of a single electron system \( H = \frac{p^2}{2m} + V(\vec{r}) \) with a periodic potential \( V(\vec{r} + \vec{R}_n) = V(\vec{r}) \) can be written as

\[
\left| \Psi_{\alpha, \vec{k}}(\vec{r}) \right\rangle = e^{i\vec{k} \cdot \vec{r}} \left| u_{\alpha, \vec{k}}(\vec{r}) \right\rangle ,
\]

\[ (2.1) \]
where \( |u_{\alpha,\vec{k}}(\vec{r} + \vec{R}_n)\rangle = |u_{\alpha,\vec{k}}(\vec{r})\rangle \) is a periodic function with the same periodicity as the potential, \( \alpha \) is the band index and \( \vec{k} \) is the crystal momentum restricted within the first Brillouin Zone. Here \( \vec{R}_n \) denotes an arbitrary translation vector of the lattice, which can be expressed as the following:

\[
\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \tag{2.2}
\]

where \( \vec{a}_1, \vec{a}_2, \vec{a}_3 \) are the lattice unit vectors. As a result, the eigenstates of the single particle Hamiltonian \( H \) satisfy the property

\[
|\Psi_{\alpha,\vec{k}}(\vec{r} + \vec{R}_n)\rangle = e^{i\vec{k} \cdot \vec{R}_n} |\Psi_{\alpha,\vec{k}}(\vec{r})\rangle. \tag{2.3}
\]

Now, if the energy eigenvalues of the Hamiltonian \( H \) is given by \( E_{\alpha,\vec{k}} \), then

\[
H |\Psi_{\alpha,\vec{k}}(\vec{r})\rangle = E_{\alpha,\vec{k}} |\Psi_{\alpha,\vec{k}}(\vec{r})\rangle \Rightarrow e^{-i\vec{k} \cdot \vec{r}} H e^{i\vec{k} \cdot \vec{r}} |u_{\alpha,\vec{k}}(\vec{r})\rangle = E_{\alpha,\vec{k}} |u_{\alpha,\vec{k}}(\vec{r})\rangle. \tag{2.5}
\]

Now, the Bloch Hamiltonian then can be constructed by writing [31]

\[
\mathcal{H}(k) = e^{-i\vec{k} \cdot \vec{r}} H e^{i\vec{k} \cdot \vec{r}}, \tag{2.6}
\]

whose eigenstates are just the periodic part of the Bloch function. Since the momentum vectors belong to the first Brillouin zone, it acts as the parameter space of the Bloch Hamiltonian \( \mathcal{H}(k) \) and the parameterized eigenstates \( |u(\alpha, \vec{k})\rangle \) pick up a Berry phase [32–34] as a result of adiabatic evolution in this parameter space. The construction of the Berry phase for a closed path \( C \) is given by the following equation:

\[
\gamma_C = \oint_C \mathcal{A}_\alpha(\vec{k}) \cdot d\vec{k}, \tag{2.7}
\]
where $A_{\alpha}(\vec{k})$ is the Berry connection in the $\alpha$th band, which is defined by

$$A_{\alpha}(\vec{k}) = \left\langle u(\alpha, \vec{k}) \right| -i \nabla_{\vec{k}} \left| u(\alpha, \vec{k}) \right\rangle.$$  \hspace{1cm} (2.8)

The Berry phase in the parameter space which is the momentum space for the Bloch Hamiltonians of the solids characterizes the non-trivial topology of the Bloch bands. Since there is an ambiguity in the phase choice of the Bloch eigenstates, a gauge-invariant quantity can be constructed from the Berry connection which is denoted as the Berry curvature:

$$\Omega^\alpha(\vec{k}) = \nabla_{\vec{k}} \times A_{\alpha}(\vec{k}).$$ \hspace{1cm} (2.9)

The Berry phase can be written using the Stokes theorem in the following manner:

$$\gamma_C = \int_S d\vec{S} \cdot \Omega^\alpha(\vec{k}).$$ \hspace{1cm} (2.10)

Although, generally the Berry phase can be of any real value and therefore does not always work as a topological invariant, in the presence of certain symmetries it can be quantized, and then it can give rise to a topological invariant. Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) \[3\] first introduced such a topological number which later was expressed as the Chern number of the integer quantum Hall states. In general, for two-dimensional (2D) systems the Chern number of the $\alpha$th band can be written with the help of the previously-defined Berry Curvature in the following way:

$$C_\alpha = \frac{1}{2\pi} \int_{2DBZ} dk_x dk_y \Omega^\alpha_{xy}(\vec{k}),$$ \hspace{1cm} (2.11)

where the integration is performed over the 2D Brillouin zone. For the 2D insulators, it can be shown that the Hall conductance of the system is related to the total Chern number of the filled-up
bands by

$$\sigma_{xy} = \frac{e^2}{h} \sum_{E_\alpha < E_F} C_\alpha,$$

(2.12)

where $E_\alpha$ is the energy of the $\alpha$th band and $E_F$ is the Fermi energy. The symmetry of the Bloch Hamiltonian also takes a crucial role in determining the topology of the states which are filled up. Without any symmetry of the Hamiltonian, there exists only one possible topological phase up to three dimensions (3D) which is the integer quantum Hall state. Therefore in the next part, we try to understand the effect of symmetry and topology in the simplest one-dimensional (1D) model.

**SSH model**

The Su-Schrieffer-Heeger (SSH) model [35] is a simple one-dimensional model which was first proposed to describe how electrons behave in a polyacetylene chain. The SSH chain consists of $N$ unit cells with each cell having two sublattices $A$ and $B$ as shown in the following figure. The model describes an electron hopping with staggered hopping amplitude from one sublattice to another. The single particle Hamiltonian for the SSH model is given by

$$H = \sum_{i=1}^{N} \left[ (t + \delta t)c_{Ai}^\dagger c_{Bi} + h.c. \right] + \sum_{i=1}^{N-1} \left[ (t - \delta t)c_{Ai+1}^\dagger c_{Bi} + h.c. \right].$$

(2.13)
We can use Fourier transform to write the above Hamiltonian in momentum space due to the translational invariance of the bulk, which results in the following:

\[
H(k) = \sum_{k \in BZ} \sum_{\alpha, \beta = A, B} c_{\alpha k}^\dagger h_{\alpha \beta}(k) c_{\beta k}.
\]  

(2.14)

The $2 \times 2$ Bloch Hamiltonian reads

\[
H(k) = \begin{pmatrix}
0 & (t + \delta t) + (t - \delta t)e^{-ik} \\
(t + \delta t) + (t - \delta t)e^{ik} & 0
\end{pmatrix}.
\]  

(2.15)

We define $v = t + \delta t$, $w = t - \delta t$ and $H(k) = \vec{d}(k) \cdot \vec{\sigma}$, where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and

\[
d_x(k) = v + w \cos(k)
\]

(2.16)

\[
d_y(k) = w \sin(k)
\]

(2.17)

\[
d_z(k) = 0.
\]

(2.18)

The spectrum of the above Hamiltonian $H(k)$ is described by two bands which are given as

\[
E_{\pm}(k) = \pm |\vec{d}(k)| = \pm \sqrt{v^2 + w^2 + 2vw \cos(k)}.
\]

(2.19)

The two corresponding eigenstates are

\[
|\psi_{\pm k}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{i\phi(k)} \end{pmatrix},
\]

(2.20)

where $\tan \phi(k) = (w \sin k)/(v + w \cos k)$.

Now for the bulk system to remain gapped, we need to have $|\vec{d}(k)| \neq 0$ which implies that the
Figure 2.2: Dispersion of SSH model according to Eq. (2.19) for different values of $v$ and $w$. The wavenumber belongs to the first Brillouin zone.

trajectory of the endpoints of the vector $\mathbf{d}(k)$, in the $d_x, d_y$ plane has to exclude the origin. One important point to be noticed here is the absence of the diagonal term in the Hamiltonian, which is a result of the existing symmetries in the SSH model, which we list below.

- Chiral symmetry is represented in the following way:

$$SH(k)S^{-1} = -H(k),$$

(2.21)

with $S = \sigma_z$. 

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• Time reversal symmetry $\mathcal{T}$ is just complex conjugation since the SSH model only has spinless fermions:

$$\mathcal{T}H(k)\mathcal{T}^{-1} = H(-k).$$  \hspace{1cm} (2.22)

• Inversion symmetry is imposed by the following condition:

$$\mathcal{I}H(k)\mathcal{I}^{-1} = H(-k),$$  \hspace{1cm} (2.23)

with $\mathcal{I} = \sigma_x$.

From the energy spectrum in Eq. 2.19, it is to be noticed that the gap in the spectrum is closed and the bulk can transport electrons only when there are no staggered hopping amplitudes, i.e., $(v = w)$ and at $k = \pm \pi i$. So, to go from the gapped insulating phase at parameter limit $v > w$ to the other gapped insulating phase at $v < w$, the system has to close the gap at $v = w$ which indicates a gapless metallic state. We can now calculate the Berry connection for the eigenstate $|\psi_{-k}\rangle$ using Eq. (2.8),

$$\mathcal{A}_{-k} = \langle \psi_{-k}|i \nabla_k|\psi_{-k}\rangle = \frac{1}{2} \frac{d\phi(k)}{dk}.$$  \hspace{1cm} (2.24)

We consider the circular path in the 1D Brillouin zone and integrate over it to get the winding number for the different parameter values

$$\frac{1}{\pi} \int \mathcal{A}_{-k} dk = \begin{cases} 1 & \text{if } v < w \\ 0 & \text{if } v > w \\ \text{undefined} & \text{if } v = w. \end{cases}$$  \hspace{1cm} (2.25)

Therefore, the winding number can act as the bulk topological invariant for the SSH chain which characterizes two different kinds of gapped insulators. Now for the open SSH chain in 1D, it can
be understood that in the limit \( w = 0 \) and \( v \neq 0 \) the chain is broken down into dimers with each dimer having the A site and the B site. In the other extreme limit \( v = 0 \) and \( w \neq 0 \), however, there are two zero energy states localized at the edges of the chain. The localized zero energy edge modes exist, as long as \( v < w \) and then delocalize once \( v > w \). So although these two limits both are gapped insulators in the bulk, only one of them does have edge states with a finite winding number. This is called "bulk-boundary correspondence". Thus the 1D SSH model captures all the essential features of a topological insulator.

**Topological Superconductor and Majorana Fermion**

The Bardeen, Cooper, and Schrieffer (BCS) mean-field theory of superconductivity [36, 37] allows one to write down an interacting problem to a single particle non-interacting problem. The BCS mean-field Hamiltonian can be written in the Bogoulibov-de Gennes(BdG) form in the following way:

\[
H = \frac{1}{2} \sum_k \begin{pmatrix} \epsilon_k & \Delta_k \\ \Delta_k^\dagger & -\epsilon_k \end{pmatrix} \mathcal{H}_{\text{BdG}} \begin{pmatrix} c_k \\ c_k^\dagger \end{pmatrix},
\]

where \( \mathcal{H}_{\text{BdG}} = \begin{pmatrix} \epsilon_k & \Delta_k \\ \Delta_k^\dagger & -\epsilon_k \end{pmatrix} \) with \( \Delta_k = -\Delta(-k) \). This particular form of the BdG Hamiltonian has a symmetry which is called particle-hole symmetry. The anti-unitary operator \( \mathcal{P} \), which is defined as,

\[
\mathcal{P} = \sigma_x \mathcal{K},
\]

with \( \mathcal{K} \) as the complex conjugation operator, transforms the Hamiltonian as

\[
\mathcal{P} H(k) \mathcal{P}^{-1} = -H(-k).
\]
Since this single particle Bloch-BdG Hamiltonian has particle-hole symmetry, adding a particle to the upper band at energy $E$ is the same as removing a particle from the symmetric lower band at energy $-E$. Now a specific situation arises when the BdG Hamiltonian has a single mode with exactly zero energy. In this case, the creation and annihilation operators for the state are related by

$$\Gamma_{E=0}^\dagger = \Gamma_{E=0} = \gamma.$$  \hspace{1cm} (2.29)

By doing continuous deformation of the Bloch-BdG Hamiltonian it is impossible to remove a zero mode to non-zero energy since it requires opening up a gap in the spectrum. So, if a zero mode exists in a superconductor with a particle-hole symmetry, it is topologically protected. Each of these single zero modes is called a Majorana zero mode $\gamma$ with the following property:

$$\gamma^\dagger = \gamma.$$  \hspace{1cm} (2.30)

The Majorana zero modes are exactly half of a fermion and two of them are needed to define a single two-level system. If a fermionic operator is given by $f$ then the corresponding two Majorana operators are

$$\gamma_1 = f + f^\dagger$$  \hspace{1cm} (2.31)

and

$$\gamma_2 = -i(f - f^\dagger),$$  \hspace{1cm} (2.32)

with the following properties:

$$\gamma_i^2 = 1$$  \hspace{1cm} (2.33)

and

$$\{\gamma_i, \gamma_j\} = 2\delta_{ij}.$$  \hspace{1cm} (2.34)
Although the fermion operator \( f = (\gamma_1 + i\gamma_2)/2 \) looks like a conventional fermion, it is non-trivial because of the ability of the two Majorana zero modes \( \gamma_1 \) and \( \gamma_2 \) to localize far apart from one another. The occupation number of the state constructed by this fermion \( f^\dagger f = 0, 1 \) as usual. However, this state requires zero energy to fill up or empty and thereby resulting in ground state degeneracy. As a result of the non-locality and the existence of the degenerate ground state, one can think about storing quantum information non-locally to a given ground state. Now, adiabatic transformations can be also carried out to the system in such a way that the Majorana zero modes (MZM) exchange positions but the system remains in the ground state manifold. This is possible because of the presence of the non-abelian statistics for Majorana zero modes. This idea as first explored by Kitaev, in his work, formulates the stepping ground for making a fault-tolerant topological quantum computer.

Kitaev chain in 1D

Kitaev introduced this idea of the existence of Majorana zero modes in a 1D toy model of spinless fermions in a p-wave superconductor [7]. This is the simplest model in 1D where two Majorana zero modes appear at two edges of the 1D wire. The Kitaev Hamiltonian is described by the following Hamiltonian:

\[
H_{\text{Kitaev}} = \sum_{l=1}^{L-1} \left[ -t(a^\dagger_{l+1}a_{l+1} + a^\dagger_{l}a_{l}) + |\Delta|(e^{i\phi}a_{l}a_{l+1} + e^{-i\phi}a^\dagger_{l+1}a^\dagger_{l}) \right] - \mu \sum_{l=1}^{L} \left( a^\dagger_{l}a_{l} - \frac{1}{2} \right),
\]

(2.35)

where \( a^\dagger, a \) are spinless fermion creation and annihilation operators, \( |\Delta| \) and \( \phi \) are the chain’s superconductor order parameter amplitude and phase, respectively, \( t \) is the hopping amplitude between the nearest-neighbor sites, and \( \mu \) is the chemical potential. We define each fermion operator.
Figure 2.3: (a): Pictorial representation of the trivial case where $t = |\Delta| = 0$. (b) The topological phase in the limit $|\Delta| = t > 0$ and $\mu = 0$. The two modes at the ends of the wire $\gamma_{A,1}$ and $\gamma_{B,N}$ are the Majorana zero modes.

$a_l$ in terms two Majorana operators $\gamma_{A,l}$ and $\gamma_{B,l}$ as

$$a_l = \frac{1}{2} e^{-\phi/2} (\gamma_{A,l} + i \gamma_{B,l}).$$

(2.36)

Using this transformation we can rewrite the Kitaev Hamiltonian as

$$H_{\text{Kitaev}} = \frac{i}{2} \sum_l ( - \mu \gamma_{A,l} \gamma_{B,l} + (|\Delta| + t) \gamma_{B,l} \gamma_{A,l+1} + (|\Delta| - t) \gamma_{A,l} \gamma_{B,l+1} ).$$

(2.37)

There are two special cases to consider:

a) The trivial case: $t = |\Delta| = 0$. So,

$$H_{\text{Kitaev}} = - \mu \sum_l (a_l^\dagger a_l - \frac{1}{2})$$

$$= \frac{i}{2} (-\mu) \sum_l \gamma_{A,l} \gamma_{B,l}.$$
In this case, the ground state is formed by the Majorana operators $\gamma_{A,l}$ and $\gamma_{B,l}$ from the same site $l$. For the ground state, the occupation number of each fermionic state is either $0$ ($\mu < 0$) or $1$ ($\mu > 0$). This is, therefore, clearly a trivial state.

b) Now for $|\Delta| = t > 0$ and $\mu = 0$,

$$H_{\text{Kitaev}} = it \sum_l \gamma_{B,l} \gamma_{A,l+1}. \quad (2.40)$$

Here, it is clear that the two Majorana operators $\gamma_{B,l}$ and $\gamma_{A,l+1}$ are from different sites. The ground state of this Hamiltonian can be constructed by forming a new set of fermionic operators,

$$b_l = \frac{1}{2} (\gamma_{B,l} + i \gamma_{A,l+1}) \quad \text{and} \quad b_l^\dagger = \frac{1}{2} (\gamma_{B,l} - i \gamma_{A,l+1}), \quad (2.41)$$

for $l = 1, 2, \cdots, N - 1$. Now the Hamiltonian can be rewritten in terms of these new operators,

$$H_{\text{Kitaev}} = 2t \sum_{l=1}^{N-1} \left( b_l^\dagger b_l - \frac{1}{2} \right), \quad (2.42)$$

for which the ground state is given by the vacuum of the newly defined operator $b_l$. So the ground state $|\psi\rangle$ satisfies $b_l |\psi\rangle = 0$ for $l = 1, 2, \cdots, N - 1$. Notice that the Majorana operators $\gamma_{A,1}$ and $\gamma_{B,N}$ are not included in the Hamiltonian. These represent the zero-energy Majorana zero modes, localized at both ends of the 1D chain. This is the topological phase of the Kitaev model, where two unpaired Majorana zero modes are localized at both ends of the wire. The degenerate ground state manifold of this Hamiltonian has, therefore, two orthogonal states, $|\psi_g\rangle$ and $|\psi_{g'}\rangle$, with different fermion parity such that

$$-i \gamma_{A,1} \gamma_{B,N} |\psi_g\rangle = |\psi_g\rangle \quad \text{and} \quad -i \gamma_{A,1} \gamma_{B,N} |\psi_{g'}\rangle = - |\psi_{g'}\rangle. \quad (2.43)$$
Now, to connect these two phases (trivial and topological) to the bulk Kitaev Hamiltonian, we can take a periodic Kitaev chain and use Fourier transform to write down the Hamiltonian in the momentum space as

\[ H_{\text{Kitaev}}(k) = \sum_k [(-2t \cos k - \mu) c_k^\dagger c_k + |\Delta| (i \sin k c_k c_{-k} + \text{H.c.})]. \]  

(2.44)

This can then be diagonalized using the BdG method, to get the energy levels

\[ E(k) = \pm \sqrt{(-2t \cos k - \mu)^2 + 4|\Delta|^2 \sin^2 k}. \]

(2.45)

Now, if the superconducting phase \(|\Delta| \neq 0\), the excitation spectrum remains fully gapped, unless \(\mu = 2t\), for \(k = \pm \pi\) or \(\mu = -2t\), for \(k = 0\). Therefore, \(\mu = \pm 2t\) is the phase boundary between the trivial gapped and non-trivial topological phase.

One way to calculate the topological number, which distinguishes the trivial and the topological
phase is to determine the following quantity

\[ M = (-1)^{\nu}, \]  

(2.46)

where \( \nu \) is the number of pairs of Fermi points of the normal system when \( |\Delta| = 0 \). Since, for \( |\Delta| = 0, E(k) = -2t \cos k - \mu \). This ensures that the number of pairs of Fermi points is 1 only when \( |\mu| < 2t \) making \( M = -1 \). Thus the Kitaev 1D Hamiltonian yields a topological phase only when \( |\mu| < 2t \). We now diagonalize a finite Kitaev chain of length \( N = 25 \) as shown in Fig. 2.4 to show that the two zero mode wavefunctions localize at both ends of the Kitaev chain.

Physical realization of Kitaev Hamiltonian in 1D

For the realization of such a 1D model of topological superconductors, we require a spinless fermionic system that has only one pair of Fermi points at the Fermi energy. Now, in naturally occurring material realizations of the 1D chains, electron spin causes double degeneracy for all the bands, and therefore the condition of having only one pair of Fermi points is not satisfied. Also, almost all the superconductors available in nature have s-wave pairing. We need to have p-wave pairing for the realization of the Kitaev chain, which is extremely rare.

These issues were then resolved by introducing a spin-orbit-coupled semiconducting nanowire deposited on an s-wave superconductor. The superconductivity is produced by the proximity effect on the nanowire. This system then can be driven to a topological superconducting state by appropriately controlling the chemical potential and applying an external magnetic field [15, 16]. The continuum Hamiltonian for a single-channel nanowire with an electron effective mass \( m^* \), Rashba spin-orbit coupling \( \lambda \) and applied Zeeman field \( B_z \), proximitized with an s-wave superconductor
with a pairing amplitude $\Delta_s$, with a chemical potential $\mu_w$ can be written as

$$H_{\text{wire}} = \frac{1}{2} \int dx \Psi(x)^\dagger \left[ \left( -\frac{\hbar^2 \partial^2}{2m^*} - i \lambda \partial_x \sigma_y - \mu_w \right) \tau_z + \frac{g \mu_B |B_z|}{2} \sigma_z + |\Delta_s| \tau_x \right] \Psi(x) \quad (2.47)$$

in the BdG formulation. Here we use the Nambu spinor formulation where

$$\Psi(x)^T = (\psi_\uparrow(x), \psi_\downarrow(x), \psi_\downarrow^\dagger(x), -\psi_\uparrow^\dagger(x)) \quad (2.48)$$

and $\psi_\sigma^\dagger(x)$ and $\psi_\sigma(x)$ are fermionic creation and annihilation field operators. We use periodic boundary condition to get the $k$-space Hamiltonian of the nanowire,

$$H_{\text{wire}} = \frac{1}{2} \sum_k \psi_k^\dagger H_{\text{wire}}^k \psi_k, \quad (2.49)$$

where

$$H_{\text{wire}}^k = (\varepsilon_k + \lambda k \sigma_y - \mu) \tau_z + E_Z \sigma_z + \Delta_s \tau_x, \quad (2.50)$$
\( \varepsilon_k = \hbar^2 k^2 / 2m \), and \( E_Z = g\mu_B |B_z|/2 \). In matrix form,

\[
H_{\text{wire}}^k = \begin{pmatrix}
\varepsilon_k - \mu + E_Z & -i\lambda k & \Delta_s & 0 \\
i\lambda k & \varepsilon_k - \mu - E_Z & 0 & \Delta_s \\
\Delta_s & 0 & -\varepsilon_k + \mu + E_Z & i\lambda k \\
0 & \Delta_s & -i\lambda k & -\varepsilon_k + \mu - E_Z
\end{pmatrix}.
\] (2.51)

Let \( E_k \) be the energy eigenvalue. After some algebra, we find the secular equation

\[
[4E_k^2 - (\varepsilon_k - \mu - E_Z)^2][4E_k^2 - (\varepsilon_k - \mu + E_Z)^2] - 2\Delta_s^2 [4E_k^2 + E_Z^2 - (\varepsilon_k - \mu)^2]
\]

\[
- 2\lambda^2 k^2 [4E_k^2 - E_Z^2 + (\varepsilon_k - \mu)^2] + (\Delta_s^2 + \lambda^2 k^2)^2 = 0. \quad (2.52)
\]

The solutions are

\[
E_k = \pm \sqrt{(\varepsilon_k - \mu)^2 + E_Z^2 + \Delta_s^2 + \lambda^2 k^2} \pm 2 \sqrt{(\varepsilon_k - \mu)^2 (E_Z^2 + \lambda^2 k^2) + \Delta_s^2 E_Z^2}. \quad (2.53)
\]

We can understand the physics of Eq.(2.53) by taking the limit where \( |B_z| = |\Delta_s| = 0 \). Now, once the magnetic field is non-zero a gap appears at \( k = 0 \). If the chemical potential \( \mu \) is adjusted in such a way that it lies inside this gap, the system again becomes similar to the Kitaev model described in the previous section and fulfills the condition of having a pair of Fermi points. Therefore, once the s-wave superconducting pairing \( |\Delta_s| \) is introduced through the proximity effect in such a way that the gap is maintained, the nanowire goes into the topological phase as an effective p-wave pairing takes place between the fermions at momentum \( k \) and \(-k\). The excitation gap at \( k = 0 \) is given by

\[
E_{\text{gap}}(k = 0) = \left| \frac{g\mu_B |B_z|}{2} - \sqrt{|\Delta|^2 + \mu^2} \right|. \quad (2.54)
\]

Hence, the Majorana zero modes appear if the chemical potential maintains the following condi-
$|\mu_w| < \mu_c = \sqrt{\left(\frac{g\mu_B|B_z|}{2}\right)^2 - |\Delta|^2}$. \hfill (2.55)

Majorana fermions inside a vortex

In two dimensions, Majorana fermions occur as a zero energy excitation inside a vortex in a spinless chiral p wave $(k_x + i k_y)$ superconductor. Fu and Kane [38] first showed that as a result of the proximity effect from an s-wave superconductor, the surface of a strong topological insulator can work like a spinless $(k_x + i k_y)$ superconductor. The BdG Hamiltonian for the spinless $k_x + i k_y$ superconductor is written as [39]

$$H_{\text{BdG}} = \frac{1}{2} \sum_k \psi_k^\dagger \begin{pmatrix} (k_x^2 - \mu) & 2i\Delta (k_x + i k_y) \\ -2i\Delta^* (k_x - i k_y) & -(k_x^2 - \mu) \end{pmatrix} \psi_k. \hfill (2.56)$$

Now, this BdG Hamiltonian can be solved in case of a vortex being present at $r = 0$, in the polar co-ordinates. The superconducting order parameter in the presence of a vortex is expressed as $\Delta(r) = \Delta_0(r)e^{i\phi}$, where $\Delta_0(r) \to 0$ as $r \to 0$. Since $k_x \pm ik_y = -i(\partial_x \pm i\partial_y)$, the BdG Hamiltonian in polar co-ordinate is

$$H_{\text{BdG}} = \frac{1}{2} \begin{pmatrix} -\mu & 2\Delta(r)e^{i\phi} \left( \frac{\partial}{\partial r} + \frac{i}{r} \frac{\partial}{\partial \phi} \right) \\ -2\Delta(r)e^{-i\phi} \left( \frac{\partial}{\partial r} - \frac{i}{r} \frac{\partial}{\partial \phi} \right) & \mu \end{pmatrix}. \hfill (2.57)$$

Now, once we solve for $H_{\text{BdG}}\psi_0 = E\psi_0 = 0$, we can show that the zero mode operator can be expressed as

$$\gamma = \int r dr d\phi \frac{i}{\sqrt{rN}} e^{\mu(r') \int_0^r \frac{\mu(r'^{\prime})}{\Delta(r'^{\prime})} \left( -e^{i\phi/2}c(r, \phi) + e^{-i\phi/2}c^\dagger(r, \phi) \right)}, \hfill (2.58)$$
from which it clear that $\gamma = \gamma^\dagger$. So, in a chiral p-wave superconductor, a Majorana bound state can be trapped inside the vortex core at zero energy.
CHAPTER 3: MAJORANA NANOWIRE NETWORK


Although there have been numerous experiments on how to realize the nanowire proposal for the experiments, there are still ongoing debates on developing a proper protocol to separate the Majorana zero modes in the topological phase of the nanowire from the non-topological Andreev bound states. In the quest of building a topological quantum computer, the next step after making a topological qubit with the Majorana zero modes is to be able to move them and perform the braiding operation in 2D. Since the non-abelian nature of the statistics of the Majorana zero modes, one can perform braiding to realize a gate operation. The problem with the nanowire proposal is that the Majorana zero modes appearing in two edges of a nanowire are fixed in location for a finite length wire. Fisher et al. [40] first proposed an idea based on T-junctions of Majorana chains to be able to perform braiding adiabatically with the help of tunable keyboard-like gates which can change the chemical potential of the part of a nanowire. There are also alternate protocols that are based on the variation of the magnetic flux [41]. Alternatively, in this chapter, we will describe a protocol to construct logical Majorana zero modes in a 2D wire network.

Hierarchical construction of "logical" Majorana zero mode

In the last chapter, we discussed the existence of Majorana zero modes in a finite-size semiconductor nanowire that is proximitized by an s-wave superconductor. Here in this section, the "logical" Majorana zero modes are not the zero modes that exist at both ends of a nanowire. Instead the
“logical” Majorana zero modes are emergent zero modes, which live inside a Kekule vortex as a topological defect in a 2D brickwall or honeycomb lattice, constructed by the 1D nanowires. The rationale for this construction includes three steps:

• In the first step, each finite-length nanowire in the network is brought to a regime where there is a single Majorana zero mode at each nanowire end. At the vertices of the network, where three nanowires meet, the Majorana zero modes hybridize. As a result, two of the zero modes are gapped out and only one survives, leaving one Majorana zero mode per vertex.

• In the second step, by tuning the gate voltages on each wire, these surviving zero modes are made to weakly overlap, creating a band.

• In the third and final step, a Kekulé vortex modulation of gate voltages is employed to open a spectral gap everywhere but on the vortex, which binds a topological zero mode.

Two conditions are essential for obtaining a “Majorana graphene” system on which to build the logical Majorana zero mode at the vortex core: (i) having a single Majorana mode on each site of the honeycomb lattice, and (ii) hybridizing this mode with all three neighboring sites. In Ref. [12] this was achieved by a fixed pattern of breaking time-reversal symmetry (TRS) at the junction of the three wires connecting at each site. While breaking TRS is not a problem in practice, breaking it in a prescribed pattern on the lattice – in opposite ways in the two sublattices of the honeycomb lattice – could be difficult to achieve. In this paper, we provide a concrete realization of the “Majorana graphene” system of Ref. [12] that requires no breaking of TRS. Here we show that it is impossible, in systems with TRS, to satisfy both conditions (i) and (ii) with junctions of three wires, such as Y- or T-junctions. To satisfy both conditions requires the use of junctions with five wires, where two wires “sister” a third central wire in one of the legs of the Y- or T-junctions, as depicted in Fig. 3.1.

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Figure 3.1: A unit cell of the brickwall network. Every junction consists of five nanowires and the polarity (± signs) correspond to whether the zero mode at a given endpoint of a wire is even or odd under time-reversal symmetry. Notice that the five wires are arranged in such a way that two wires “sister” a (third) central wire in one of the legs of the brickwall lattice. The presence of a nonzero Majorana zero mode amplitude at a nanowire end is indicated by a circular line around a solid circle. The polarities on the nanowires are such that there is only one zero mode per lattice site, and this mode hybridizes with all three neighboring sites. The red circle shows a zoom-in of the interwire couplings at a junction.

Design rationale of the nanowire network

In this section, we justify the design of the nanowire network in Fig. 3.1. Our goal is to obtain an artificial “Majorana graphene” platform, i.e., a system in which single Majorana (quasi-)zero mode sits on the sites of a brickwall or a honeycomb lattice and hybridizes with the three neighboring sites. This platform shares many of the features of graphene but with Majorana (not complex) fermions on the sites. The programmable hoppings (via gate voltages) allow us to imprint Kekulé vortices in the dimerization pattern, thereby trapping logical Majorana zero modes.
The conditions to realize the “Majorana graphene” platform, namely, (i) that a single (quasi-)zero mode sits on each site, and (ii) that these modes hybridize with the three neighbors, and are connected to two indices that we discuss in this section. Here we shall focus solely on an effective model of Majorana end modes on the nanowires, without diving into any microscopic model of the nanowires or the junctions; that discussion is reserved for the subsequent sections.

Let us start from a single nanowire in a phase in which two Majorana zero modes sit at the wire endpoints, which we label $\gamma_{\pm}$. Under the TRS operation $T$, one of these modes is even and the other is odd:

$$T \gamma_{\pm} T^{-1} = \pm \gamma_{\pm}. \quad (3.1)$$

The $\pm$ sign associated with the parity of the endpoint zero modes can be thought of as a polarity for that endpoint. Notice that the only possible coupling that can be added to the effective model in which there are only the Majorana endpoints left in the wire is $H = i \gamma_+ \gamma_-$, which is non-local and gaps the wire. That $\gamma_{\pm}$ have opposite polarity is needed for this $H$ to be both Hermitian and respect TRS.

Consider now a junction where endpoints of multiple wires come together, of which $n_+$ have positive polarity and $n_-$ have negative polarity, as shown in Fig. 3.2. The tunneling Hamiltonian $H_{\text{junction}}$ is quadratic in $\gamma_{a+}$, $a = 1, \ldots, n_+$ and $\gamma_{b-}$, $b = 1, \ldots, n_-$. Moreover, to respect TRS, $H_{\text{junction}}$ must only couple even with odd, or $+$ with $-$, modes, i.e., the Hamiltonian must have the form

$$H_{\text{junction}} = i \sum_{a=1}^{n_+} \sum_{b=1}^{n_-} \gamma_{a+} \Gamma_{ab} \gamma_{b-} + H.c., \quad (3.2)$$

where $\Gamma_{ab} \in \mathcal{R}$. The eigenmodes can be obtained from the spectrum of the $(n_+ + n_-) \times (n_+ + n_-)$
The number of zero modes of this block matrix (in the generic case) is given by the index

$$\nu = |n_+ - n_-|.$$  \hfill (3.4)

One can trace this index to the fact that the system of 1D wires with TRS symmetry belongs to class BDI in the classification of topological insulators and superconductors [42]. Class BDI is indexed by a topological invariant $\nu \in \mathbb{Z}$. (Interactions, which we do not include here, break the classification down to $\mathbb{Z}_8$ [43].)
Besides the number of zero eigenvalues, we can also obtain from $h$ in Eq. (3.3) the number of wires in which the wave function has support, i.e., the number of non-zero components of the $(n_+ + n_-)$-dimensional eigenvectors with eigenvalue zero. The number of these non-zero components is given by

$$\rho = \max(n_+, n_-). \quad (3.5)$$

With the two indices $\nu$ and $\rho$ in hand, we can justify the geometry, Fig. 3.1, that we choose for the wire network. Notice that three (vertical) wires comprise one of the links of the brickwall lattice in Fig. 3.1, so the lattice connectivity is three even though five wires meet at each junction. Given the polarity assignments of the network, we have at each site of the brickwall lattice $\nu = |3 - 2| = 1$ and $\rho = \max(3, 2) = 3$. These values allow us to satisfy both conditions (i) and (ii) above: we have a single zero mode in each site ($\nu = 1$) and that mode leaks through three wires, which connect to three sites ($\rho = 3$). (Notice that the polarity assignments in the network are such that each of the three links connecting to a site has at least one wire with polarity in the majority set for that site, and hence the wave function of a mode leaks in the direction of all three neighboring sites.)

We remark that it is not possible to build a nanowire network that only uses three-wire junctions because one cannot satisfy both conditions (i) and (ii) simultaneously. For example, $n_+ = 2$ and $n_- = 1$ yield a single mode at a site, but then the wave function would only leak to two out of three neighboring sites. In this example, instead of a system with 2D connectivity, the network would behave as a set of decoupled 1D systems.

The arguments above are our rationale for proposing the design in Fig. 3.1 as a way to realize the 2D artificial “Majorana graphene” platform on which to build logical Majorana zero modes. In the next sections, we present a detailed analysis of the wire network using an electronic tight-binding
model of the nanowires and junctions.

Time reversal symmetric Kitaev chains

Majorana modes appear as zero-energy excitations in a spinless one-dimensional p-wave superconductor, as shown by Kitaev [7]. The Hamiltonian model for a 1D chain based on Kitaev’s idea is given by

\[ H_{\text{Kitaev}} = \sum_{l=1}^{L-1} \left[ -t(a_{l+1}^\dagger a_l + a_l^\dagger a_{l+1}) + |\Delta| (e^{i\phi}a_{l+1} a_l + e^{-i\phi} a_{l+1}^\dagger a_l^\dagger) \right] - \mu \sum_{l=1}^{L} \left( a_l^\dagger a_l - \frac{1}{2} \right), \] (3.6)

where \( a_l^\dagger, a_l \) are spinless fermion creation and annihilation operators, \(|\Delta|\) and \(\phi\) are the chain’s superconductor order parameter amplitude and phase, respectively, \(t\) is the hopping amplitude between the nearest-neighbor sites, and \(\mu\) is the chemical potential. For this Hamiltonian, provided that \(|\mu| < 2t\), it can be shown that the two Majorana zero modes are localized at both endpoints of the chain within a characteristic length

\[ \ell_0 = \max(\ell_0^+, \ell_0^-), \] (3.7)

where

\[ \ell_0^\pm = \left| \ln \left( -\mu \pm \sqrt{\mu^2 - 4t^2 + 4|\Delta|^2} \right) \right|^{-1}. \] (3.8)

Thus, for a finite chain there is always some residual interaction between the two zero modes at the chain endpoints.
Under the TRS symmetry operation, the spinless fermionic operators transform as

\[ T a_l T^{-1} = a_l \]  
(3.9)

\[ T a_l^\dagger T^{-1} = a_l^\dagger, \]  
(3.10)

while a scalar \( z \) transforms as

\[ T z T^{-1} = z^*. \]  
(3.11)

Therefore, applying the TRS operation on the chain Hamiltonian we obtain

\[
T H_{\text{Kitaev}} T^{-1} = \sum_{l=1}^{L-1} \left[ -t(a_l^\dagger a_{l+1} + a_{l+1}^\dagger a_l) + |\Delta| \left( e^{-i\phi} a_l a_{l+1} + e^{i\phi} a_{l+1}^\dagger a_l^\dagger \right) \right] - \mu \sum_{l=1}^{L} \left( a_l^\dagger a_l - \frac{1}{2} \right),
\]  
(3.12)

We can easily verify that in order for the Hamiltonian to be time-reversal symmetric we must have \( \phi = \pi n \), where \( n = 0, \pm 1, \pm 2, \ldots \). In this case, we can write \( \Delta = \pm |\Delta| \) (positive or negative). However, since \( a_l a_{l+1} = -a_{l+1}^\dagger a_l \), we can turn a “negative” sign in \( \Delta \) into a positive one by running the index \( l \) from \( L \) to 1 instead of 1 to \( L \). Therefore, the orientation of the hopping in the superconductor term and the sign of \( \Delta \) are related. We can take this into account by classifying time-reversal symmetric Kitaev chain into two classes: “right” and “left”. Thus, in general, for time-reversal symmetric chains we have

\[
H_{\text{Kitaev}} = \sum_{l=1}^{L-1} \left[ -t(a_l^\dagger a_{l+1} + a_{l+1}^\dagger a_l) + \eta |\Delta| (a_l a_{l+1} + a_{l+1}^\dagger a_l^\dagger) \right] - \mu \sum_{l=1}^{L} \left( a_l^\dagger a_l - \frac{1}{2} \right),
\]  
(3.13)

where \( \eta = \pm 1 \). In fact, we can introduce the concept of chain “polarity”, see Fig. 3.3, where ± signs are associated to the endpoints of the chain (i.e, site coordinates \( l = 1 \) or \( l = L \)), as well as an arrow, depending on the sign of \( \eta \). As we showed in Sec. 3, the polarity of the chain is connected
to how the Majorana zero modes at the chain endpoints transform under time reversal.

\[
\gamma^+ \quad \gamma^- \quad \gamma^- \quad \gamma^+ \\
1 \quad \eta = 1 \quad L \quad \eta = -1 \quad L
\]

Figure 3.3: Schematic illustration of the concept of polarity for time-reversal symmetric Kitaev chains. \( \eta = \pm 1 \) correspond to whether the Majorana zero modes at the chain endpoints (here indicated by \( \gamma_{\pm} \)) are even/odd or odd/even under time-reversal symmetry.

Electronic tight-binding model of nanowires and junctions

We start by investigating junctions of time-reversal symmetric Kitaev nanowires. We only consider junctions in the all-connected configuration, where all nanowire endpoints are coupled to each other.

We employ an electronic, single-band electronic tight-binding model based on the Hamiltonian of Eq. (3.6) to model nanowires and their junctions. We adopt a BdG representation for the fermion operators

\[
\psi_{l,\alpha} = \begin{pmatrix} a_{l,\alpha} \\ -a_{l,\alpha}^\dagger \end{pmatrix}, \quad \psi_{l,\alpha}^\dagger = \begin{pmatrix} a_{l,\alpha}^\dagger \\ -a_{l,\alpha} \end{pmatrix},
\]

where \( l = 1, \ldots, L \) is the site coordinate and \( \alpha = 1, \ldots, n \) is the nanowire index. We number the sites by starting from the junction end of the nanowire. The total Hamiltonian of a \( n \)-nanowire junction system is written as

\[
H_{\text{total}} = \sum_{\alpha=1}^{n} H_{\alpha} + H_{\text{junction}},
\]

where

\[
H_{\alpha} = \sum_{l=1}^{L-1} \psi_{l,\alpha}^\dagger \left( -t_\tau z + i\eta_{\alpha} |\Delta| \tau_y \right) \psi_{l+1,\alpha} - \frac{\mu}{2} \sum_{l=1}^{L} \psi_{l,\alpha}^\dagger \tau_z \psi_{l,\alpha}
\]
describes the $\alpha$-th wire and

$$H_{\text{junction}} = -\frac{1}{2} \sum_{\alpha \neq \beta} \Gamma_{\alpha\beta} \psi_1^\dagger \tau_z \psi_{1,\beta}$$

(3.17)

describes the couplings at the junction, where $\Gamma_{\alpha\beta}$ is the pairwise hopping amplitude between the endpoints of the $\alpha$-th and $\beta$-th nanowires. For the simulations discussed in this section, we adopt $\mu = 0.5t$, $L = 20$ and $\Delta = 0.5t$, which sets the nanowires in the topological regime and exponentially localize the Majorana zero modes at the nanowire ends, with $\ell_0 \approx 1.82$. We have performed all the numerical simulations in this paper by implementing the tight-binding Hamiltonian of Eq. (3.15) in Kwant [44]

**Majorana junction of 3 wires**

We note that for two Majorana zero modes on different time-reversal symmetric nanowires to hybridize and to combine into a finite-energy fermion, they must to be of different polarity. This restricts how the zero modes can be distributed among the junction nanowires. In the case of a three-wire junction, two possible cases exist. When all the Majorana zero modes in the junction are of the same polarity, none of the zero modes couple and all six zero modes on the ends of three nanowires survive. However, when one of the nanowires has a different polarity than the other two nanowires, for example, in a $(+ + -)$ or $(- + -)$ configuration, there is only one zero mode at the junction and the wave function amplitude for that zero mode is shared between the majority polarization sites.

This analysis in terms of Majorana operators is corroborated by a numerical simulation of the underlying electronic system. The results are presented in Fig. 3.4, where the electronic local density of states (LDOS) at zero energy for the $(- - -)$ and $(+-+)$ junction configurations
Figure 3.4: Numerical results for a three-wire junction with two different choices of polarity. Solid lines indicate the location of the nanowires (site coordinates are shown), while dotted lines connect neighboring nanowire endpoints. To facilitate visualization, neighboring endpoints are set farther apart than one chain lattice constant unit. In panels (a) and (b) the electronic local density of states (LDOS) at zero energy and the energy eigenstates are plotted, respectively, for the \((- - -)\) case, while in panels (c) and (d) the same quantities are plotted for the \((+ + +)\) case. The wires are identified by the subscripts \(A, B, C\). In (a), it is noticeable that the zero-energy wave function has amplitude in the three junction sites and the total number of zero modes is six, with three sitting at the junction and three other modes sitting at the outer ends of the wires. In (c), the zero-energy wave function has amplitude in the majority polarity sites of the junction but there is only zero mode at the junction. The other three modes sit at the outer ends of the nanowires.

are shown when \(\Gamma_{\alpha\beta} = (1 - \delta_{\alpha,\beta})\Gamma\) with \(\Gamma = t\). It is clear that for the \((- - -)\) configuration a total of six Majorana zero modes are present, including three at the junction. For the \((- + +)\) configuration, there is a single zero mode at the junction and it is shared only by the nanowires with majority polarity.
Figure 3.5: Schematic illustration of a brickwall network of nanowires with well-defined polarizations and three-wire junctions of the \((-++\) and \((++-\) types. The presence of a nonzero Majorana zero mode amplitude at a nanowire end is indicated by a circular line around a solid circle. Nanowire polarities are indicated by arrows and ± signs.

The wave function distribution in the majority-polarized nanowires makes it impossible to satisfy simultaneously the two necessary conditions for the realization of a single-band Majorana network. This illustrated in Fig. 3.5 where a brickwall network out of the nanowires with only one Majorana zero mode at each junction is shown. The Majorana zero mode located on the majority nanowires of a junction is disconnected from the zero mode on the junction across the minority nanowire. As a result, when hybridization within the nanowires is turned on, the network breaks up into an array of disconnected chains with no inter-chain coupling.
We now consider the case of five nanowires and when $n_+ = 2$ and $n_- = 3$. We simulate such a junction similarly to the three-nanowire junction using the following choice for the $\Gamma_{\alpha\beta}$ coupling parameters:

$$
\Gamma_{\alpha\beta} = \frac{\Gamma}{\sqrt{6}} \times \begin{pmatrix}
0 & 0 & 1 & 1 & -2 \\
0 & 0 & \sqrt{3} & -\sqrt{3} & 0 \\
1 & \sqrt{3} & 0 & 0 & 0 \\
1 & -\sqrt{3} & 0 & 0 & 0 \\
-2 & 0 & 0 & 0 & 0
\end{pmatrix}.
$$

(3.18)

This choice of coupling matrix elements lifts all by one mode from zero energy. The remaining zero mode has equal amplitude among the three majority-polarity nanowires. The results are shown in Fig. 3.6. In this case, the single Majorana zero mode wave function is distributed among the negative endpoints of the majority polarization nanowires in the junction, fully connecting the three links of the network that emanate from the junction and condition (i) of Sec. 3 is satisfied. Moreover, all junction zero modes can be connected to zero modes located at the outer endpoints of the junction nanowires, satisfying condition (ii). This configuration is therefore chosen for the simulation of a “Majorana graphene” network, which we discuss in the following section. While others choices of coupling matrix elements are possible, as long as the diagonal blocks in Eq. (3.18) are zero, only one zero mode exists at the junction. Small deviations from the coupling matrix elements in Eq. (3.18) are possible: due to TRS, Dirac cones in the dispersion relation survive as long as the matrix elements satisfy the triangle rule, which says that the magnitude of each of the tunnel couplings is smaller than the sum of the magnitudes of the other two couplings [39]. Moreover, Dirac cones are also robust to inhomogeneities in $\Gamma$ from one junction to another, as there is no equivalent to on-site disorder in a Majorana “graphene” system.
Figure 3.6: Numerical results for a five-wire junction consisting of two positive and three negative polarity nanowires coupled according to Eq. (3.18). The same conventions as in Fig. 3.4 are followed here. In panel (a), the electronic local density of states (LDOS) at zero energy is plotted while in panel (b) the relevant energy eigenstates are plotted. The wires are identified by the subscripts $K, L, M, N, O$. It is clear from the electronic LDOS that the zero energy wave function in the junction has nonzero amplitude only in the majority polarity sites. There is no impediment for the zero mode located at a junction can hybridize with the zero modes in neighboring junctions.

Majorana network

In Sec. 3, we established that, using a five-wire junction, it is possible to (i) have a single Majorana (quasi-)zero mode per site of the brickwall lattice, and (ii) hybridize this mode with those on the three neighboring sites. These results justify using the brickwall structure in Fig. 3.1 to realize the “Majorana graphene” network. Here we proceed to construct the logical Majorana zero mode using this structure, modeling every nanowire in the network by the Kitaev Hamiltonian in the BdG formulation, as in Eq. (3.16).
“Majorana graphene” network

The characteristic length of the zero modes in the Kitaev nanowires depends on the chemical potential, as indicated in Eq. (3.7). It is thus possible to increase the overlap between the zero modes in neighboring sites of the network, i.e., effective hopping of the Majorana zero modes in the brickwall lattice, by controlling a gate voltage $V_g$ in every nanowire.

We consider first the case with uniform hopping matrix elements (i.e., uniform gate voltages) across the entire network. In this case, the Majorana system on the brickwall lattice contains features similar to those of graphene, such as a Dirac-type dispersion. To illustrate this point, we computed the electronic energy bands of an infinite honeycomb network of 5-nanowire junctions.

*Model Hamiltonian for the unit cell*

The Hamiltonian for the unit cell consists of two 5-wire Majorana junctions. The ends are connected by periodic boundary conditions to simulate the whole system which is tiled by the unit cell. The Hamiltonian of the unit cell can be written as:

\[
H_{\text{unit}} = \sum_{\varepsilon=1}^{4} H_{\varepsilon} + \sum_{\varepsilon'=5}^{9} H_{\varepsilon'} + \sum_{\alpha, \beta} \Gamma_{\alpha, \beta} a_\alpha^\dagger a_\beta - t(e^{i\vec{k} \cdot \vec{a}_1} a_0^\dagger a_{3L-1} + \text{h.c.}) - t(e^{-i\vec{k} \cdot \vec{a}_2} a_{4L-1}^\dagger a_{2L-1} + \text{h.c.}) + \Delta (e^{i\vec{k} \cdot \vec{a}_1} a_0^\dagger a_{3L-1} + \text{h.c.}) + \Delta (e^{-i\vec{k} \cdot \vec{a}_2} a_{4L-1}^\dagger a_{2L-1} + \text{h.c.}), \tag{3.19}
\]

where $H_{\varepsilon}$ and $H_{\varepsilon'}$ are Kitaev chains of length $L$ and $2L$, and $\alpha$ and $\beta$ are the site indices of the two junctions.

In Fig. 3.8a we show the energy bands close to zero energy, where the six pairs of Dirac cones at the $K_\pm$ points are clearly visible. The nanowire parameters are $L = 20$, $\Delta = 0.5t$, and $\mu = 0.5t$;
Figure 3.7: (a): Graph model of each unit cell with two 5-wire junctions. One of them has polarity (++−−) and another one has the polarity choice (++−+). $\Gamma$ is the hopping matrix as mentioned in 3.18 (b) Periodic honeycomb lattice with each unit cell connected by the lattice vectors $\vec{a}_1$ and $\vec{a}_2$. The hopping phase factors are given by $\phi_1 = e^{i\vec{k} \cdot \vec{a}_1}$, and $\phi_2 = e^{-i\vec{k} \cdot \vec{a}_2}$.

the junction couplings follow Eq. (3.18), with $\Gamma = t$. In Fig. 3.8b, we show that the Fermi velocity for the Dirac dispersion depends on the nanowire chemical potential, which in turn controls the effective hopping amplitude between Majorana zero modes located at the opposite ends of the nanowire.

Returning to the finite-size network of Fig. 3.1 with open boundaries, in Fig. 3.9 we show its electronic LDOS at zero energy for the network when $\mu = 0.4t$, $\Delta = 0.8t$, and $\Gamma = t$, employing the junction coupling matrix of Eq. (3.18). The LDOS shows zero energy modes at the boundary and in the bulk of the system. These zero modes correspond to the states at the Dirac nodes (i.e., the apexes of the cones in the energy bands of Fig. 3.8). Due to the open boundary conditions,
Figure 3.8: (a) Electronic energy bands near zero energy for an infinite network of five-wire junctions consisting of two positive and three negative polarity nanowires. The nanowire parameters are \( L = 20, \Delta = 0.5t, \) and \( \mu = 0.5t. \) The junction coupling parameters are chosen according to Eq. (3.18) with \( \Gamma = t. \) The brickwall lattice is reshaped as a honeycomb lattice in order to create a triangular reciprocal lattice unit cell to facilitate visualization of the bands. (b) Energy bands along the reciprocal space dashed line path are shown in the inset. Bands are various chemical potential values are shown to illustrate their impact on the Fermi velocity at the \( K_\pm \) points.

zero modes appear at the boundary sites. They can be removed by switching to periodic boundary conditions, as we show in Fig. 3.10.

**Kekulé modulation in the brickwall lattice**

Introducing a Kekulé dimerization pattern in a graphene lattice opens up a gaps in the Dirac spectrum \([12, 45]\). The Kekulé modulation can be realized by imposing the following perturbation to the local chemical potential (via gate voltages):

\[
\mu = \mu_0 + \delta \mu_{r, \alpha},
\]  

(3.20)
Figure 3.9: Electronic LDOS for a $7 \times 10$ brickwall lattice of Majorana nanowires with open boundary conditions and a single zero mode at each junction. Horizontal links in the lattice consist of a single nanowire while vertical links contain three wires. Every nanowire is described by a Kitaev chain Hamiltonian with $L = 5$ sites, $\mu = 0.4t$, and $\Delta = 0.8t$. Junction couplings follow Eq. (3.18) with $\Gamma = t$.

where

$$\delta \mu^\text{Kekule}_{r,\alpha} = \mu_K \cos (\varphi_{r,\alpha}).$$

(3.21)

and

$$\varphi_{r,\alpha} = K_+ \cdot s_\alpha + (K_+ - K_-) \cdot r. \quad (3.22)$$

To implement this modulation, we return momentarily to the equivalent honeycomb lattice and its coordinate system. The position vector $r$ has a fixed (arbitrary) origin and points to the sites of one of the triangular sublattices. The three vectors $s_\alpha (\alpha = x, y, z)$ connect sites of that sublattice to their nearest neighbors on the other sublattice. $K_+ = -K_-$ are the distinct vectors connecting the $\Gamma$ to the $K$ points in the reduced Brillouin zone in reciprocal space for the honeycomb lattice. In Fig. 3.11 we show the pattern induced by the Kekulé distortion.
Figure 3.10: Electronic LDOS for a $3 \times 4$ brickwall lattice of Majorana nanowires similar to that of Fig. 3.9 but with periodic boundary conditions and $L = 8$. Notice the absence of zero modes at the boundaries. The smaller lattice has been used to show that the boundary Majorana-zero modes disappear when using periodic boundary conditions.

In Fig. 3.12, we show the effect resulting from the Kekulé dimerization pattern on the electronic LDOS at zero energy for the wire network in Fig. 3.1. For these calculations, the junction coupling amplitude $\Gamma = t$, the superconductor order parameter amplitude $\Delta = 0.8t$, and the chemical potential parameters are set as $\mu_0 = t$ and $\mu_K = 0.98t$. We choose the maximum value of the chemical potential ($\mu_{\text{max}} = \mu_0 + \mu_K$) to be very near the boundary of the topological range, $\mu_{\text{max}} = 1.98t < \mu_c = 2t$ to ensure a sizable overlap between the Majorana zero modes on both ends of the same nanowire, with the Majorana characteristic length reaching $\ell_0 \approx 80$ on those nanowires [see Eq. (3.7)]. Notice that the bulk zero modes are now absent because of the bulk gap, while the boundary zero modes remain. The boundary zero modes disappear under periodic boundary conditions. To illustrate this point, in Fig. 3.13 we show the energy eigenvalues of a Majorana zero-mode lattice of 4 layers with each layer consists of 5 horizontal wires with periodic
Figure 3.11: The Kekulé dimerization in a honeycomb lattice. The single (double) links correspond to weak (strong) bond amplitudes. The red and blue dots represent the two sublattices of the honeycomb lattice. As a result of the dimerization, three kinds of plaquettes are created which are labeled by A, B and C.

boundary conditions in the presence and in the absence of the Kekulé modulation. We adopt the same parameters as in Fig. 3.9 and Fig. 3.12. for the absence and presence of Kekulé modulation respectively.

Zero modes bound to Kekulé vortices

The Kekulé dimerization pattern can support defects in the form of vortices. As noted in Ref. [12], a vortex can be imprinted via an additional modulation of the Kekulé pattern,

\[
\varphi_{r,\alpha} = K_+ \cdot s_\alpha + (K_+ - K_-) \cdot r + \varphi_{r,\text{vortex}},
\]

(3.23)
Figure 3.12: Electronic LDOS of a brickwall network of Majorana nanowires with a Kekulé distortion on the chemical potentials. Chain and junction parameters are the same as in Fig. 3.9, with the baseline chemical potential $\mu_0 = t$ and the added Kekulé modulation $\mu_K = 0.98t$.

Figure 3.13: The energy spectrum of a brickwall lattice with quasi-Majorana zero modes at each vertex and periodic boundary conditions without (a) and with (b) a Kekulé modulation for $L = 8$ and the same network size as in Fig. 3.10. The parameters used in panels (a) and (b) are the same as those in Fig. 3.9 and Fig. 3.12, respectively.
where

$$\varphi_r^{\text{vortex}} = \sum_{n=1}^{\nu} q_n \arg(r - R_n).$$

(3.24)

One important advantage of this construction is that the vorticities $q_n = \pm 1$ ($n = 1, \cdots, \nu$) and the positions of the vortices $R_n$ are also programmable via the applied gate voltage on each wire. The Kekulé vortices bind zero energy modes at their location – these are the *logical* Majorana zero mode. These logical Majoranas can be moved by applying gate voltages that correspond to changing the value of $R_n$ in Eq. (3.23).

In Fig. 3.14 a,c we show the electronic LDOS at zero energy for the wire network in Fig. 3.1 with a Kekulé vortex pattern of applied gate voltages. In Fig. 3.14 b,d we plot the intensity of eigenfunctions associated to the zero modes bound to the Kekulé vortex. We choose the vorticity to be $-1$. Other parameters are the same as those in Fig. 3.12.

The results described above establish that the wire network presented in Fig. 3.1 is a concrete realization of the proposal in Ref. [12] to obtain logical Majorana zero modes in a hierarchical manner. The architecture in Fig. 3.1 enables the placement of multiple vortices and the movement of those vortices by simply changing the gate voltage on the wires according to Eq. (3.23). In particular, this construction allows the logical Majorana zero modes to be braided adiabatically by the modulation of the gate voltages.

**Experimental realization**

We now connect the idealized tight-binding model used to describe the Majorana network with a more realistic model of semiconductor system proximitized with s-wave superconductors. We return to the Hamiltonian in Eq. (2.47) and consider an infinite nanowire in the momentum space.
Figure 3.14: Vortex in a Majorana network. The electronic LDOS at zero energy is plotted in panels (a) and (c) for the two different vortex positions indicated by red circles. The intensity of the eigenstates located within the red circles is plotted in panels (b) and (d). Notice that the eigenstate are the same for both vortex positions. The Majorana zero modes in the bulk are bound to the Kekulé vortex and they move around lattice together with the vortex. The location of the vortex is controlled by gate voltages on the nanowires. Here the vortex has charge $q = -1$. All other parameters are the same as in Fig. 3.9.

representation, yielding

$$H_{\text{wire}} = \frac{1}{2} \sum_k \psi_k^+ H_k \psi_k,$$

(3.25)

where

$$H_k = (\varepsilon_k + \lambda k \sigma_y - \mu_w)\tau_z + E_Z \sigma_z + \Delta_s \tau_x,$$

(3.26)
\[ \varepsilon_k = \hbar^2 k^2 / 2m^*, \text{ and } E_Z = g\mu_B|B|/2. \] The eigenvalues of this matrix are

\[ E_k = \pm \sqrt{(\varepsilon_k - \mu)^2 + E_Z^2 + \Delta_s^2 + \lambda^2 k^2 + 2R_k}, \tag{3.27} \]

where

\[ R_k = \sqrt{(\varepsilon_k - \mu)^2(E_Z^2 + \lambda^2 k^2) + \Delta_s^2 E_Z^2}. \tag{3.28} \]

Each one of the four eigenvalues generates a band in \( k \)-space. The exact shape of these bands depends sensitively on the values of the parameters \( m^*, E_Z, \Delta_s, \lambda, \) and \( \mu_w \). Therefore, it is fundamental to seek parameter values that match experimental systems. For that purpose, we choose InSb-NbTiN hybrid nanowires, which are currently used to realize Majorana zero modes. They have a proximity-effect induced superconductor gap \( \Delta \approx 1 \) meV. The effective mass of bulk InSb is \( m^* = 0.014 m_e \), where \( m_e \) is the electron bare mass [46]. The Rashba spin-orbit coupling parameter for bulk InSb is \( \lambda = 0.1 \) eV·nm and the g-factor is 50 [47]. Since it is advantageous to use a large magnetic field and the critical field for bulk NbTiN is approximately 10 T, we pick this value for our analysis. Thus, following Eq. (2.55), the range of chemical potential values for which the nanowire remains in the topological phase is \( |\mu_w| \lesssim 11 \) meV.

After substituting those experimental parameter values into Eq. (3.27) we find low-lying energy bands which can be well approximated by the dispersion relation

\[ E_k \approx \sqrt{\alpha(k \pm k_0)^2 + \beta}, \tag{3.29} \]

with \( \alpha \approx 0.140 \) eV²·nm², \( k_0 \approx 0.0777 \) eV²·nm, and \( \beta \approx 2.23 \times 10^{-7} \) eV².

We can similarly derive a low-lying band structure from the Kitaev chain Hamiltonian in Eq. (3.13). In the long wave-length limit, we find an expression that matches Eq. (3.29), allowing us
to connect its coefficients with the Kitaev chain parameters as follows:

\[ t a^2 = \frac{\sqrt{\alpha}}{k_0}, \]  
\[ t - \frac{\mu}{2} - \frac{\Delta^2}{t} = \frac{\sqrt{\alpha} k_0}{2}, \]  
\[ \beta = \frac{\Delta^2}{2t} \left[ 2t - \mu - \frac{2\Delta^2}{t} \right], \]  

(3.30)  
(3.31)  
(3.32)

where \( a \) is the chain lattice constant. These relations are obtained under the assumption that \( \mu < 2t - \Delta^2/t \). Inserting the experimental values for \( \alpha, k_0, \) and \( \beta \) into these relations, we find that a realistic Kitaev model parameters satisfy

\[ t a^2 \approx 4.8 \text{ eV} \cdot \text{nm}^2 \]  
\[ t - \frac{\mu}{2} - \frac{\Delta^2}{t} = 0.015 \text{ eV}. \]  

(3.33)  
(3.34)

Let us consider the case when \( \Delta = 0.5t \) and \( \mu = 0.5t \), corresponding to the regime of Figs. 3.4 and 3.6. Substituting these values into the above equations we find \( t = 7.3 \text{ meV} \) and \( a = 26 \text{ nm} \); the latter value, when combined with a length of 20 sites (\( L = 20 \)) yields a wire of approximately 500 nm in length, which is quite reasonable when considering a realistic nanowire. Equation (3.32) serves as a consistency check: The r.h.s. yields 1 meV, which is about 5 times larger than the fitted value for \( \beta \). This discrepancy comes primarily from \( \Delta \), which is set to a relatively high value in the numerical calculations to keep the Majorana zero modes sufficiently isolated at the ends of the chains. Smaller values of \( \Delta \) could be implemented at the expense of using longer chains (i.e., more sites) and performing exact diagonalizing of larger systems. However, given that the values obtained for \( a \) and \( t \) in comparison to the realistic nanowire model are reasonable, and they
dependent only weakly on $\Delta$ when $\Delta \ll t$, our considerations show that it is possible to achieve the necessary conditions for the realization of Majorana zero modes in current experimental setups.

Figure 3.15: Energy eigenstates for the brickwall lattice in the presence of a vortex. The $E_{1913}$ eigenstate along with its particle-hole partner is the vortex eigenstate. The closest state which does not contribute to the boundary zero modes is the state $E_{1930}$.

Another important aspect to consider in connection to the experimental observation of Majorana zero modes is the necessary energy resolution. In Fig. 3.15, we show a portion of the energy spectrum for the brickwall lattice for the specific vortex position in Fig. 3.14a. We notice that the difference in energy between the nearest bulk zero mode state is $0.00257t$. Using the value of $t$ obtained from the fitting to the realistic nanowire model, this energy separation equals approximately $19 \mu$eV, or, equivalently, 220 mK, which is a very accessible temperature.
Conclusion

In this work, we present a nanowire architecture, shown in Fig. 3.1, where it is possible to realize logical Majorana zero modes that are movable in 2D by changing gate voltages on the nanowires. This architecture realizes the hierarchical construction of Ref. [12], without the need for breaking time-reversal symmetry (TRS).

The basis for building the logical Majorana zero modes is a programmable “Majorana graphene” platform, where a single Majorana quasi-zero mode at each site of a brickwall or of a honeycomb lattice hybridizes with modes on the three neighboring sites. The degree of hybridization, and hence the effective hopping, is controlled by gate voltages. To arrive at the geometry in Fig. 3.1, we showed that junctions of five nanowires meeting at each site are necessary so that (i) there is a single (quasi-)zero mode in each site; and (ii) this single mode hybridizes with the three neighboring sites. The number of nanowires needed at the junction follows from two indices constructed from the polarities of the zero modes at the end of nanowires. (A positive polarity corresponds to zero modes that are even under TRS, while a negative polarity corresponds to modes that are odd under TRS.) For a junction where $n_+$ positive and $n_-$ negative polarities meet, the number of zero modes at the junction is $\nu = |n_+ - n_-|$ and the wave function of the zero modes spread over $\rho = \max(n_+, n_-)$ wires. We thus satisfy conditions (i) and (ii) with either $n_+ = 3$ and $n_- = 2$, or $n_+ = 2$ and $n_- = 3$, which are the cases in the two sublattices of the brickwall network shown in Fig. 3.1. In the paper, we show that numerical results obtained from electronic tight-binding models of nanowire junctions agree with this counting.

We further carried out numerical studies of a tight-binding model for all nanowires and junctions of the network in Fig. 3.1. In particular, we decorated the tight-binding model with a Kekulé dimerization pattern and showed that it is possible to make the bulk of the system gapped. We achieved the final stage in the hierarchical construction of Ref. [12] by including vortices in the
Kekulé dimerization pattern and showed that there exists a zero mode – the logical Majorana mode – at the core of the Kekulé vortex. Finally, we provided estimates of the experimental values for the parameters used in the numerical calculations and argued that it is possible to detect the logical Majorana zero modes using low-temperature local probes.

In closing, we stress that the construction of movable logical Majorana zero modes in 2D would enable direct and controllable experiments where Majoranas are braided. This realization of braiding may require less stringent conditions on the nanowires than other proposals in the literature.
CHAPTER 4: MANY-BODY LOCALIZATION AND PROTECTION OF QUANTUM INFORMATION BY DISORDER

In this chapter, we will switch gears from the topological protection of quantum information to the disorder-induced protection of quantum information. As mentioned in one of the DiVincenzo criteria [20] in the first chapter, it is necessary for the qubits to have a long coherence time such that enough quantum operations can be performed. In addition to that, it is also necessary to construct lossless quantum channels for communication. Now as mentioned in the work by Vishwanath et al. [48], constructing such a decoherence-free quantum channel from an interacting quantum many-body system, is very hard. Therefore, usually, coherence is maintained either by operating at very low temperatures and freezing out all the degrees of freedom that causes decoherence or by making a very specific few-body system. In this chapter, we will discuss in detail the phenomena of “many-body localization” (MBL), where, in a strongly interacting disordered system local information is preserved due to the non-ergodicity. We will also comment on the phase transition from the ergodic (thermalized) to non-ergodic (many-body localized) behavior in an infinite temperature limit. The ideas of this paragraph are largely based on the work by Vishwanath et al. [48].

Equilibration and thermalization

How an isolated quantum many-body system reaches thermal equilibrium [13, 49] is a fundamental question in statistical mechanics. Starting from an initial state, how the unitary evolution makes it a thermal state, is a longstanding question that invoked theoretical, numerical, and most recently experimental studies. Recent studies on these systems [9, 50, 51] have also found many systems which do not necessarily thermalize in the presence of strong disorder. The interplay of interaction and disorder in these systems causes a quantum phase transition between the thermalized and the
non-thermalized (localized) phase [10, 52]. In order to study the dynamics, the method of quantum quenching is used, which can also be successfully implemented in experiments. Below, we provide a detailed discussion on equilibration, thermalization, and localization in isolated quantum many-body systems. For one-dimensional quantum many-body systems, integrability basically means that the system is solvable by the Bethe Ansatz [53]. Integrable systems possess additional conserved charges on top of the common conserved quantities. The conservation of these extra charges constrains the dynamics of the integrable systems so that they can not relax to a thermal state. In fact, a pioneering experiment by Kinoshita, Wenger, and Weiss [54] on a one-dimensional Bose gas showed that the steady state measured in the experiment was different from the thermal state. However, these systems can relax to a long-time asymptotic stationary state given by the following density matrix [55]:

\[
\rho = Z^{-1} \exp \left( - \sum_m \lambda_m I_m \right),
\]

where \( \{ I_m \} \) is the complete set of conserved quantities, \( Z = \text{Tr} \left[ \exp \left( - \sum_m \lambda_m I_m \right) \right] \) is the partition function, and \( \{ \lambda_m \} \) are the Lagrange multipliers fixed by the initial conditions,

\[
\text{Tr} \{ I_m \rho \} = \langle I_m \rangle (t = 0).
\]

The ensemble in 4.1 is called the generalized Gibbs ensemble and it can be reduced to a grand-canonical ensemble in the case of a generic system, where total energy and the number of particles are the only conserved quantities. However, for a strongly correlated interacting quantum system, it is very hard to construct the ensemble. Therefore, the initial theoretical studies on the relaxation of quantum integrable systems only included those whose Hamiltonians could be written in terms of free fermions. Recently, interacting integrable systems like the one-dimensional Bose gas and the XXZ Heisenberg spin chain [56], have been studied both theoretically and numerically for the
validation of the generalized Gibbs ensemble (GGE). Field-theoretical methods have also been
developed in these scenarios. Although there is excellent agreement between the numerical studies
and the GGE in such integrable models, there have been cases where another proposed method
named overlap-incorporating thermodynamic Bethe ansatz (OTBA) [57] has been stated to be a
correct alternative.

Equilibration

Here we explain the process of equilibration in isolated quantum many-body systems evolving
under unitary evolution [58, 59]. We consider the initial state of the system expanded in the
eigenbasis of the Hamiltonian,

\[ |\Psi(0)\rangle = \sum_\alpha C_\alpha |E_\alpha\rangle \]

\[ |\Psi(t)\rangle = e^{-iHt/\hbar} |\Psi(0)\rangle = \sum_\alpha C_\alpha e^{-iE_\alpha t/\hbar} |E_\alpha\rangle. \]

The expectation value of any operator at any later time will be

\[ \langle A(t) \rangle = \langle \Psi(t) | A | \Psi(t) \rangle = \sum_{\alpha,\beta} C_\alpha C_\beta^* e^{-i(E_\alpha - E_\beta) t/\hbar} A_{\alpha\beta}. \]

Now, if the system relaxes to equilibrium, \( \langle A(t) \rangle \) must reach its long-time average behavior with
minimal fluctuations,

\[ \overline{\langle A(t) \rangle} = \lim_{t \to \infty} \frac{1}{t} \int_0^t \langle A(t') \rangle \, dt' = \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha}. \]
Also, the density matrix will relax to its long-time average form,

\[
\overline{\rho(t)} = \lim_{t \to \infty} \frac{1}{t} \int_0^t \rho(t') dt'
\]

(4.7)

\[
= \lim_{t \to \infty} \frac{1}{t} \int_0^t \sum_{\alpha, \beta} C_\alpha C^*_\beta e^{-i(E_\alpha - E_\beta) t'/\hbar} dt'
\]

(4.8)

\[
= \sum_\alpha \rho_{\alpha \alpha} |E_\alpha \rangle \langle E_\alpha| = \sum_\alpha \Pi_\alpha \rho \Pi_\alpha.
\]

(4.9)

where \( \rho_{\alpha \alpha} = |C_\alpha|^2 \) are the relative population of the initial state in the basis of the Hamiltonian and \( \{ \Pi_\alpha = |E_\alpha \rangle \langle E_\alpha| \} \) are the projectors onto the eigenstate of the Hamiltonian. We can see that if we take the long-time average we get a completely dephased state which loses all the off-diagonal terms in the density matrix. This is what is meant by an equilibrium state. The equilibrium expectation value of an operator can be written in the following manner:

\[
A_{eq} = \langle A(t) \rangle = \text{Tr}\{ A \overline{\rho(t)} \} = \text{Tr}\{ A \overline{\rho^{eq}} \}.
\]

(4.10)

However, equilibration is at most approximately valid for a specific class of observables \( A \) and initial conditions \( \rho(0) \). According to the discussion in ref. [59], if we consider any \( \rho(t) \) that is not completely independent of \( t \), then there exists, at least one \( \rho_{mn}(0) \neq 0 \) with \( \omega := [E_n - E_m]/\hbar \neq 0 \). Now, if we consider an observable such as

\[
A = \frac{|n \rangle \langle m| + |m \rangle \langle n|}{\rho_{mn}(0)},
\]

(4.11)

then

\[
\text{Tr}\{ \rho(t)A \} = 2 \cos \omega t.
\]

(4.12)

This clearly indicates that \( \langle A(t) \rangle \) shows oscillation instead of equilibration. Therefore, it is very clear that equilibration only happens for a restricted class of observables. Since any experimentally
realistic observable has a finite range of possible measurements, we only choose those observables whose measured outcome has a definite range:

\[ \Delta_A = \max(\langle \Psi | A | \Psi \rangle) - \min(\langle \Psi | A | \Psi \rangle) \]

\[ = a_{\text{max}} - a_{\text{min}}, \]

where \( a_{\text{max}} \) and \( a_{\text{min}} \) are the maximum and the minimum eigenvalues of \( A \). It can be proven that for realistic initial states and generic Hamiltonians, the system behaves as it was exactly in the equilibrium state for a vast majority of the time, [59] which implies that the expectation value of reasonable operators (for which \( \Delta_A / \epsilon \leq 10^2 \)) are always close to their equilibrium values:

\[ \text{Prob}[|\text{Tr}\{A\rho(t)\} - \text{Tr}\{A\rho^{eq}\}| \geq \epsilon] \leq \frac{\Delta_A^2}{\epsilon^2} 10^{-O(\epsilon)}, \]

where \( \epsilon \) is the number of degrees of freedom in the system. Thus the probability of measuring a local operator away from its equilibrium value is very small at any finite time. This is how one understands equilibration in quantum mechanics.

**Thermalization**

Thermalization [13, 49, 50] in a sense is a stronger requirement than equilibration. We have seen that the expectation value of local observables equilibrate, but to thermalize they need to equilibrate to their thermal expectation value, namely,

\[ \text{Tr}\{A\rho(t)\} = \text{Tr}\{A e^{-\beta H} \} \]

\[ \text{Tr}\{A\rho(t)\} = \text{Tr}\{A e^{-\beta H} \} \]

(4.16)
for some \( \beta \). The thermal state does not remember any detailed information about the initial state as opposed to the equilibrium state. However, the information about the initial state is not erased by unitary evolution. Since there is slow entanglement spreading in the system, the information becomes inaccessible just from measuring any local operator. This is called decoherence. In particular, for an isolated quantum system to thermalize, any small subsystem will see the rest of the system as its own reservoir. If we consider \( M \) a subsystem and \( N \) as the bath such that \( S = M \cup N \) is the full system, we can write the following condition for thermalization: the system thermalizes if, in the long-time and large-system limit

\[
\rho_M(t) = \rho_{eq}^{M}(t) = \text{Tr}_N\{\rho^{eq}\}
\] (4.17)

for any subsystem \( M \). One way of explaining thermalization is through the eigenstate thermalization hypothesis (ETH), first proposed by Deutsch and Srednicki [13, 49]. ETH asserts that in the case where the system thermalizes, individual excited eigenstates have thermal expectation values. For an eigenstate \( |n\rangle, (H |n\rangle = E_n |n\rangle) \), \( E_n \) is the thermal equilibrium energy \( E_n = \langle H \rangle_{T_n} \) at some temperature \( T_n \) and the state of the subsystem is given by \( \rho_{eq}^{M}(t) = \text{Tr}_N\{|n\rangle \langle n|\} \). Also, the thermal entropy at that temperature is given by the entanglement entropy of \( \rho_{eq}^{M} \) which is the von Neumann entropy

\[
S(M) = -k_B \text{Tr}\{\rho_{eq}^{M} \ln \rho_{eq}^{M}\}.
\] (4.18)

Since the thermodynamic entropy generally scales with the system’s volume, in ETH, the entanglement entropy of an eigenstate also scales with the system’s volume. ETH also yields an ansatz about the matrix element of any local operator in the eigenbasis of the system,

\[
A_{\alpha\beta} = A(E)\delta_{\alpha\beta} + e^{-S(E)/2} f(E, w) R_{\alpha\beta},
\] (4.19)
where $A(E)$ is a smooth function and $S(E)$ is the thermodynamic entropy of the average energy $E = \frac{(E_\alpha + E_\beta)}{2}$. $f(E, w)$ is also a smooth function of $E$ and the energy difference $w = (E_\alpha - E_\beta)$ and $R_{\alpha\beta}$ is random number with zero mean and unit variance. This ansatz for the matrix element has been verified in quite a few models that were assumed to thermalize. Thus ETH introduces single-eigenstate ensembles each consisting of a single eigenstate of the full Hamiltonian. When a system obeys ETH, each of these ensembles can give the thermal expectation value of any local operator.

**Localization**

*Anderson localization*

A large class of systems where the concept of ETH and thermalization fails are the systems that are Anderson-localized [60]. The problem of single-particle localization was introduced by Anderson [60] and can be described by a simple tight-binding Hamiltonian,

$$H = t \sum_{<ij>} (c_i^\dagger c_j + c_i c_j^\dagger) + \sum_i U_i c_i^\dagger c_i,$$

where non-interacting particles hop on a lattice with an amplitude $t$ and $U_i$ is the on-site random potential uniformly distributed in the interval $[\frac{-U}{2}, \frac{U}{2}]$. When the disorder strength $U$ is increased, the nature of the eigenstates changes. Instead of extended Bloch waves, they get localized around some point $R_\alpha$ in the lattice, such that the amplitude of the single-particle wave function has the form, $|\psi_\alpha(r)|^2 \propto \exp\{ -|r - R_\alpha|/\xi \}$. The localization length $\xi$ depends on the disorder strength and energy of the eigenstate. In one and two dimensions, all states are localized even when the disorder is weak, $U << t$. However, in three dimensions we only see localization when the disorder is strong, $U/t > U_c$. In three dimensions at weaker disorder, the states near the band
edges are localized; however, the middle states are extended.

**Many-body localization**

As an extension of Anderson localization for interacting quantum many-body systems, the phenomenon of many-body localization [9, 10] has been introduced in a one-dimensional disordered Heisenberg spin chain. The standard model of many-body localization is the following

$$H = \sum_{n=1}^{L-1} J \vec{S}_n \cdot \vec{S}_{n+1} + \sum_{n=1}^{L} h_n S^z_n, \quad (4.21)$$

where the random magnetic fields $h_n$ are chosen from a uniform distribution of width $W$. In the trivial limit, when the interaction term $(J)$ is zero, then the complete set of conserved, localized operators is given by

$$[H, S^n_z] = 0 = [S^n_z, S^m_z] \quad (4.22)$$

and all the eigenstates of the system are the product of the eigenstates of the $S^n_z$ operator. Now, in the limit where $J/W$ is small, the $\{S^n_z\}$ operators can be dressed to make the pseudospin operators $\{\tau^z_n\}$. These dressed operators are called the "l-bits", and they obey the following property in this limit:

$$[H, \tau^z_n] = 0 = [\tau^z_n, \tau^z_m], \quad (4.23)$$

and each $\{\tau^z_n\}$ is localized.

The current understanding is that for the limit $J/W >> 1$, the system is quantum chaotic, and it thermalizes and therefore no localized l-bits remain. Therefore, there exists a critical $(J/W)_c$, where the system goes from a many-body localized (MBL) phase to a thermal phase through a transient pre-thermal regime. Although, there have been both numerical and renormalization group-
based studies to understand this phase transition, the details are yet to be understood completely [61, 62]. The numerical simulations are restricted to small system sizes which do not actually replicate the asymptotic behavior of this phase transition in large systems, whereas, the analytical renormalization group-based methods mostly just capture phenomenological properties.

Experimental realization

MBL has been experimentally studied recently in ultra-cold atomic and molecular systems (cold atoms, trapped ions, etc). In most of these experiments, the quantum evolution is monitored after a quantum quench.

Bloch’s [63] group studied dynamics starting from an initial charge density wave state (alternated filled and empty particles) in a one-dimensional fermionic gas with a quasi-periodic potential (Hubbard model). From the imbalance $I(t) = \langle |N_{\text{even}} - N_{\text{odd}}|/(N_{\text{even}} - N_{\text{odd}}) \rangle$ measurement, they found that, in the absence of the quasi-periodic potential, imbalance rapidly decays, whereas in the case of MBL a non-vanishing value of the imbalance signifies that the system retained the information about the initial state.

Monroe’s group [64] performed an experiment on trapped ions in one dimension simulating a long-range Ising model with a random transverse field and probing the existence of MBL.

Recently one experiment on a two-dimensional bosonic optical lattice confirmed the existence of MBL in two dimensions [65]. Theoretically [66], it is still an important question whether a stable many-body localized phase can exist in more than one dimension [67]. Numerical studies in more than one dimension are also very limited because of our inability to probe into large system sizes. Phenomenological renormalization group [68–70] studies have not been done in more than one dimension.
Quantum coherence quantifies the amount of superposition a quantum state can have on a given basis. Since there is a difference in the structure of eigenstates of the ergodic and many-body localized systems, we expect them also to differ in terms of their coherences on a given basis. Here, we numerically calculate different measures of quantum coherence in the excited eigenstates of an interacting disordered Hamiltonian as a function of the disorder. We show that quantum coherence can be used as an order parameter to detect the well-studied ergodic to the many-body-localized phase transition. We also perform quantum quench studies to distinguish the behavior of coherence in thermalized and localized phases. We then present a protocol to calculate measurement-based localizable coherence to investigate the thermal and many-body localized phases. The protocol allows one to investigate quantum correlations experimentally in a non-destructive way, in contrast to measures that require tracing out a subsystem, which always destroys coherence and correlation.

Introduction

Advances in experimental realizations of closed quantum many-body systems such as ultra-cold atoms, trapped ions, or superconducting qubits undergoing unitary evolution over long time scales [71–75] have lead to the study of quantum dynamical phenomena like the dynamical quantum phase transitions [76, 77], discrete time crystals [78], and many-body localization (MBL) [79]. One of the main focuses of these studies is to examine the way isolated systems reach thermal
equilibrium. Deutsch [49] and Srednicki [13] discussed the process of thermalization and the eigenstate thermalization hypothesis (ETH) [13] was put forward as a strong criterion for thermalization to occur in closed quantum many-body systems. MBL [9, 10, 50, 52, 69, 80, 81] has emerged as an extension of the much-studied Anderson localization [60], applicable in the case of closed interacting systems. MBL systems fail to thermalize due to the presence of local integrals of motion [68, 70, 82] and hence the MBL eigenstates violate the ETH hypothesis, according to which all the eigenstates of a thermalizing system have to be locally thermal. ETH also postulates that the matrix elements of any local observable $O$, between two eigenstates $i, j$ of the Hamiltonian can be expressed as 

$$
\langle i | O | j \rangle = O(\bar{E}) \delta_{ij} + \exp(-S(\bar{E})/2) f_O(\bar{E}, \omega) R_{ij},
$$

where $\bar{E} \equiv (E_i + E_j)/2$, $\omega = E_j - E_i$, and $S(E)$ is the thermodynamic entropy at energy $E$. It is also important to note that both $O(\bar{E})$ and $f_O(\bar{E}, \omega)$ are smooth functions of their arguments and $R_{ij}$ is a random real or complex variable with zero mean and unit variance.

The effort of keeping a quantum system decoupled from the environment and thus undergoing unitary dynamics is done with the goal of preserving coherence in the many-body wave-function. Coherence quantifies the amount of superposition of a particular state in any fixed basis sets. A rigorous framework for quantum coherence as a resource has been developed recently[83–86]. The study of quantum coherence in closed quantum systems is relevant because quantum coherence is exactly what is responsible for quantum fluctuations and correlations. In a many-body quantum system, local degrees of freedom are described by a tensor product structure (TPS). Coherent superposition of basis states in a TPS results in quantum entanglement and this is why, in recent years, entanglement has been widely studied as a diagnostic tool for quantum phase transitions in many-body systems [87] or as a probe to exotic quantum orders like topological order [14, 88–93]. In the context of the ETH-MBL phase transition in spin chains, entanglement has been used as a useful marker of the transition [94–97]. In quantum many-body dynamics, the nature of the growth of entanglement entropy has been considered as an important tool for characterizing
different dynamical phases. It has been shown that MBL offers slow logarithmic growth while ETH has a linear growth of entanglement entropy [98, 99].

In this paper, we study the role that quantum coherence plays in the MBL-ETH transition. As coherence is a function of the wave function, one should expect that some of its moments should be able to capture any kind of transition. We first show that coherence (in the computational basis) in a high energy eigenstate and its variance due to sample-to-sample fluctuations do indeed signal the MBL-ETH transition. Second, we look at the coherence/decoherence power of dynamics generated by MBL and ETH Hamiltonians. We find that ergodic dynamics induced by ETH has more coherence/decoherence power in a basis that is incompatible with that of the energy, while the dynamics induced by MBL has a low coherence/decoherence power, or, in other words, retain the memory of the initial conditions.

However, quantum coherence does not contain any information about the TPS is, by itself, useless to discriminate the localized versus the unlocalized structure of quantum states. To this end, we exploit the notion of localizable coherence that has recently been put forward in [100]. Localizing coherence to two blocks of spins, we can then compute the coherence in these two blocks as a function of their distance $d(A, B)$, as a coherence-connected correlation function $C_d$. We show that while this quantity does depend on $d$ within the dynamics induced by an MBL Hamiltonian, the ergodic dynamics induced by the ETH Hamiltonian is insensitive to the distance between the two blocks. We finally note that due to the projective nature of coherence measures, they are more suitable to the experimental investigation than entanglement entropy, making our results amenable to testing beyond numerical computations.
Quantum coherence is a notion relative to a specific basis. A (Hermitian) operator is called incoherent if it is diagonal in a particular basis $B = \{|i\rangle\}$. We call $I_B$ the set of incoherent states in $B$. As an example, the Gibbs state is incoherent in the energy eigenbasis $E$ since its completely diagonal in it. Every completely dephased operator in $B$ is also incoherent in that basis. The set $I_B$ is given by just any probability distribution over $\pi_i$, where $\pi_i = |i\rangle \langle i|$ are the projectors in the basis $B$. Thus we can say that any completely dephased operator $X \in I_B$ can be expressed as $X = \sum_i p_i \pi_i$. Therefore, a coherence measure for a state $\rho$ is the quantity

$$C_B(l_p)(\rho) := \|\rho - D_B(\rho)\|_{l_p},$$

(5.1)

where $D_B(\rho) = \sum_i \pi_i \rho \pi_i$ is the completely dephased state and the measure is based on the $l_p$ norm. According to this definition, a state $\rho$ has zero coherence, $C_B(\rho) = 0$, if and only if $\rho \in I_B$. We use two different matrix norms as measure for coherence [83, 86]. Using the $l_1$ norm, coherence is expressed as the sum of all the off-diagonal elements of the quantum state, that is, $C_B(l_1)(\rho) = \sum_{i \neq j} |\langle i | \rho | j \rangle|$. Similarly, using the $l_2$ norm measure we obtain $C_B(l_2)(\rho) = \sum_{i \neq j} |\langle i | \rho | j \rangle|^2$.

Another way of measuring coherence in a basis $B$, which we also employ, is through the Kullback-Leibler divergence from the completely dephased state,

$$C_B^{KL}(\rho) := S(D_B(\rho)) - S(\rho),$$

(5.2)

where $S(\rho)$ indicates the entropy of the state $\rho$. 
Quantum Coherence in disordered spin chain

In order to study the role of coherence in the ETH-MBL transition, we consider the disordered Heisenberg 1/2-spin chain [101] described by the Hamiltonian

\[ H = \sum_{i=1}^{N} J (S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + S^z_i S^z_{i+1}) + h_i S^z_i + h_x S^x_i \]  \hspace{1cm} (5.3)

with periodic boundary conditions. We set \( J = 1 \) in the numerical computation. The static random fields \( h_i \) are chosen from a uniform distribution in \([-W, W]\). A transverse constant field \( h_x = 0.1 \) is introduced to break the total \( S_z \) conservation so that no sector with conserved quantities that break ergodicity explicitly exists [96, 102].

\textit{ETH-MBL transition point from level statistics}

The model Hamiltonian in Eq. (5.3) without the small transverse field \((h_x)\) is known to undergo an ergodic to MBL transition for strong disorder [10, 94, 95]. Here, in order to locate the transition point between the eigenstate thermalization hypothesis (ETH) to many-body localization (MBL) regimes, we diagonalize the full Hamiltonian in Eq.5.3 and calculate the energy level spacing \( \delta_n = |E^n_\alpha - E^{n+1}_\alpha| \), where \( E^n_\alpha \) is the energy of the \( n \)-th eigenstate in the \( \alpha \)-th disorder sample. The ratio of the adjacent gaps or level spacings \( r^n_\alpha = \min\{\delta^n_\alpha, \delta^{n+1}_\alpha\}/\max\{\delta^n_\alpha, \delta^{n+1}_\alpha\} \) is averaged over the samples to yield \( \langle r_{\text{avg}} \rangle \). In random matrix theory [103, 104], when the statistical distribution of level spacing follows the the predictions of the Gaussian Orthogonal Ensemble (GOE) \( \langle r_{\text{avg}} \rangle \) converges to \( r_{\text{GOE}} \approx 0.53 \) for \( N \to \infty \). We find that, deep in the ergodic phase, the average ratio \( \langle r_{\text{avg}} \rangle \) does approach the GOE (Gaussian Orthogonal Ensemble) value (see Fig. 5.1). On the other hand, deep in the localized phase, it reaches the value derived from a Poisson distribution of level spacings, and \( \langle r_{\text{avg}} \rangle \) converges to \( r_{\text{Poisson}} \approx 0.39 \). Finite-size scaling gives an estimate of the
Figure 5.1: Average level spacing ratio $\langle r_{\text{avg}} \rangle$ versus the disorder strength $W$ for different system sizes ($N$ identifies the number of spins in the chain). We obtain $\langle r_{\text{avg}} \rangle$ by first averaging over 10 eigenstates near the middle of the spectrum for each disorder realization and then averaging over different realizations. We employed 8000 disorder samples for $N = 8, 9$, 4000 for $N = 10, 11$, and 1000 for $N = 12$.

critical value of disorder to drive the transition from ETH to MBL at $W \approx 3.5$.

ETH-MBL transition point from quantum coherence

We now show that one can also extract information about this transition from measures of coherence. Recently [105], it was shown that the escape probability and dynamical conductivity are connected by measures of coherence that can effectively probe the localization transition. Since the ETH and MBL phases are characterized by the different structures of the high-energy eigenstates,
we start by evaluating the coherence present in an eigenstate in the middle of the spectrum. As a basis, we choose the computational (z) basis for the tensor product of the spins as the preferred basis in which one can observe quantum fluctuations. Here we calculate coherence using $l_1$. The disorder-averaged normalized coherence $\langle \text{Coh} \rangle = \langle C_{B,J_1} (\rho) \rangle / (2^N - 1)$ for different system sizes feature a crossing at a disorder value around $W = 2.5$, see Fig. 5.2a. The standard deviation of the normalized coherence due to sample-to-sample variations also show critical behavior around $W = 2.5$, see inset in Fig. 5.2a.

Next, we calculate the average Kullback-Leibler divergence between the completely dephased state and a high-energy eigenstate, see Eq. (5.2). In this case, $\langle C_{KL}^B (\rho) \rangle$ does not reveal any crossing point for different system sizes, see Fig. 5.2b. However, similarly to $\langle C_{B,J_1} (\rho) \rangle$ in the inset of Fig. 5.2a, the standard deviation does show a well-defined peak, but in this case the peak is centered at $W = 3.2$ for the system sizes we investigated. Although a peak is much easier to follow and employ for finite-size scaling analyzes than a line crossing (Fig. 5.1), larger systems would nevertheless be for an accurate estimate of the transition point location.

**Coherence after a quantum quench**

Now consider a situation away from equilibrium, e.g., a quantum quench. After initial preparation, we let the state evolve unitarily under the Hamiltonian in Eq. (5.3) for different strengths of the disorder $W$. In the ergodic phase, the long-time evolution should take the state to equilibrate as a thermal ensemble of the eigenstates of the Hamiltonian. Since these are very delocalized in the eigenbasis of the local spins – that is, in the computational basis – we expect that evolution under the ETH Hamiltonian will have more of both coherence and decoherence power than that of the MBL Hamiltonian. We prepare the initial state as either (i) the maximally coherent state $|\Psi\rangle = d^{-1/2} \sum_{i=1}^{d} |i\rangle$ (in the computational basis), in which case the time evolution will decohere
Figure 5.2: Average normalized coherences: (a) $\langle C_{B,l} (\rho) \rangle$ and (b) $\langle C_{B}^{KL} (\rho) \rangle$ of an excited state as a function of disorder for different chain sizes. We use the eigenstate exactly at the middle of the spectrum for each case. The data are averaged over 8000 disorder samples for $N = 8, 9$, 4000 for $N = 10, 11$, and 1000 for $N = 12, 13$. The inset shows the standard deviation of the normalized coherence as a function of disorder for the specific eigenstates mentioned earlier.
Figure 5.3: Time evolution of the average normalized coherence \( \langle C_{B,l} (\rho) / (2^N - 1) \rangle \) starting from: (a) the maximal coherent state \( |\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle \) in the computational basis, (b) the state \( |\Psi\rangle = |\uparrow\uparrow \ldots \uparrow\rangle \), and (c) the state \( |\Psi\rangle = |\uparrow\downarrow\uparrow\downarrow \ldots \rangle \). Here, \( N = 12 \) and 200 disorder realizations are employed.

The different behaviors of coherence and decoherence induced by the ETH and MBL Hamiltonians are strikingly different. The ETH Hamiltonian decoheres in a more efficient way to a very coherent state, and, at the same time, it is capable of building up more coherence from an incoherent state.

Hence by studying the dynamics of quantum coherence for different initial states, we confirm quite clearly that the MBL phase retains the memory of the initial state [106–108].
Localizable coherence

In a quantum many-body system the Hamiltonian is the sum of local terms, and local terms have support on local Hilbert spaces, e.g., the spins. The total Hilbert space \( \mathcal{H} = \bigotimes_i \mathcal{H}_i \) is the tensor product of the local Hilbert spaces. In other words, quantum many-body systems create a tensor product structure. Following Ref. [100], we want to quantify the coherence that is localizable in a subsystem \( S \) comprising a subset of all the spins. For this purpose, we adopt the bipartition \( \mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R \) ("system" and "rest") with \( \dim(\mathcal{H}) = d = d_S d_R \). We then localize coherence in the subsystem \( S \) by performing a measurement on \( R \). The latter step consists of the following. Let \( B_R := \{ |i\rangle \}_{i=1}^{d_R} \) be some preferred basis in the subsystem, where \( \omega_i := |i\rangle \langle i| \) form a complete set of rank-one projectors over \( \mathcal{H}_R \). A projective measurement on \( \mathcal{H}_R \) transforms a density matrix \( \rho \) to a tensor product state of the form

\[
\rho'_i = \frac{\text{Tr}_R (\rho I_S \otimes \omega_i)}{\text{Tr} (\rho I_S \otimes \omega_i)} \otimes \omega_i. \tag{5.4}
\]

Each \( \rho_i \) is obtained with the probability \( p_i = \text{Tr} (\rho I_S \otimes \omega_i) \). One can then trace out the system \( R \) without having the state decohere and compute the coherence in \( S \) in any basis of the system \( B_S \), now described by

\[
\rho'_{S,i} = \text{Tr}_R \rho'_i = \frac{\text{Tr}_R (\rho \omega_i)}{\text{Tr}(\rho \omega_i)}. \tag{5.5}
\]

Finally, the average coherence in the post-measurement states of the the system can be defined as

\[
C_{\text{avg}}(\rho) := \sum_{i=1}^{d_R} p_i C_{B_S}(\rho'_{S,i}). \tag{5.6}
\]

The calculation of the above quantity is carried out using matrix product states (MPS) [17]. The protocol of measurement on MPS was first discussed by Popp and coworkers [109] in the context of localizable entanglement. Here we extend that formalism and calculate the average local coherence.
for a particular subsystem.

We again consider the disordered Heisenberg spin 1/2 in Eq. (5.3) as a model Hamiltonian. We prepare the initial state in an incoherent state and let it evolve. For the time-evolved state, we calculate the localizable coherence in a subsystem consisting of two blocks \((A, B)\) each consisting of two spins placed at a distance \(d(A, B)\) from each other. Our goal is to show that whereas the ergodic delocalized phase should be insensitive to \(d(A, B)\), in the MBL phase the localizable coherence should be higher when the two blocks are closer together. In order to localize coherence in the \((A, B)\) blocks, we perform projective measurements in the rest of the system. Let us describe the procedure for the projection in the MPS formalism. Here we consider two blocks to be separated by three spins, \(d(A, B) = 3\), but we can use similar methods for other separations. The exact quantum state of the \(N\)-spin system is represented by an MPS,

\[
|\Psi\rangle = \sum_{x_N=\uparrow,\downarrow} \cdots \sum_{x_1=\uparrow,\downarrow} M_N^{x_N} \cdots M_1^{x_1} |x_N \cdots x_1\rangle.
\]  

(5.7)

Here we will consider the localized coherence between two blocks each consisting of two spins and separated by distance \(d(A, B) = 3\). Block A consists of matrices \(M_N^{x_N/2-2}\) and \(M_N^{x_N/2-1}\). Block B consists of matrices \(M_N^{x_N/2+2}\) and \(M_N^{x_N/2+3}\). We calculate all possible projectors on the rest of the system which is given by the tuple \(\{s\} = \{x_N, x_{N-1}, \cdots, x_1\} - \{x_{N/2-2}, x_{N/2-1}\} - \{x_{N/2+2}, x_{N/2+3}\}\), consisting of \(N - 4\) spins. Therefore, we have a total of \(2^{N-4}\) projectors. Thus, the pure state after any projection can be written as

\[
|\phi_{\{s\}}\rangle = \langle \{s\} | \Psi \rangle
\]  

(5.8)

\[
= \sum_{x_{N/2-2}=\uparrow,\downarrow} \sum_{x_{N/2-1}=\uparrow,\downarrow} \sum_{x_{N/2+2}=\uparrow,\downarrow} \sum_{x_{N/2+3}=\uparrow,\downarrow} R \cdot M_N^{x_N/2+3} \cdot M_N^{x_N/2+2} \cdot Q \cdot M_N^{x_N/2-1} \cdot M_N^{x_N/2-2} \cdot P \times |x_{N/2+3}, x_{N/2+2}\rangle |x_{N/2-1}, x_{N/2-2}\rangle,
\]  

(5.9)
where the three auxiliary matrices $R$, $Q$, and $P$ are defined as following:

$$R = \sum_{\{x_N, \ldots, x_{N/2+4}\}} M_{x_N}^x \cdot M_{x_N-1}^{x_N} \cdots M_{x_{N/2+4}}^{x_{N/2+4}}. \quad (5.10)$$

$$Q = \sum_{\{x_{N/2+1}, x_{N/2}\}} M_{x_{N/2+1}}^{x_{N/2+1}} \cdot M_{x_{N/2}}^{x_{N/2}}. \quad (5.11)$$

and

$$P = \sum_{\{x_{N/2-3}, \ldots, x_1\}} M_{x_{N/2-3}}^{x_{N/2-3}} \cdots M_{x_1}^{x_1}. \quad (5.12)$$

$R$, $Q$, and $P$ are computed by carrying out the matrix multiplications for each tuple $\{x_N, \ldots, x_{N/2+4}\} = s_1$, $\{x_{N/2+1}, x_{N/2}\} = s_2$, and $\{x_{N/2-3}, \ldots, x_1\} = s_3$ respectively. There are total $2^{N-4}$ possible combinations for $s_1$, $s_2$, and $s_3$ combined, each of which corresponds to a different projector. The probability of a specific projector is then given by

$$\Pr(\{s\}) = \langle \phi_{\{s\}} | \phi_{\{s\}} \rangle = |\langle \{s\} | \Psi \rangle|^2, \quad (5.13)$$

and the density matrix corresponding to the projected pure state is

$$\rho(\{s\}) = \frac{1}{\Pr(\{s\})} |\phi_{\{s\}}\rangle \langle \phi_{\{s\}}|. \quad (5.14)$$

The average local coherence of the two blocks is then computed according to the expression

$$C_{\ell_2}(\text{avg}) = \sum_{i=1}^{2^{N-4}} \Pr_i(\{s\}) \times C_{\ell_2}(\rho_i(\{s\})). \quad (5.15)$$

To obtain the correlation of local coherence among these two-spin blocks one needs to subtract the effect of these individual blocks. An an effective way to do that is to calculate the local coherence of the two-spin blocks in different locations of the disordered spin chain, while considering the ap-
Figure 5.4: Average localizable coherence after a quantum quench with (a) the ETH Hamiltonian ($W = 1$) and (b) the MBL Hamiltonian ($W = 10$). The quantity $\langle \text{Coh}(d) \rangle$ is computed for two blocks $A$ and $B$ of two spins each at different distance $d(A, B) = 3, 5, \ldots$. The total number of spins is $N = 14$. The initial state is the product state $|\downarrow\downarrow \cdots \downarrow\rangle$. The $l_2$ norm of coherence is evaluated on the computational basis. The results represent an average of over 480 disordered samples. In the case of the MBL Hamiltonian (b) we perform the quench for a longer time to specify the nature of distance dependence of average localizable coherence over longer timescale.
appropriate set of projective measurements on the respective Hilbert spaces, and then take an average over the results. One then subtracts the calculated average coherence of the individual blocks from the local coherence of the two two-spin blocks to define \( \text{Coh}(d) \) as localizable coherence, namely,

\[
\text{Coh}(d) = \text{C}_{l_2}(\text{avg}) - \frac{1}{4} \sum_{i=1}^{4} \text{C}_{l_2}(p_i).
\]

Here, \( \text{C}_{l_2}(p_i) \) refers to the coherence of the individual two-spin blocks in several different locations along the spin chain.

In order to compute the time evolution after the quantum quench we utilize the time-evolving block decimation (TEBD) method [18, 110]. For the TEBD, we have used a second-order Suzuki-Trotter decomposition with a time step \( \delta t = 0.1 \) and open boundary condition. We let the bond dimension increase to the maximum \( D = 2^{N/2} \), which in the case of 5.4 is 128, during time evolution. The time evolution reveals an important feature of the local structure of the wave function in the ETH or MBL phase. In ETH the many-body wave function is extended, resulting in distance-independent behavior of the average local coherence between different blocks, which is clearly shown in Fig. 5.4a. In contrast, in MBL we can see that the average local coherence between two blocks decreases with distance when they are farther apart than the localization length (see Fig. 5.4b). Considering these results, we can say that the maximum local coherence of two blocks is higher in ETH than in the MBL phase. Since all the coherence has been measured on the computational basis, the lower local coherence in MBL indicates the localized structure of the wave function in the Hilbert space.
Conclusions and outlook

In this chapter, we showed that measures of coherence are effective in distinguishing the ergodic (ETH) and many-body localized (MBL) phases and their dynamics after a quantum quench. In particular, we showed that the standard deviation of the coherence and the entropy of coherence for a high-energy eigenstate mark the localization transition. We also showed that the time evolution of the coherence characterizes the different dynamics of the two phases. We then utilized the notion of correlation of coherence based on the localizable coherence introduced in Ref. [100], to show that the ergodic phase is insensitive to the distance between the subsystems, while it decays for the localized phase.

We conclude that localizable coherence can be a useful instrument in the investigation of quantum many-body systems. For example, one could look at the fluctuations of this quantity as a probe for scrambling and the onset of chaotic behavior in a closed quantum system [111–114]. Moreover, one can think of studying in this way topological phases, as the coherence localizable in the topological degrees of freedom should be more robust after a quantum quench [115] compared to the one localizable to local topologically trivial subsystems. Finally, as coherence is a more experimentally accessible quantity [116–118] compared to other quantities used to probe into quantum many-body dynamics such as entanglement entropy [119, 120], these results should be of wide interest to the community of quantum many-body physics.
CHAPTER 6: SUMMARY AND FUTURE DIRECTION

List of relevant publications


Providing a physical platform for topological quantum computing is a long-standing challenge. The usual way is to look for the existence of Majorana zero modes in topological superconductors, which is still an experimental challenge due to the similar behavior with other low energy Andreev bound states in such systems. In our work, we showed that it is possible to build a “nanowire network” from a collection of physical Majorana zero-mode carrying wires, by allowing them to hybridize in every sublattice of a honeycomb or a brick-wall lattice. We have identified the symmetry class and the topological index for such a multi-wire topological Majorana junction which was constructed by several time-reversal symmetric Kitaev wires.

Next, we have demonstrated numerically by constructing a tight-binding model of the nanowire network, that a Kekulé perturbation allows to include a vortex inside the two-dimensional lattice in any position by controlling the applied voltage. We have also provided experimental parameters for the realization of such important vortex states which carry the ”logical Majorana zero mode” and therefore allow them to perform braiding adiabatically. In future work, we would like to show the braiding operation happening in an adiabatic manner between the Majorana zero modes inside the vortices.
In the next work, we have demonstrated that the coherence of an excited eigenstate in the computational basis can carry a lot of information about the state and can be used as an order parameter to access the ergodic to a many-body localization phase transition. We have also shown by quantum quench studies that the many-body localized phase can protect the coherence information of the initial state in the computational basis state.

Next, we have developed a protocol to calculate localized coherence with the help of the MPS. Such measurement base protocol is much more accessible in experiments than measuring any entanglement entropy. This localized coherence-based correlation can then be used to inquire properties of quantum many-body states. In the future, we will try to explore how this coherence-based method might be useful for providing knowledge for the time-periodic disordered Floquet system.
APPENDIX A: KWANT IMPLEMENTATION AND NUMERICAL SIMULATION DETAILS OF MAJORANA NETWORK
Simulation of 3-wire and 5-wire junction

We use "Kwant" [44], which is a numerical package in python. "Kwant" is capable of representing tight-binding Hamiltonians by creating a graph structure that corresponds to the sparse matrix associated with the Hamiltonian. Each site of the tight-binding model works as a node in the graph and hopping matrix elements are denoted by edges. For simulating the 3 and 5-wire junction, we use the general Hamiltonian in Eq. (3.15). Each individual wire of the junction described by a time-reversal symmetric Kitaev chain has the choice of polarity as mentioned in Fig. 3.3. The onsite and hopping matrix element for the $\alpha$th wire is given by the following:

$$\langle l | H_{\alpha} | l \rangle = -\mu \tau_z \quad \langle l | H_{\alpha} | l + 1 \rangle = -(t \tau_z + \eta_\alpha i \Delta \tau_y). \quad (A.1)$$

For any hopping element among the junction sites $\alpha, \beta \in \text{junction}$, the hopping matrix element is

$$\langle \alpha | H_{\text{junction}} | \beta \rangle = -\Gamma_{\alpha,\beta} \tau_z. \quad (A.2)$$

Figure A.1: Kwant implementation of the BdG Hamiltonian for a 3-wire junction. Here the blue dots represent the node in the graph and hopping matrix elements are denoted by the orange arrows. The black arrows represent the hopping matrix elements of the junction.
Kekulé modulation and vortex in the brickwall lattice

To imprint the Kekulé modulation in the brickwall lattice as described in Fig. 3.9, we first transform the brickwall lattice to an equivalent honeycomb lattice. We then label one of the sublattices of the honeycomb lattice with integer coordinates as the following Fig.A.2. The Kekulé modulation

![Honeycomb lattice diagram](image)

Figure A.2: A honeycomb lattice where the "A" sublattice points are represented by the green dots. These are marked by integer coordinates with respect to an arbitrarily chosen center $(0, 0)$. Every one of these sublattice points is connected to the nearest neighbor, which is the other sublattice, by the vectors $s_\alpha (\alpha = x, y, z)$.

according to Eq. (3.21) is expressed as

$$\delta \mu_{K,\alpha}^{\text{Kekulé}} = \mu_K \cos (\varphi_{r,\alpha}).$$

(A.3)
where

$$\varphi_{r, \alpha} = K_+ \cdot s_\alpha + (K_+ - K_-) \cdot r.$$ \hspace{1cm} (A.4)

The Brillouin zone of the honeycomb lattice has two types of corner points given as

$$K_\pm = \frac{4\pi}{3\sqrt{3}} \left[ \begin{array}{c} \pm 1 \\ 0 \end{array} \right].$$ \hspace{1cm} (A.5)

The real coordinate of the sublattice \((r)\) can be expressed in terms of the integer coordinate tuple \((m, n)\) in Fig.A.2 as

$$r = \left( \begin{array}{c} \frac{\sqrt{3}}{2} m \\ \frac{3}{2} n \end{array} \right).$$ \hspace{1cm} (A.6)

Therefore, the three phases along the three nearest neighbor vectors of the ”A” sublattice points are the following:

$$\varphi_{m,n,\alpha=x} = \frac{2\pi}{3} + \frac{4\pi}{3} m$$ \hspace{1cm} (A.7)

$$\varphi_{m,n,\alpha=y} = -\frac{2\pi}{3} + \frac{4\pi}{3} m$$ \hspace{1cm} (A.8)

$$\varphi_{m,n,\alpha=z} = \frac{4\pi}{3} m.$$ \hspace{1cm} (A.9)

Now once the above equations are iterated over all the sublattice coordinates \((m, n)\), it generates the phases needed for the Kekulé modulation. As an example, for the point \((m = 0, n = 0)\), the chemical potentials along the three nearest neighboring vectors are,

$$\mu_0 + \mu_K \cos(\varphi_{m=0,n=0, \alpha = x}) = \mu_0 + \mu_K \cos\left(\frac{2\pi}{3}\right) = \mu_0 - \frac{\mu_K}{2}$$ \hspace{1cm} (A.10)

$$\mu_0 + \mu_K \cos(\varphi_{m=0,n=0, \alpha = y}) = \mu_0 + \mu_K \cos\left(-\frac{2\pi}{3}\right) = \mu_0 - \frac{\mu_K}{2}$$ \hspace{1cm} (A.11)

$$\mu_0 + \mu_K \cos(\varphi_{m=0,n=0, \alpha = z}) = \mu_0 + \mu_K \cos(0) = \mu_0 + \mu_K.$$ \hspace{1cm} (A.12)
APPENDIX B: LOCALIZABLE COHERENCE CALCULATION WITH
MATRIX PRODUCT STATES (MPS)
Localizable coherence of two spins

We start with the MPS representation of the quantum state,

$$|\Psi\rangle = \sum_{x_N=\uparrow,\downarrow} \sum_{x_{N-1}=\uparrow,\downarrow} \cdots \sum_{x_2=\uparrow,\downarrow} \sum_{x_1=\uparrow,\downarrow} M_N^{x_N} M_{N-1}^{x_{N-1}} \cdots M_2^{x_2} M_1^{x_1} |x_N x_{N-1} \cdots x_2 x_1\rangle. \quad (B.1)$$

Now we say that the projectors in the $C$ subspace are given by $P_i$’s. The action of a single projector on the MPS is the following:

$$P |\Psi\rangle = \sum_{x_N=\uparrow,\downarrow} \sum_{x_1=\uparrow,\downarrow} M_N^{x_N} Q M_1^{x_1} |x_N\rangle \otimes |P\rangle \otimes |x_1\rangle, \quad (B.2)$$

where

$$Q = \sum_{x_{N-1},\cdots,x_2} M_{N-1}^{x_{N-1}} \cdots M_2^{x_2} \quad (B.3)$$

is a $D \times D$ matrix corresponding to the projected state $|P\rangle$. Each tuple $\{x_{N-1}, \cdots, x_2\}$ corresponds to a projector. So the total number of possible projectors is $2^{N-2}$. The density matrix of the projected state of two spins is given by

$$\rho = P |\Psi\rangle \langle \Psi| P = \sum_{x_N=\uparrow,\downarrow} \sum_{x_1=\uparrow,\downarrow} \sum_{\tilde{x}_N=\uparrow,\downarrow} \sum_{\tilde{x}_1=\uparrow,\downarrow} M_N^{x_N} Q M_1^{x_1} M_1^{\tilde{x}_1} Q^\dagger M_N^{\tilde{x}_N} |x_N \tilde{x}_N \tilde{x}_1\rangle \langle \tilde{x}_N \tilde{x}_1|. \quad (B.4)$$

We thus get a $4 \times 4$ matrix for which we can calculate the coherence. Now we can choose a satisfactory number of projectors from the available $2^{N-2}$. Then the total average coherence is

$$\text{Coh}(\Psi) = \sum_i q_i \cdot \text{Coh}(\rho_{AB}^{(i)}), \quad (B.5)$$

where $q_i = \langle \Psi | P_i | \Psi \rangle$ and $\rho_{AB}^{(i)}$ is the normalized state after measurement.
Localizable coherence of two 2-spin blocks

The exact quantum state of the N-spin system is represented by the so-called matrix product state (MPS),

$$|\Psi\rangle = \sum_{x_N=0,1} \sum_{x_{N-1}=0,1} \cdots \sum_{x_2=0,1} \sum_{x_1=0,1} M_N^{x_N} M_{N-1}^{x_{N-1}} \cdots M_2^{x_2} M_1^{x_1} |x_N x_{N-1} \cdots x_2 x_1\rangle.$$  \hspace{1cm} (B.6)

Here we will consider the localized coherence between two blocks, each consisting of two spins and separated by distance 3 \((d(A, B) = 3)\). The block A consists of spins \(M_N^{\frac{x_N-2}{2}}\) and \(M_{\frac{x_N-1}{2}}\). The block B consists of spins \(M_N^{\frac{x_N+2}{2}}\) and \(M_{\frac{x_N+3}{2}}\). We calculate all possible projectors on the rest of the system which is given by the \(N-4\) tuple \(\{s\} = \{x_N, x_{N-1}, \cdots, x_1\} - \{x_N-2, x_{N-1}\} - \{x_N+2, x_{N+3}\}\). Therefore, we have a total of \(2^{N-4}\) projectors. The pure state of the two 2-spin blocks after a local projective measurement is done on the subsystem is given by

$$|\phi_{\{s\}}\rangle = \langle\{s\}|\Psi\rangle =$$

$$\sum_{x_N-2=0,1} \sum_{x_{N-1}=0,1} \sum_{x_{N+2}=0,1} \sum_{x_3=0,1} M_N^{x_N} M_{N-1}^{x_{N-1}} \cdots M_2^{x_2} M_1^{x_1}$$

$$|x_N+3, x_{N+2}\rangle |x_N-1, x_{N-2}\rangle.$$  \hspace{1cm} (B.7)

Now we define three matrices \(R, Q, P\) as following:

$$R = \sum_{x_N, \cdots, x_N/2+4} M_N^{x_N} M_{N-1}^{x_{N-1}} \cdots M_{N/2+4}^{x_{N/2+4}}.$$  \hspace{1cm} (B.8)

$$Q = \sum_{x_{N/2+1}, x_{N/2}} M_{x_N/2+1}^{x_N/2} M_N^{x_N/2}.$$  \hspace{1cm} (B.9)

$$P = \sum_{x_{N/2-3}, \cdots, x_1} M_N^{x_N/2-3} \cdots M_1^{x_1}.$$  \hspace{1cm} (B.10)
where \( \{x_N, \cdots, x_{N/2+4}\} = s1, \{x_{N/2+1}, x_{N/2}\} = s2 \) and \( \{x_{N/2-3}, \cdots, x_1\} = s3 \) are three tuples of 0 and 1. There are total \( 2^{N-4} \) possible combinations for \( s1, s2, \) and \( s3, \) each of which corresponds to a different projector. So the pure state after any projection can be written as

\[
|\phi_{\{s\}}\rangle = \langle\{s\} | \Psi \rangle = \sum_{x_N/2-2=0,1}^{x_N/2+2} \sum_{x_N/2-1=0,1}^{x_N/2+1} \sum_{x_N/2+3=0,1}^{x_N/2+3} R \cdot M_{x_N/2+3}^{x_N/2+3} M_{x_N/2+2}^{x_N/2+2} \cdot Q \cdot M_{x_N/2+1}^{x_N/2+1} M_{x_N/2+2}^{x_N/2+2} \cdot P \cdot |x_N/2+3, x_N/2+2\rangle \langle x_N/2-1, x_N/2-2| . \tag{B.11}
\]

The probability of the specific projector is then given by

\[
Pr(\{s\}) = \langle \phi_{\{s\}} | \phi_{\{s\}} \rangle = |\langle \{s\} | \Psi \rangle|^2 . \tag{B.12}
\]

Also, the density matrix corresponding to the projected pure state is

\[
\rho(\{s\}) = \frac{1}{Pr(\{s\})} |\phi_{\{s\}}\rangle \langle \phi_{\{s\}}| . \tag{B.13}
\]

The average localizable coherence of the two blocks is then given by

\[
C_{L2}(avg) = \sum_{i=1}^{2^{N-4}} Pr_i(\{s\}) \times Coh_{L2}(\rho_i(\{s\})) . \tag{B.14}
\]

Algorithm to implement the calculation of localizable coherence with MPS
Algorithm 1: To calculate localizable coherence

Result: avg. localizable coherence of two blocks of 2-spins
Cohbl = 0.d0;
for (subspace 1:)
  for (subspace 2:)
    for (subspace 3:)
      Calculate the matrix R;
      Calculate the matrix Q;
      Calculate the matrix P;
      Calculate the projected state vector: $|\phi_{\{s\}}\rangle = \langle\{s\}|\Psi\rangle$;
      Calculate $Pr(\{s\}) = \langle\phi_{\{s\}}|\phi_{\{s\}}\rangle = |\langle\{s\}|\Psi\rangle|^2$;
      Calculate $\rho(\{s\}) = \frac{1}{Pr(\{s\})}|\phi_{\{s\}}\rangle\langle\phi_{\{s\}}|$;
      $C_{L2} = \sum_{i\neq j}|\rho_{ij}(\{s\})|^2$;
      Cohbl = Cohbl + Pr . $C_{L2}$;
LIST OF REFERENCES


117. Girolami, D. Observable Measure of Quantum Coherence in Finite Dimensional Systems. 

