MANY-BODY LOCALIZATION AND
TENSOR NETWORKS

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DISSERTATION
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Abstract

This thesis is focused on many-body localization (MBL) and the development of algorithms using the tensor networks representation for many-body localized systems. Chapter 1 is a detailed discussion on the MBL phenomenon. Chapter 2 gives an introduction to the numerical techniques that are frequently used in studying many-body quantum systems. Chapter 3 studies the shift-and-invert matrix product state method for obtaining highly excited states of MBL systems. Chapter 4 studies an efficient full diagonalization method using Wegner unitary gates. Chapter 5 studies the distribution of the entanglement entropy in the MBL-ergodic transition region. Chapter 6 studies the the influence of pseudo-spin $SU(2)$ symmetry on the MBL phase. Chapter 7 is a side project that studies the influence of the duality-twisted boundary conditions on the critical twist defect chains.

The MBL-ergodic transition is a dynamical phase transition which happens at finite energy density for a disordered and isolated many-body interacting system. It is a natural extension of Anderson localization where the localized phase survives the inter-particle interaction. In Chapter 1, we describe its relation to quantum thermalization, typical lattice models that harbor a MBL phase, MBL system’s phenomenological description, the characteristics of the MBL phase, experimental studies of MBL phenomenon in 1D and higher dimensions, the latest developments and the open questions on the nature of the MBL-ergodic transition.

In Chapter 2, we provide a short but self-contained discussion of basic numerical methods that are frequently used in studying MBL physics. We mainly focus on the exact diagonalization methods and the matrix product state (MPS) representation, and explain their advantages and disadvantages.

In Chapter 3, because obtaining the interior eigenstates of MBL Hamiltonians is a key step to studying the MBL phases and the transitions, we develop algorithms that can capture individual excited states to high fidelity. Using the fact that eigenstates of many-body localized systems have area-law entanglement and can therefore be efficiently represented as a matrix product state (MPS), we designed two algorithms that can generate excited states in the MPS representation, and use them to test the basic properties of MBL in the regime of large one-dimensional random field Heisenberg chains that were previously inaccessible due to the limitations of exact diagonalization (ED).
In Chapter 4, we investigate an efficient way to diagonalize a fully many-body localized (FMBL) Hamiltonian. Using the Wegner flow technique for subsystems, we constructively build unitary gates that can greedily transform a local part of the FMBL Hamiltonian with the aim of lowering its average energy variance. Applying the Wegner unitary successively can make the system “flow” towards the diagonalized form. We find that the performance of this method is mainly controlled by the length of each individual Wegner unitary gate, and gets better with increasing length of the gate. We compare the performance of this constructive method with previous methods based on quasi-Newtonian optimization methods, and find that they have similar performance, while our constructive method is far more efficient. We also comment the possibility of constructing a tensor network state that resembles a multi-scale entanglement renormalization ansatz (MERA) using this constructive method.

In Chapter 5, using strong subadditivity (SSA) theorem, we develop two order parameters – cut-averaged entanglement entropy (CAEE) and its slope (SCAEE), and show that they can be used to directly identify the volume or area law scaling in single eigenstates. We study the distribution of the SCAEE over disorder realizations. This distribution appears Gaussian at weak disorder, while on the MBL side, the distribution of the SCAEE is peaked at zero slope and has an exponential tail. In the critical regime we find that the distribution of the SCAEE is bimodal both over multiple disorder realizations as well as for single disorder realizations. The variance of the SCAEE distribution in the transition region seems to grow with system size when considered over disorder realizations. Our system sizes are too small to pin down its maximal value, but they are consistent with (among other possibilities) the maximal variance possible which would lead to half the states having zero SCAEE and half having maximal SCAEE. This scenario would lead to an entanglement entropy at the transition which scales as a volume law with half its thermal value.

In Chapter 6, we consider the strongly disordered one-dimensional Hubbard model with spin disorder, which, as we argue, cannot be categorized as a conventional MBL phase. Though the spin rotation $SU(2)$ symmetry is broken by the spin disorder, this model still preserves the pseudo-spin $SU(2)$ symmetry under periodic boundary conditions. On the theoretical side, using the pseudo-spin algebra we show that a significant number of the excited states at any disorder strength have logarithmic correction to their von Neumann entanglement entropy, which violates the area-law entanglement for a typical MBL phase. A common feature of this group of excited states is that they usually have far more double occupancies than single occupancies. On the numerical side, we studied the time evolution after quantum quench from two extreme cases of product states – all single occupancies at quarter filling, and all double occupancies at half filling. We find in the former case entanglement entropy behaves as in a typical MBL system, while the latter is clearly delocalized, which suggests the existence of incomplete set of local integrals of motion. With the
above evidence, it is convincing that this model provides a playground for studying a non-ergodic, non-MBL phase, and its relation to continuous $SU(2)$ symmetry.

Chapter 7 deviates from the common scene of MBL physics. In this chapter, we consider a series of one-dimensional critical twist defect models with various boundary conditions. These twist defects are embedded in the background of a generalization of Kitaev $Z_2$ toric code model, and can also be understood as a discrete $Z_k$ gauge theory in its deconfined phase. We analytically construct the duality transformation of these critical models, and use numerical methods to extract information on the central charges, sound velocities, and conformal dimensions. With the numerical data, we show the relation between the CFT contents of the critical chains with periodic boundary conditions and the critical chains with duality-twisted boundary conditions.
To Mother and Chi.
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Chapter 1

Introduction to Many-body localization

1.1 Origin of many-body localization

The phenomenon of Anderson localization exists in closed low-dimensional quantum systems with disordered on-site potentials and no interactions between particles [1, 2]. It is an intriguing example where systems do not reach thermal equilibrium but rather show an absence of transport. This phenomenon has been experimentally verified in various systems [3–5]. In one-dimensional systems, arbitrarily small disorders will lead to localization [1, 6].

As a natural extension, the concept of many-body localization (MBL) grew out of a desire to understand the fate of Anderson localization in the presence of interactions between particles. In the seminal works by D.M. Basko, I.L. Aleiner, and B.L. Altshuler [7], and I. V. Gornyi, A. D. Mirlin, and D. G. Polyakov [8], the authors concluded that the electron-electron interaction alone is not sufficient to destabilize the localized one-particle orbitals, and postulated a many-body mobility threshold. Specifically, they performed perturbative analysis to show that the DC conductivity of such systems would, at all orders, remains exactly zero below a finite temperature, leading to the conclusion that there exists a many-body localized phase, and a possible melting transition at certain temperature or disorder. This newly hypothesized “quantum phase transition” is characterized by the change of dynamical properties of the many-body wave functions, rather than the existence of singular equilibrium observables, making it qualitatively different from conventional thermal and quantum phase transitions. However, due to the perturbative nature of the analysis, they could not rule out the possibility that such a phase is meta-stable. This discovery soon gathered enormous interest from the condensed matter physics community, and led to many intriguing discoveries on MBL. The latest developments and summaries of important findings can be found in recent review articles [9–14].

In the following, I will give a short survey of MBL physics, starting with how it fits into the concept of quantum thermalization.
1.2 Quantum thermalization

In classical statistical mechanics, ergodicity is often related to thermalization, and means the equivalence between ensemble average and time average. This ergodic hypothesis is the key to unite the laboratory measurements and theoretical analysis.

A similar understanding of ergodicity exists in quantum mechanics, but its interpretation is more subtle. In the following I will motivate the eigenstate thermalization hypothesis (ETH) from the angle of unitary time evolution of an ergodic system, and discuss its implications for thermalization of eigenstates.

1.2.1 Unitary time evolution and eigenstate thermalization hypothesis

The following argument mainly follows Ref. [15]. Given a many-body quantum system $H$ isolated from any heat bath, its unitary time evolution is

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle. \quad (1.1)$$

If $|\psi_0\rangle$ is an eigenstate, time evolution only adds a phase factor to the wave function instead of letting it explore more of the Hilbert space. To properly discuss the system’s dynamics, we instead consider a quantum quench [16], where a closed system is prepared in an initial state with high energy density but low entanglement, which is likely to be far from equilibrium. From the classical statistical mechanics point of view, one can assume that an ergodic system will thermalize and equilibrate as a canonical ensemble in the long time limit. This relative simple assumption has important consequences as will be illustrated below.

Assume we have a normalized initial state with energy expectation value $E$ and expanded in the eigenbasis as

$$|\psi_0\rangle = \sum_i C_i |E_i\rangle. \quad (1.2)$$

As a constraint, we want $|\psi_0\rangle$ to be distributed narrowly around $E$, meaning that it has a small energy standard deviation $\Delta E$. For a local few-body observable $A$, we have

$$\langle A(t) \rangle = \sum_{ij} C_i^* C_j e^{i(E_i - E_j)t} A_{ij}. \quad (1.3)$$

where $A_{ij} = \langle E_i | A | E_j \rangle$. Since we are only interested in the long time limit, we can define the infinite time average of $A$ as

$$\bar{A} = \lim_{t \to \infty} \frac{1}{t} \int_0^t \langle A(\tau) \rangle d\tau = \sum_i |C_i|^2 A_{ii}, \quad (1.4)$$

where it only receives diagonal contributions.
In another line of reasoning, since the system is believed to be ergodic, it is reasonable to argue that in the long time limit, the expected value of $A$ is determined by the statistical average over a micro canonical ensemble with an energy window $I = [E - \Delta E, E + \Delta E]$. So

$$\mathcal{A}_{mc} = \frac{1}{N_{E,\Delta E}} \sum_{E_i \in I} A_{ii},$$

(1.5)

where $N_{E,\Delta E}$ is the number of eigenstates in that energy window.

To match the two results above, we need

$$\sum_i |C_i|^2 A_{ii} = \frac{1}{N_{E,\Delta E}} \sum_{E_i \in I} A_{ii}.$$

(1.6)

It should be noticed that the L.H.S. of this equation strongly depends on the initial state’s distribution in the eigen basis, while the R.H.S. mainly depends on its energy expectation value and the width of the energy window. The only way of reconciliation is to assume that within a small energy window, $\langle E_i | A | E_i \rangle$ almost does not vary from eigenstate to eigenstate, which leads to the eigenstate thermalization hypothesis (ETH) \[15, 17–19\]

$$A_{ij} = A(E)\delta_{ij} + e^{-S(E)/2} f(E, \omega) R_{ij},$$

(1.7)

where $E = (E_i + E_j)/2$ and $\omega = E_i - E_j$. For Eq. (1.7), the first term on the R.H.S. means that $A$’s expectation value should be a smooth function of energy which varies little within the energy window. The second term describes the off-diagonal fluctuations, where $S(E)$ is the thermodynamic entropy of at energy $E$, $f(E, \omega)$ governs the relaxation of $A$ to $A(E)$ as in Ref. [18], and $R_{ij}$ is sampled from a random distribution of zero mean and unit variance. Because of the factor of $e^{-S(E)/2}$, the off-diagonal fluctuations are more suppressed at larger system sizes.

### 1.2.2 Thermalization of eigenstates

With the above discussion on ETH, there is a seemingly paradoxical issue as detailed in Ref. [9]. Given an isolated ergodic many-body quantum system after a long time evolution, ETH says that one cannot determine its initial state using any local measurements, which indicates that thermalization erases memory. But since the time evolution is unitary, one would expect all quantum information to be preserved. The key to resolve the contradiction is to realize that unitary time evolution hides but does not erase memory of the initial state. Local information of the initial state spreads to other parts of the system over time, which builds up entanglement entropy among subsystems. After a long time, the subsystems become so strongly
entangled that information about the initial state is only accessible if one measures non-local or global observables. The above example perfectly illustrates the relation between thermalization and entanglement entropy, and points to how one can understand thermalization for the eigenstates.

Simply speaking, for an isolated quantum system in an eigenstate to be thermal, different subsystems should be strongly entangled and act as each other’s heat bath. For convenience, let’s denote the full system’s energy as $E$, its energy density as $\varepsilon$. For an arbitrary small local subsystem $A$ (the rest of the system denoted as $B$), since $A$ is expected to be thermal, the reduced density matrix of $A$

$$\rho_A = \text{Tr}_B |\psi\rangle \langle \psi|$$

should becomes similar to the thermal density matrix of $A$

$$\rho_A = e^{-\beta H_A},$$

where $H_A$ is the full Hamiltonian $H$ restricted to subsystem $A$, and $\beta$ is determined by matching $A$’s energy density to $\varepsilon$ via

$$\varepsilon = \frac{1}{V_A Z_A} \text{Tr} \left( e^{-\beta H_A} H_A \right)$$

where $V_A$ is the “volume” of $A$ and $Z_A$ is the partition function. Since $\rho_A$ is thermal, the thermal entropy of $A$, or equivalently the von Neumann entanglement entropy of $A$,

$$S_A = -\text{Tr}_A (\rho_A \ln \rho_A)$$

should also be extensive.

The thermal reduced density matrix has direct connection to ETH. Since any local observable $O$ in subsystem $A$ can be estimated as

$$\langle O \rangle = \text{Tr}_A (\rho_A O) = \frac{1}{Z_A} \text{Tr} \left( e^{-\beta H_A} O \right).$$

As long as there are no other thermal/quantum phase transitions in $H_A$, the expectation value $\langle O \rangle$ is expected to be a smooth function of $\beta$. Because of Eq. (1.10), it also has to be a smooth function of energy.

As a summary, we discussed the time evolution where the isolated many-body quantum system is ergodic. However, a many-body localized system behaves in exactly the opposite way. It fails to thermalize itself, retains memory of initial state locally, breaks the eigenstate thermalization hypothesis, and violates the
volume law of entanglement entropy. Among these, the last two points are more directly related to the eigenstates.

One usually finds two kinds of narratives of MBL. From the dynamical point of view, one can consider how quickly the entanglement entropy would spread and whether unevenly distributed local observables would relax. On the other hand, from the static point of view, one can consider if highly excited eigenstates would violate ETH and have area-law entanglement entropy.

1.3 Typical many-body localized Hamiltonian models

In order to provide a concrete discussion of the properties of MBL systems, we will introduce typical MBL Hamiltonian models. In the early works of Ref. [7, 8], MBL was not fully established as a stable phase of matter, because it was not clear if the conclusion would be changed due to non-perturbative effects. This situation was later improved by J. Z. Imbrie [20]. Using one-dimensional spin chains with large disorders and weak short-range interactions, the author took non-perturbative effects into account and concluded rigorously that all eigenstates of these type of spin Hamiltonians are MBL. Besides this, there have been numerous numerical studies on one-dimensional disordered spin chains, which constantly supported the existence of a robust MBL phase and MBL-ergodic transition.

Among all spin models, arguably the “standard model” of the MBL transition is the one-dimensional random fields Heisenberg chain [21–45]

\[ H = \sum_{i=1}^{L} \hat{S}_i \cdot \hat{S}_{i+1} + h_i \hat{S}_i^z, \quad h_i \in [-h, h]; \quad p(h_i) = \frac{1}{2h}, \tag{1.13} \]

where \( h \) (sometimes alternatively denoted as \( W \)) is the disorder strength. Fig. 1.1 (excerpted from Ref. [30]) shows the phase diagram using the exact diagonalization (ED) method. The phase diagram is plotted on a 2D plane with energy density and disorder strength. The energy density \( \epsilon \) here means the energy of eigenstates normalized by the spectrum width

\[ \epsilon = \frac{E - E_{\text{min}}}{E_{\text{max}} - E_{\text{min}}}, \tag{1.14} \]

which serves as an indicator of the “temperature”. At small disorder strength, the system stays ergodic (the violet region); but as disorder strength increases, the system eventually goes into the MBL phase (dark brown region). The “C”-shaped many-body mobility edge is clearly visible.

At the center of the spectrum (\( \epsilon = 0.5 \)), numerical evidence primarily suggests that the MBL transition
occurs at a critical disorder strength $h_c \approx 3.7$ [24, 30], although the exact value of $h_c$ is not fully settled [46].

By a Jordan-Wigner transformation, the above model is equivalent to the following spinless fermion model

$$H = \frac{1}{2} \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \sum_i n_i n_{i+1} + \sum_i \mu_i n_i,$$  \hspace{1cm} (1.15)

where $n_i = (c_i^\dagger c_i - 1/2)$, and the random fields $h_i$ is replaced with the on-site potential $\mu_i$. This spinless fermion model is convenient for the one-particle density matrix (OPDM) description of the MBL-ergodic transition [34, 47, 48].

### 1.4 Phenomenological theory of MBL phase

The benefit of having a concrete Hamiltonian model is that one has full access to its microscopic details. But the downside is that sometimes the details might distract you from discerning universal properties shared by a range of models. It is good then to have a phenomenological theory for the benefit of a simpler physical picture.

For the MBL phase, we have noticed that the systems can retain information locally. Via microscopic analysis of eigenstates of MBL systems, this vague idea of locality has been elevated to a powerful phe-
nomenological theory of “local integrals of motions” (LIOMs) [12, 26, 49–58]. The LIOMs are often referred to as the l-bits, where “l” stands for “local”. They are well-defined deep in the MBL phase. But when one comes closer to the mobility edge, the fate of the l-bits are not fully understood, because some of the eigenstates are MBL and the others are ergodic. In the discussion below, we will only consider the fully MBL phase.

For a spin-$\frac{1}{2}$ MBL system of $N$ sites, let’s denote the physical degrees of freedom using $\sigma$, and denote the set of $N$ l-bits as $\{\tau^z_i\}$. Since they are local integrals of motion, the l-bits commute with each other and with the Hamiltonian

$$[\tau^z_i, H] = [\tau^z_i, \tau^z_j] = 0, \quad 1 \leq i, j \leq N. \quad (1.16)$$

The l-bit and the physical spins are related via a unitary transformation that also diagonalizes the Hamiltonian

$$\tau^z_i = U \sigma^z_i U^\dagger, \quad U^\dagger H U = H_{diag}. \quad (1.17)$$

In general, as shown in Ref. [26], the unitary transformation $U$ can be constructed using a short quantum circuit, which means that the l-bits can be produced very efficiently. When the above equality between $\tau^z_i$ and $\sigma^z_i$ is expanded, one usually gets

$$\tau^z_i \approx \sigma^z_i + \sum_{j} \sum_{s_1, s_2} f^{s_1, s_2}_{j_1, j_2} \sigma^s_{j_1} \sigma^s_{j_2} + \cdots \quad (1.18)$$

where the coefficient $f^{s_1, s_2}_{j_1, j_2}$ normally decays exponentially fast (see Ref. [51])

$$f^{s_1, s_2}_{j_1, j_2} \sim e^{-\text{max}(|i-j|, |i-k|)/\xi}, \quad (1.19)$$

where $\xi$ is one possible way of defining the localization length.

In terms of the l-bits, the transformed Hamiltonian $H_{diag}$, sometimes called the l-bit Hamiltonian, takes the form of

$$H_{diag} = \sum_i \tilde{h}_i \tau^z_i + \sum_{ij} J_{ij} \tau^z_i \tau^z_j + \sum_{ijk} J_{ijk} \tau^z_i \tau^z_j \tau^z_k + \cdots. \quad (1.20)$$

The single body terms are dominant in the l-bit Hamiltonian, as they dictate how fast each l-bit precess around the $\tilde{h}_i$. But many physical phenomena of MBL are related to the couplings. $J_{ij}$ typically decay exponentially as

$$J_{ij} \propto e^{-|i-j|/\tilde{\xi}}, \quad (1.21)$$

where $\tilde{\xi}$ is another way of defining the localization length. Similar behavior is expected for $J_{ijk}$ and higher
order couplings.

Using the above phenomenological description, one can make some simple yet qualitatively accurate arguments on the dynamics of MBL systems. For example, given a random product state, its entanglement entropy is observed to grow logarithmically after a short amount of time[59], which is a distinctive feature of an MBL system compared to an Anderson localized system or an ergodic system. This behavior can be interpreted in the l-bit basis as follows, which is adapted from the argument in Ref [59].

Because $\sum_i \tilde{h}_i \tau_i^z$ are the dominant terms in the l-bit Hamiltonian, the l-bit on each site precess according to $\tilde{h}_i$. Given sites $i, j$ separated by a distance of $r = |i - j|$, slow dephasing is caused by couplings between the l-bits $\tau_i^z$ and $\tau_j^z$. For simplicity, we will only consider the coupling $J_{ij}$. During the time evolution according to the $e^{-iH_{\text{diag}}t}$, dephasing between $i, j$ becomes significant when the time scale $t$ satisfies

$$J_{ij} t \sim 1.$$  \hspace{1cm} (1.22)

Because of Eq. (1.21), the above equation is equivalent to

$$r \sim \xi \ln t.$$  \hspace{1cm} (1.23)

This means that at time $t$, only spins within a distance of $\ln t$ are entangled, which is in perfect agreement with the observation that entanglement entropy grows logarithmically with time.

Besides the above example, the phenomenological description can also be quantitatively applied to the decay of out-of-time-order correlators (OTOC) [60, 61].

### 1.5 Characterization of MBL phase

In this section, we will summarize the ways of characterizing the MBL phase. Most of the approaches are commonly used in numerical studies on the MBL-ergodic transition. Here we restrict to Hamiltonian models, though the same analysis can be performed for other systems.

1. In the MBL phase, ETH is no longer valid, so few-body operators under nearby eigenstates have very different expectation values, as shown in Fig. 1.2.

2. In the ergodic phase eigenstates will have volume-law entanglement entropy, while in the MBL phase they will have area-law behavior. To calculate the entanglement entropy, typically the subsystems are defined to be half of the full system. Entanglement entropy was proposed as the order parameter to
Figure 1.2: (From Ref. [40]) Local magnetization (for site 5) versus energy density $\epsilon$ for periodic random field Heisenberg chains with disorder strength $h = 1.0$ at various system sizes $L$. For $0.2 < \epsilon < 0.9$, the local magnetization clusters tighter and smoother with increasing system size. So eigenstates close in energy tend to have very similar expectation values of local observables. ETH is valid, and the systems are in ergodic phase. However, for $\epsilon > 0.9$, eigenstates close in energy have wildly different local observables irrespective of the system size, meaning that ETH is invalid and the systems are in MBL phase.

probe MBL-ergodic transition first in [62]. The reason is, for a fixed energy window when the system moves close to the transition, eigenstates within the window start to have a mixture of volume-law and area-law entanglement entropy [32]. Because of this mixture, the standard deviation of entanglement entropy is expected to be peaked at the transition, as can be seen in Fig. 1.3. The location of the peak usually changes with the system size $L$, so finite size scaling is often used with some empirical scaling ansatz to estimate the exact transition point.

3. Besides the entanglement entropy, it is argued that the gap between the largest two eigenvalues of the reduced density matrix is also a sensitive signal of the MBL-ergodic transition [63], and gives more reasonable critical exponent when performing finite size scaling analysis.

4. MBL systems have emergent integrability, revealed by an extensive number of LIOMs, which implies the lack of level repulsion in the energy spectrum. From the random matrix’s perspective [64–66], energy level spacings in MBL systems should follow Poisson statistics for the lack of level repulsion [21, 24, 30, 67, 68], compared to the Gaussian orthogonal ensemble (GOE) or Gaussian unitary ensemble (GUE) in the ergodic phase. This difference can be quantified by the gap ratios of adjacent energy levels

$$ r^{(n)} = \frac{\min(E_n - E_{n-1}, E_{n+1} - E_n)}{\max(E_n - E_{n-1}, E_{n+1} - E_n)}, \quad (1.24) $$
Figure 1.3: (From Ref. [62]) Standard deviation of the von Neumann entanglement entropy $\Delta S$ of eigenstates in the middle of the spectrum versus disorder strength $\delta J$, for the disordered $J_1$-$J_2$ transverse Ising chains at system sizes of $L = 8, 10, 12, 14$. A peak is clearly visible around $\delta J = 3$. Upper Left Inset: Disorder averaged von Neumann entanglement entropy versus disorder strength. At small disorder strength, it can be seen that the von Neumann entanglement entropy grows linearly with $L$, indicating the ergodic phase; at large disorder strength, however, the von Neumann entanglement entropy is almost system size independent, indicating the MBL phase. Upper Right Inset: Scaling collapsed standard deviation of the von Neumann entanglement entropy versus disorder strength curves. The scaling collapse gives an estimate of the critical disorder strength of $\delta J_c = 3.81$.

where $r_{GOE} \approx 0.51$ and $r_{Poisson} \approx 0.39$. An example showing the transitioning behavior of gap ratios is in Fig. 1.4. Later it was found that the level statistics of the entanglement spectrum can also be used to distinguish the MBL phase from the ergodic phase [69].

5. In the quantum quench setup, the entanglement entropy in MBL systems grows logarithmically with time [59, 70, 71], as in Fig. 1.5, while in ergodic systems it grows linearly with time.

1.6 Experimental studies on MBL

When MBL systems are discussed above, it is assumed that they are isolated from any external heat baths, so they will not become thermalized in an unintended way. In a traditional electronic material, however, it is very difficult to isolate the electronic degrees of freedom from the environment, especially from the phonons.

In comparison, ultra-cold atoms are much better isolated. Recently, there have been considerable progress in employing ultra-cold atoms to simulate disordered systems in a controllable fashion [72, 73]. Clear signs of the MBL transition were observed in one-dimensional ultra-cold atoms experiments [74, 75], as well as in higher dimensions [76, 77]. Usually these experiments are designed to simulate time evolution after a quantum quench, where the initial states are far from equilibrium. The relaxation or transport properties
can then tell whether the system is MBL or not, for example, in Fig. 1.6; In general, ultra-cold atoms experiments can provide valuable insights into the dynamical aspects of MBL physics.

### 1.7 Latest developments and open questions

#### 1.7.1 Floquet systems

Recently, MBL transitions have also been observed in Floquet systems [78–83]. Floquet systems have Hamiltonians that are periodical in time, as $H(t + T) = H(t)$. The most common setup is to choose two non-commuting disordered Hamiltonians $H_1$ and $H_2$. Then time evolve the system according to

$$H(t) = \begin{cases} 
H_1, & 0 \leq t < \frac{T}{2} \\
H_2, & \frac{T}{2} \leq t < T
\end{cases} .$$ (1.25)

Because of the explicit time dependence, energy conservation is broken in Floquet systems. It is usually expected that the the lack of energy conservation law and the periodic driving can make Floquet systems thermalize easily. However, when the disorder is large enough, or when the driving is sufficiently slow, a stable localized phase is possible.

Typically the properties of a Floquet system are reflected in the spectrum of its unitary evolution operator

$$U = T e^{-\frac{i}{\hbar} \int_0^{T/2} H(t) dt} .$$ (1.26)
Figure 1.5: (From Ref. [71]) Disorder averaged von Neumann entanglement entropy versus time after a quantum quench, of disorder XXZ chains for different interaction strength at system size $L = 20$. After $J_{\perp}t > 10$, the entanglement entropy starts to grow logarithmically. Inset: Standard deviation of von Neumann entanglement entropy versus time.

Similar analysis can be performed on the eigenstates of $U$, just as in the case of a Hamiltonian model. Because of the lack of energy conservation, it is argued that the Floquet systems thermalize faster and have sharper transition than a Hamiltonian model at the same finite system size [83].

1.7.2 Symmetry and MBL

The idea of using the MBL phase to preserve symmetry-protected topological (SPT) orders at finite energy density was first proposed in Ref. [84, 85]. The basic idea is that localization freezes the excitation modes so that they will not couple the edge modes. Later it was suggested in Ref. [86] that having SPT orders in MBL might be restricted to SPT orders protected by discrete symmetries.

For continuous non-Abelian symmetries, similar behavior was not expected. Non-Abelian symmetries usually means that the eigenstates have degenerate multiplets, which are prone to having resonances that can destabilize the localized phase. It was later shown in Ref. [87, 88] that the presence of continuous non-Abelian symmetries preclude the existence of a typical MBL phase altogether.

1.7.3 Open questions

At this moment, the MBL-ergodic transition is largely believed to be continuous, but the nature of the transition remains hard to grasp.

One issue is, for almost all exact diagonalization calculations on one-dimensional Hamiltonian models
Figure 1.6: (From Ref. [74]) Charge imbalance versus time in ultra-cold atoms experiment simulating the one-dimensional Aubry-André model, where $\Delta$ represents the disorder strength, and $U$ is the on-site interaction. The initial state is prepared as a charge density wave. In the ergodic phase, the charge imbalance (difference between charges on even sites and odd sites divided by total number of atoms) relaxes very fast to zero. In comparison, the charge imbalance stays almost constant in the ergodic phase at large $t$.

with MBL-ergodic transition, the correlation-length exponent $\nu$ obtained through finite size scaling analysis was always around or less than 1, which strongly violated the Harris-Chayes bound $\nu > 2/d$ [89], where $d$ is the spatial dimensionality.

Though having the same form, the Harris-Chayes bound is a stronger version than the original Harris criterion, in the sense that it is generalized to a larger class of disordered systems, including percolation and Anderson localization. It is generalized even further in Ref. [90] with a slightly weaker inequality, but argued to be valid for the MBL-ergodic transition with entanglement entropy as the order parameter.

This contradiction between numerical results and analytical arguments is a big open question. Currently, there are at least two possibilities as to how they can be reconciled.

1. The system sizes in previous numerical studies could be too small. Currently, the largest MBL system simulated using exact diagonalization methods has $L = 22$ [30]. It is usually believed at small system sizes the finite size scaling could be strongly affected by drift terms, so there could be errors in the critical exponents. More specifically, it is proposed in Ref. [91] that at small system size, the variance of entanglement entropy is strongly affected by intra-sample fluctuation (variance contributed by eigenstates within an energy window of the same sample), which represents a non-random fixed point not covered by the Harris-Chayes bound. The authors showed that as system size grows, the intra-sample fluctuation decreases and inter-sample fluctuation increases. So possibly the current numerical studies are not at a point to detect the fixed point relevant to the MBL-ergodic transition.
2. Another possibility is that entanglement entropy might not be a proper order parameter for doing finite size scaling analysis. In a recent study [63], Schmidt gap, which is the difference between the largest two eigenvalues of the reduced density matrix, is proposed to be a better candidate. Using Schmidt gap as an order parameter for the random field Heisenberg chain, the authors obtained a correlation-length exponent $\nu = 2.2$ and a critical disorder strength of $h_c = 5.0$, compared to $\nu = 0.8$ and $h_c = 3.7$ when using entanglement entropy as the order parameter [30].

The implications of the two proposals above should be verified carefully, because they also rely on numerical evidence gathered from finite size scaling analysis done at small system sizes ($L < 20$). But it is clear that strong finite size effects make it necessary to develop new algorithms that can be scaled to much bigger systems and can be robust near the transition region. To this end, people have explored renormalization group (RG) methods like real space RG for excited states (RSRG-X) [92] and spectrum bifurcation RG (SBRG) [93], Wegner-Wilson flows [55], as well many tensor networks methods that diagonalize the entire Hamiltonian or optimizes for individual eigenstates [31, 37–39]. These methods work efficiently in the MBL phase but so far have various problems when approaching the transition point. Besides these, there are phenomenological RG methods to avoid the computational burden associated with the model details [94], where the system is simplified to a combination of local and thermal blocks. But a microscopic theory of how thermal blocks and MBL blocks influence each other is desirable in verifying these results.

Another issue concerns the scaling behavior of entanglement entropy at criticality. It has been argued that the scaling of the disorder-averaged entanglement entropy at the critical point could follow a volume law [95], or a power law scaling as $S \propto L^\alpha$ with an exponent $\alpha < 1$ (i.e. slower than volume law) [96]. Our own numerical study shows that in the transition regime the systems have a bimodal entanglement entropy distribution [32].

Despite the difficulties, we are optimistic about future breakthroughs.
Chapter 2

Numerical methods

Every numerical method for strongly correlated many-body quantum systems needs to represent wave functions or density matrices in a certain format. Depending on whether numerically exactness is preferred and affordable, one can choose to work with an exact representation where a complete orthonormal basis is specified, or a restricted representation parameterized in a suitable subspace of the Hilbert space. Exact representations usually offer unrivaled accuracy for small systems, but suffer from the exponentially growing Hilbert space size. Restricted representations are far more efficient and feasible for larger systems, but the validity of the parameterization is situation-dependent.

In the following sections, I will give a detailed discussion about exact diagonalization (ED) methods and density matrix renormalization group (DMRG) like methods, because they are essential for my research on many-body localization phenomenon, and critical twist defect chains.

2.1 Exact diagonalization

Exact diagonalization (ED) methods encompass a range of unbiased and numerically exact ways of solving for the energy eigenstates and eigenvalues of finite size quantum systems. For a finite size Hamiltonian system on a lattice, one can choose a set of orthonormal basis, cast the Hamiltonian $H$ as a matrix and the eigenstate $|\psi\rangle$ as a vector, and then solve the time independent Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle$$

numerically. ED is straightforward in its idea, yet complicated in its implementation. The biggest problem is that the Hilbert space grows exponentially with the system size. Very quickly it becomes impractical to store a few full wave functions, let alone the matrix format of the Hamiltonian. There are quite a few techniques to deal with these problems at large system sizes. To give some context to the discussion, I will focus on the following two cases.
1. Only a few low lying eigen pairs (pair of eigenvalues and eigenstates) are sought after, as in simulating quantum phase transitions.

2. Only a few eigen pairs near a given finite energy density are sought after, as in simulating the MBL-ergodic phase transition.

As an example, the state-of-the-art ED program can solve for a few low lying eigen pairs (pair of eigenvalues and eigenstates) of a system made up of about 40 half spins, after taking advantage of symmetry sectors. Solving for excited states is relatively harder. As a matter of fact, in Ref. [30], it was only practical to get eigen pairs at the middle of the spectrum for a system made up of 22 half spins. At these system sizes, the best practice is to use the Lanczos method for diagonalizing Hermitian matrices, which will be introduced below. I will first describe the case where only a few low lying eigen pairs are sought after.

2.1.1 Low lying eigenstates

Krylov subspace

The Lanczos method belongs to a group called Krylov subspace methods. The key of any Krylov subspace method is to expand a subspace so it becomes increasingly likely to contain the desired states. In the context of solving for low lying energy eigenvalues, this works in the following way.

One can build an \( M \)-dimensional Krylov subspace starting from a random vector \( |\psi_0\rangle \) and the Hamiltonian matrix \( H \) as

\[
K^M = \text{span}( |\psi_0\rangle, H|\psi_0\rangle, \cdots, H^{M-1}|\psi_0\rangle ).
\] (2.2)

This subspace can be exploited to find low lying eigenstates with a few additional steps.

1. Intuitively, multiplying \( |\psi_0\rangle \) by \( H \) results in a vector rotated towards the eigenstate with the largest eigenvalue in magnitude. This means, as \( M \) grows, one can assert with growing confidence that the lowest or highest energy eigenstate is within \( K^M \).

2. To make sure that \( K^M \) can capture the low lying eigenstates, one projects the Hamiltonian \( H \) onto \( K^M \), and solves for the eigen pairs of the projected Hamiltonian. One then restarts the Krylov subspace using the lowest energy eigenstate of the projected Hamiltonian as \( |\psi_0\rangle \). Since \( M \) is small, the diagonalization of the projected Hamiltonian is quite easy to do, and restarting can keep the Krylov subspace with a moderate size.

3. After repeatedly growing and restarting the Krylov subspace, the eigen pairs of the projected Hamiltonian will converge to the true low lying eigen pairs.
As can be seen from above, restarting is a popular way of controlling the size of the Krylov subspace, and it makes sure that the subspace evolves towards the desired direction. The only question is, in order to project the Hamiltonian onto $K^M$, what orthonormal basis should one use? This is a problem because in general $\{ |\psi_0\rangle, H|\psi_0\rangle, \ldots, H^{M-1}|\psi_0\rangle \}$ are not orthogonal to each other, and solving the generalized eigenvalue problem where the basis vectors are not orthogonal is usually less efficient and less controlled.

**Lanczos method**

Assume we start from a normalized vector $|\psi_0\rangle$, and label the basis vector built at step $n$ as $|\psi_n\rangle$. To build $|\psi_n\rangle$, the Lanczos method relies on the Schmidt orthogonalization

$$b_n |\psi_n\rangle = H|\psi_{n-1}\rangle - \sum_{i=0}^{n-1} |\psi_i\rangle \langle \psi_i | H |\psi_{n-1}\rangle.$$ (2.3)

where $b_n$ is a real number for normalizing $|\psi_n\rangle$. After the Schmidt orthogonalization, $|\psi_n\rangle$ becomes orthogonal to all previous basis vectors. There are a few things to notice

1. $b_n = \langle \psi_n | H |\psi_{n-1}\rangle$. This can be obtained by contracting $|\psi_n\rangle$ with Eq. (2.3).

2. $\langle \psi_{n+k} | H |\psi_{n-1}\rangle = 0$ for $k \geq 1$. This can be obtained by contracting the later basis vector $|\psi_{n+k}\rangle$ with Eq. (2.3).

There are two immediate implications. Firstly, when projecting $H$ onto this set of basis vectors, we will get a symmetric tridiagonal matrix

$$H_{\text{projected}} = \begin{pmatrix}
a_0 & b_1 & 0 & 0 & \cdots \\
b_1 & a_1 & b_2 & 0 & \cdots \\
0 & b_2 & a_2 & b_3 & \cdots \\
0 & 0 & b_3 & a_3 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.$$ (2.4)

where $a_i = \langle \psi_i | H |\psi_i\rangle$.

Secondly, it means that Eq. (2.3) (for $n \geq 2$) can be simplified to

$$b_n |\psi_n\rangle = H|\psi_{n-1}\rangle - |\psi_{n-1}\rangle \langle \psi_{n-1} | H |\psi_{n-1}\rangle - |\psi_{n-2}\rangle \langle \psi_{n-2} | H |\psi_{n-1}\rangle.$$ (2.5)

As can be seen, in order to keep expanding the Krylov subspace, one only has to store the last two basis vectors. And every time when a new basis vector is added, one only needs to update a few elements of
$H_{\text{projected}}$. This is of course for the ideal situation where one can perform calculations with mathematical precision. For numerical calculations, because of rounding errors, the last two basis vectors will very quickly lose orthogonality with respect to previous basis vectors. There have been various techniques for making the Lanczos method stable. Usually, one has to keep more basis vectors, and once in a while re-orthogonalize all or part of the basis vectors, or simply restart the Krylov subspace as mentioned before.

There a few available libraries with a stable implementation of the Lanczos method. For example, the Iterative Eigensolver Template Library (IETL) [97] provides generic C++ implementations of famous eigensolvers; and the ARPACK library is an originally well-known Fortran library [98].

2.1.2 Excited states

The discussion in the previous subsection is for obtaining low lying eigenstates. But if we want an excited state whose energy is closest to a target value $\lambda$, most commonly one would use the shift-and-invert technique together with the Lanczos method, or use the newly developed FEAST algorithm [99, 100].

**Shift-and-invert technique plus Lanczos**

The shift-and-invert technique is quite simple in logic. Given a random initial state $|\psi_0\rangle$, and the Hamiltonian $H$, one builds another Krylov subspace as

\[
\tilde{K}^M = \text{span}(|\psi_0\rangle, (H - \lambda)^{-1}|\psi_0\rangle, \ldots, (H - \lambda)^{-(M-1)}|\psi_0\rangle).
\]

(2.6)

Intuitively, multiplying $|\psi_0\rangle$ by $(H - \lambda)^{-1}$ results in a vector rotated towards the eigenstate whose energy is closest to $\lambda$. This means, as $M$ grows, one can assert with growing confidence that the desired excited states are within $\tilde{K}^M$.

 practically, it is not feasible to invert the matrix $(H - \lambda)$. Instead one would solve a linear equation problem

\[
(H - \lambda)|\tilde{\psi}_1\rangle = |\psi_0\rangle
\]

(2.7)

to get $|\tilde{\psi}_1\rangle = (H - \lambda)^{-1}|\psi_0\rangle$. In general, to maintain the stability of the Lanczos method, one has to use a direct solver, which is usually based on QR factorization. Because of the matrix-matrix multiplications involved in such operations, the time cost of a direct linear solver scales as $O(N^3)$, where $N$ is the size of the vector. In comparison, the time cost of a matrix-vector multiplication only scales as $O(N^2)$. For this very reason, it is usually much more costly to solve for excited states than to solve for low lying eigenstates using the Lanczos method.
FEAST algorithm

The FEAST algorithm is a remarkably simple projection-based algorithm, yet it is more stable and efficient than the Lanczos method with the shift-and-invert technique [99, 100]. Although they both project the Hamiltonian into a small subspace, there is a key difference between the natures of the subspaces. The Lanczos method builds a Krylov subspace that gets exponentially better at approximating the extreme eigen pairs (lowest/highest/closest to \( \lambda \)) with increasing subspace size or number of restarts. But for the FEAST algorithm, it applies a projection operator that directly projects the Hamiltonian into the subspace spanned by eigenstates within a specified energy range.

The skeleton of the FEAST algorithm is as follows. It takes a specified energy window \([E_{\text{min}}, E_{\text{max}}]\), and then makes use of a projection operator

\[
P = \oint \frac{dz}{2\pi i} \frac{1}{z - H},
\]

where the contour is usually chosen as a circle with \([E_{\text{min}}, E_{\text{max}}]\) as its diameter. If one expands the Hamiltonian in the eigen basis, it is easy to see that

\[
P = \oint \frac{dz}{2\pi i} \frac{1}{z - \sum_n E_n |n\rangle \langle n|} = \sum_{E_n \in [E_{\text{min}}, E_{\text{max}}]} |n\rangle \langle n|.
\]

The idea is to apply \(P\) to a set of random, linearly independent vectors \(\{ |\psi_i\rangle \}\), which then results in a new set of vectors \(\{ \tilde{\psi}_i \}\) (presumably still linearly independent). Since \(P\) is a projection operator, \(\{ \tilde{\psi}_i \}\) resides exactly in the subspace spanned by eigenvectors within the energy window \([E_{\text{min}}, E_{\text{max}}]\). Then it is fairly easy to solve a generalized eigenvalue problem \((A v = \lambda B v)\) with the matrices \(A_{ij} = \langle \tilde{\psi}_i | H | \tilde{\psi}_j \rangle\), and \(B_{ij} = \langle \tilde{\psi}_i | \tilde{\psi}_j \rangle\).

For a good implementation, there are two issues to address.

1. Numerically, it is not easy to perform the contour integral exactly. One way is to use Legendre-Gauss quadrature with \(n\) contour points, as in the leftmost case in Fig. 2.1. This leads to an approximate projector

\[
P' = \sum_{i=1}^n \omega_i r e^{i \pi x_i} \frac{1}{2\pi} \frac{1}{r e^{i \pi x_i} - H},
\]

where \(r = (E_{\text{max}} - E_{\text{min}})/2\), \(\{x_i\}\) and \(\{\omega_i\}\) are the set of abscissas and weights given by Legendre-Gauss quadrature to order \(n\), and \(\frac{1}{r e^{i \pi x_i} - H}\) is not to be calculated as is, but to be interpreted as a linear equation problem when applied to a vector. Since \(P'\) is approximate, one would need to apply \(P'\) a few times to get converged basis vectors \(\{ \tilde{\psi}_i \}\).
2. One needs to estimate the number of eigenstates within the energy window \([E_{\text{min}}, E_{\text{max}}]\). It is harmless to use an excessive number of initial random vectors, since one can purge the redundant ones after the projection. But the algorithm will fail if insufficient initial random vectors are supplied.

![Figure 2.1](image)

Figure 2.1: (From Ref. [100]) 3 contours for building up the projection operators for the enclosed eigen modes (marked as crosses on the real axis). For each contour, among the 10 contour points, one only needs to perform calculations on 5 of them (solid dots), because the others (empty dots) are related by a complex conjugation.

As an example, to obtain a dozen eigenvectors of length \(2^{14}\) within some energy window, using 8 contour points, one usually needs to apply \(P'\) to \(\{|\psi_i\rangle\}\) for about 10 times. An optimized implementation of FEAST is provided in Intel Math Kernel Library (MKL) under the name of extended eigensolver, which makes use of the sparse matrix functionality provided by the Intel Parallel Direct Sparse Solver Interface (PARDISO).

### 2.2 Matrix product representation

Density matrix renormalization group (DMRG) is a ground breaking numerical method for simulating one-dimensional many-body quantum systems [101]. It is capable of solving for low lying eigenstates of large one-dimensional systems not accessible to ED methods. Although the original DMRG did not use the MPS representation, it was soon realized that the success of DMRG was directly linked to the efficiency of expressing the wave function in the MPS format [102]. Since then the MPS representation has been widely used to efficiently represent the low lying eigenstates of one-dimensional gapped or critical systems.

A pedagogical survey of DMRG and the matrix product representation is available in the review article of Ref. [103]. In the following, I will give a relatively short, but self-contained introduction to MPS, MPO, and DMRG. To provide a little bit of intuition, MPSs and an MPOs are often visualized as in Fig. 2.2.
2.2.1 Matrix product states

For simplicity, we consider 1D $N$-site spin-$\frac{1}{2}$ systems with open boundary conditions, which reside in a Hilbert space of size $2^N$. Given a general wave function in the $\sigma^z$ basis

$$|\psi\rangle = \sum_{\sigma} c_{\sigma_1 \sigma_2 \cdots \sigma_N} |\sigma_1 \sigma_2 \cdots \sigma_N\rangle$$  \hspace{1cm} (2.11)$$

($\sigma$ can be either $\uparrow$ or $\downarrow$), one can view the coefficient $c_{\sigma_1 \sigma_2 \cdots \sigma_N}$ as a rank-$N$ tensor. Although there were many existing algorithms to factorize higher-rank tensors into lower-rank ones before the invention of MPS, none of them took advantage of the simple spatial relation that $\sigma_i$ is to the right of $\sigma_{i-1}$ and to the left of $\sigma_{i+1}$, thus scrambling the local degrees of freedom in a bad way. In some sense, the MPS representation is a better way to factorize $c_{\sigma_1 \sigma_2 \cdots \sigma_N}$ for 1D systems because it aligns the lower-rank tensors according to their spatial locations.

To produce an MPS, one needs to perform successive singular value decompositions (SVD). SVD allows one to factorize a matrix $A$ as $A = USV^\dagger$, but for simplicity of notation I will use the other definition that

$$A = USV, \quad s.t. \quad U^\dagger U = \mathbb{I}, \quad VV^\dagger = \mathbb{I}, \quad S_{ij} = s_i \delta_{ij}, \quad s_i \geq 0, \hspace{1cm} (2.12)$$

where the $s_i$’s are called the singular values. We will use SVD in a step by step illustration on how to turn a general wave function into the MPS format.

1. Let’s start with the leftmost degree of freedom $\sigma_1$. Reshape the tensor $c_{\sigma_1 \sigma_2 \cdots \sigma_N}$ into a 2-by-$2^{N-1}$ matrix $c_{\sigma_1,(\sigma_2 \cdots \sigma_N)}$ by grouping $(N-1)$ indices together. Perform an SVD on this matrix as

$$c_{\sigma_1,(\sigma_2 \cdots \sigma_N)} = (U_1)_{\sigma_1,a_1} (S_1)_{a_1,a_1'} (V_1)_{a_1',(\sigma_2 \cdots \sigma_N)}, \hspace{1cm} (2.13)$$
where the Einstein summation rule is assumed and will be used from here on unless stated otherwise.

Usually one would rewrite \((U_1)_{\sigma_1,a_1}\) as \((U_1^{\sigma_1})_{a_1}\) to emphasize the ordering of the indices, and to distinguish the physical degree of freedom \(\sigma_1\) from the virtual degree of freedom \(a_1\). This way, \((U_1^{\sigma_1})_{a_1}\) and \((U_1^a)_{a_1}\) are both 1-by-2 matrices (row vectors), where the virtual bond denoted by \(a_1\) has size of 2. The sizes of the virtual bonds are usually called bond dimensions. Then multiply \((S_1)_{a_1,a_1'}\) and \((V_1)_{a_1,(\sigma_2\cdots\sigma_N)}\) together and denote the result as \((R_1)_{a_1,(\sigma_2\cdots\sigma_N)}\).

2. Reshape \((R_1)_{a_1,(\sigma_2\cdots\sigma_N)}\) as a 2\(^2\)-by-2\(^N-2\) matrix \((R_1)(a_1\sigma_2),(\sigma_3\cdots\sigma_N)\). Perform an SVD on this matrix

\[
(R_1)(a_1\sigma_2),(\sigma_3\cdots\sigma_N) = (U_2)(a_1\sigma_2),a_2 \cdot (S_2)(a_2,a_2')(V_2)a_2'(\sigma_3\cdots\sigma_N).
\]  

(2.14)

Usually one would rewrite the matrix \((U_2)(a_1\sigma_2),a_2\) as \(a_1(U_2^{\sigma_2})a_2\). In this form, \(a_1(U_2^{\sigma_2})a_2\) and \(a_1(U_2^a)a_2\) are both 2-by-2 matrices. Notice that the virtual bond denoted by \(a_2\) has a bond dimension of \(2^2\). Then multiply \((S_2)_{a_2,a_2'}\) and \((V_2)a_2'(\sigma_3\cdots\sigma_N)\) together as \((R_2)_{a_2,(\sigma_3\cdots\sigma_N)}\).

3. Repeat until one reaches the rightmost degree of freedom \(\sigma_1\).

\[
c_{\sigma_1\sigma_2\cdots\sigma_N} = (U_1^{\sigma_1})_{a_1} \cdot a_1(U_2^{\sigma_2})a_2 \cdots a_{N-2}(U_{N-1}^{\sigma_N-1})a_{N-1} \cdot a_{N-1}(R_N^{\sigma_N}).
\]  

(2.15)

At this point, the tensor \(c_{\sigma_1\sigma_2\cdots\sigma_N}\) has been turned into a product of lower-rank tensors

\[
|\psi\rangle = \sum_{\{\sigma\}} U_1^{\sigma_1} U_2^{\sigma_2} \cdots U_{N-1}^{\sigma_{N-1}} R_N^{\sigma_N} |\sigma_1\sigma_2\cdots\sigma_n\rangle,
\]  

(2.16)

where the virtual indices are hidden from sight.

If we fix a spin configuration \(\{\sigma\}\), the coefficient \(c_{\sigma_1\sigma_2\cdots\sigma_N}\) is equal to a product of matrices, hence the name “matrix product state”.

**Left, right, and mixed canonization**

As we will see, there are many ways of expressing the same wave function using the MPS representation. This is often called the gauge degrees of freedom of the MPS representation. The procedure in the previous section is called left canonization. The successive SVDs leave the MPS in the left canonical gauge, This can simplify the evaluation of local observables to some extent. For example, given a local operator \(O\) with
support on site\(K\) only, we have

\[
\langle \psi | O | \psi \rangle = \sum_{\{\sigma\}} \left[ U_{1}^{\sigma_{1}} U_{2}^{\sigma_{2}} \cdots U_{N-1}^{\sigma_{N-1}} R_{n}^{\sigma_{n}} \right]^{\dagger} O_{\sigma_{K}, \sigma_{K}} \left[ U_{1}^{\sigma_{1}} U_{2}^{\sigma_{2}} \cdots U_{N-1}^{\sigma_{N-1}} R_{n}^{\sigma_{n}} \right]
\]

\[
= \sum_{\{\sigma\}} O_{\sigma_{K}, \sigma_{K}} \left( R_{n}^{\sigma_{n}} \right)^{\dagger} \cdots \left( U_{2}^{\sigma_{2}} \right)^{\dagger} \left[ \left( U_{1}^{\sigma_{1}} \right)^{\dagger} U_{1}^{\sigma_{1}} \right] U_{2}^{\sigma_{2}} \cdots R_{n}^{\sigma_{n}} \tag{2.17}
\]

\[
= \sum_{\sigma_{K}, \cdots, \sigma_{N}} \left( R_{n}^{\sigma_{n}} \right)^{\dagger} \cdots \left( U_{K}^{\sigma_{K}} \right)^{\dagger} O_{\sigma_{N}, \sigma_{N}} U_{K}^{\sigma_{K}} \cdots R_{n}^{\sigma_{n}}.
\]

Essentially the tensors to the left of site \(K\) are all contracted to identities.

Similarly, one can also perform successive SVDs from the rightmost site, which is called right canonicalization

\[
\langle \psi | O | \psi \rangle = \sum_{\{\sigma\}} R_{1}^{\sigma_{1}} V_{2}^{\sigma_{2}} \cdots V_{N-1}^{\sigma_{N-1}} \left( V_{n}^{\sigma_{n}} \right)^{\dagger} \sigma_{1} \sigma_{2} \cdots \sigma_{n} \tag{2.18}
\]

But by far the most important gauge choice is the mixed canonical gauge, where one performs successive

\[
\langle \psi | O | \psi \rangle = \sum_{\{\sigma\}} U_{1}^{\sigma_{1}} \cdots U_{K-1}^{\sigma_{K-1}} R_{K}^{\sigma_{K}} V_{K+1}^{\sigma_{K+1}} \cdots \left( V_{N}^{\sigma_{N}} \right)^{\dagger} \sigma_{1} \sigma_{2} \cdots \sigma_{n} \tag{2.19}
\]

With mixed canonization, it is easy to show for a local operator \(O\) with support on site \(K\) that

\[
\langle \psi | O | \psi \rangle = \sum_{\sigma_{K}} \left( R_{K}^{\sigma_{K}} \right)^{\dagger} O_{\sigma_{K}, \sigma_{N}} R_{K}^{\sigma_{K}}, \tag{2.20}
\]

which is far simpler compared to other canonization choices. A schematic diagram is shown in Fig. 2.3.

\[
\begin{align*}
\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \;
\end{align*}
\]

Figure 2.3: Schematic diagram showing how the evaluation of a local observable can be simplified with the mixed canonical gauge. Notice that other than the site where \(O\) is applied, pairs of top and bottom blocks on all other sites contract to identities.

This simplification essentially comes from the fact that to the left (and right) of site \(K\), one already
has a set of orthonormal basis vectors for that subsystem. This has direct consequences on the Schmidt
decomposition of \(|\psi\rangle\). Given a bipartition into subsystems \(A\) and \(B\), the Schmidt decomposition of \(|\psi\rangle\) is
defined as

\[ |\psi\rangle = \sum_i \lambda_i |a_i\rangle |b_i\rangle, \quad \text{s.t.} \quad \langle a_i | a_j \rangle = \delta_{ij}, \quad \langle b_i | b_j \rangle = \delta_{ij}, \quad \sum_i \lambda_i^2 = 1, \quad (2.21) \]

where \( |a_i\rangle \) and \( |b_i\rangle \) are restricted to \( A \) and \( B \) respectively, and \( \lambda_i \)'s are called Schmidt coefficients. The Schmidt coefficients squared are equal to the eigenvalues of the reduced density matrix for the same bipartition, and are related to the von Neumann entanglement entropy according to

\[ S = \sum_i -\lambda_i^2 \ln(\lambda_i^2). \quad (2.22) \]

Figure 2.4: Schematic diagram showing how to calculate the Schmidt coefficients via SVD. The dashed vertical line on the L.H.S. denotes the cut position. The red block \( R \) is decomposed as \( R = U_3SV \), where the matrix \( V \) is absorbed into \( V_4 \). The Schmidt coefficients are on the diagonal of the diagonal matrix \( S \).

The mixed canonization provides a perfect way to calculate the Schmidt coefficients. It is easy to show that

1. If one labels the subsystem from site 1 to site \( K \) as \( A \), and the subsystem from site \( (K+1) \) to site \( N \) as \( B \), it is easy to show that the Schmidt decomposition of \( |\psi\rangle \) will have Schmidt coefficients equal to the singular values of \( (R_K)_{a_k,\sigma_K},a_{K+1} \), as illustrated in Fig. 2.4.

2. If one labels the subsystem from site 1 to site \( (K-1) \) as \( A \), and the subsystem from site \( K \) to site \( N \) as \( B \), it is easy to show that the Schmidt decomposition of \( |\psi\rangle \) will have Schmidt coefficients equal to the singular values of \( (R_K)_{a_k,\sigma_K,a_{K+1}} \), as illustrated in Fig. 2.5.

Figure 2.5: Schematic diagram showing how to calculate the Schmidt coefficients via SVD. The dashed vertical line on the L.H.S. denotes the cut position. The red block \( R \) is decomposed as \( R = USV_3 \), where the matrix \( U \) is absorbed into \( U_2 \). The Schmidt coefficients are on the diagonal of the diagonal matrix \( S \).
Efficiency and bond dimensions

When we turn a wave function into an MPS using the left canonization described previously, the bond dimension $M$ would grow exponentially from the edge to the center. So we have

$$M_i = \min(2^i, 2^{N-1}), \quad i \in [1, N-1]. \quad (2.23)$$

So far we have not taken any measures to reduce the computational cost. One possible way to increase efficiency is to drop some of the smallest singular values when performing successive SVDs, which drives the bond dimensions smaller. Since the singular values in the mixed canonical gauge is equal to the Schmidt coefficients of a corresponding bipartition, the reliability of this approach strongly depends on how fast the Schmidt coefficients drops, which is related the entanglement property of the wave function.

In the extreme case where all Schmidt coefficients are nearly the same, then there is no small ones to drop, which is basically the worst case scenario. In this case, if one cuts the system at virtual bond $K$ to separate the system into two pieces, it is easy to see that the von Neumann entanglement entropy as a function of $K$ is

$$S = \sum_{i=1}^{2^K} \frac{1}{2^K \ln(\frac{1}{2^K})} = K \ln 2, \quad K < \frac{N}{2}. \quad (2.24)$$

$S$ scales linearly with the subsystem size $K$, which is usually called volume-law entanglement entropy.

Of course there is a best case scenario where one can drop a significant number of the Schmidt coefficients without noticeable loss of precision. This is when the wave function has area-law entanglement entropy. For this case usually the Schmidt coefficients drop exponentially fast, and one can keep a small number of them at any cut position. Basically the bond dimension $M$ can be kept a constant at every virtual bond, which does not scale at all with the total system size $N$. Fortunately, for many of the problems we are interested in, such as the ground states of gapped 1D systems [104] and eigenstates of fully many-body localized systems, the wave functions all have area-law entanglement.

Another special case is the ground states of 1D critical systems, where the entanglement entropy scales logarithmically with respect to the subsystem size. Here the bond dimensions required to capture the wave functions accurately would grow linearly with the total system size $N$. But it is still quite affordable.

Periodic boundary conditions

The case discussed above is usually called the open-boundary MPS, as the degrees of freedom on site 1 and site $N$ are not directly connected. Despite the name, it is still possible to represent wave functions of periodic systems with open-boundary MPSs. It just becomes trickier because the MPS needs to bridge the
short-ranged correlation between site 1 and site \( N \) through all the other sites.

Alternatively one can define a periodic MPS as

\[
|\psi\rangle = \sum_{\{\sigma\}} \text{Tr}\left(A_1^{\sigma_1}A_2^{\sigma_2} \cdots A_n^{\sigma_n}\right) |\sigma_1\sigma_2 \cdots \sigma_n\rangle.
\] (2.25)

where the trace provides a connection between site 1 and site \( N \).

Despite the simple definition, the periodic MPS has limited usage compared to the open-boundary MPS. Since the sense of left and right is lost, it is impossible to canonize a periodic MPS. As a result, there is no direct method to turn a normal wave function into a periodic MPS. Even if one succeeds, one needs to rely on transfer matrices to evaluate local observables with periodic MPS, and there is no easy way to calculate entanglement entropy.

### 2.2.2 Matrix product operators

An operator \( O \) with support on all \( N \) sites can be represented as a matrix product operator

\[
O = \sum_{\{\sigma\},\{\sigma'\}} O_1^{\sigma_1,\sigma_1'} O_2^{\sigma_2,\sigma_2'} \cdots O_n^{\sigma_n,\sigma_n'} |\sigma_1\sigma_2 \cdots \sigma_n\rangle \langle \sigma'_1\sigma'_2 \cdots \sigma'_n|,
\] (2.26)

where for any site \( i \), there are four matrices \( O_i^{\uparrow\uparrow}, O_i^{\downarrow\downarrow}, O_i^{\uparrow\downarrow}, O_i^{\downarrow\uparrow} \). Operators which consist of short-range interactions can be very efficiently represented as MPOs, where the size of the matrices usually grows linear with the interaction range. Most commonly, one needs to turn a Hamiltonian \( H \) into an MPO, like in the DMRG algorithm. Unlike the MPS case, turning an 1D Hamiltonian \( H \) into an MPO should never rely on the matrix form of \( H \) and SVDs. Often the MPO is constructed by reading how an operator on site \( i \) is connected to operators on other sites in \( H \).

For example, the Hamiltonian in Eq. (1.13) with open boundary conditions can be represented as the following MPO

\[
O_i^{\sigma_i,\sigma_i'} = |\sigma_i| \begin{bmatrix}
I & S_i^z & S_i^- & S_i^+
\end{bmatrix} |\sigma_i'\rangle,
\] (2.27)

\[
O_i^{\sigma_i,\sigma_i'} = |\sigma_i| \begin{bmatrix}
I & S_i^z & S_i^- & S_i^+
\end{bmatrix} |\sigma_i'\rangle, \quad (1 < i < N),
\] (2.28)
\[
O^{\sigma_N,\sigma_N'}_{N} = \langle \sigma_N | \begin{bmatrix}
I \\
h_N S^z_N \\
S^+_N \\
S^-_N 
\end{bmatrix} | \sigma_N' \rangle. 
\]

(2.29)

Ignoring the \( \langle \sigma_i | \) and \( | \sigma_i' \rangle \), it is easy to verify that multiplying the above matrices together one after another results exactly in the Hamiltonian in Eq. (1.13).

A simple observation of the above MPO (on sites 1 < i < N) is that the first column connects operators on site \( i \) to operators to its left, while the second row connects operators on site \( i \) to operators to its right. More examples can be found in Ref. [103].

### 2.2.3 Density matrix renormalization group

In previous sections, we discussed how to transform a given exact wave function into the MPS format. In numerical simulations, however, the MPS representation is prominently used as a variational ansatz, where the matrices on every site are viewed as variational parameters. Using the MPS as a variational ansatz, the DMRG algorithm can be made very easy to understand.

![Diagram](image)

Figure 2.6: Variational prescription of the DMRG algorithm. The red block represents the matrices to be optimized at this step. The mixed canonical gauge is used so the white blocks of the MPS contract to identity. If one regards the red block as a “vector”, and the remaining part of the L.H.S. diagram as a “matrix” (or the effective Hamiltonian), then the diagrammatic equation above is exactly an eigenvalue equation. To update the red block, one replaces the original matrices with the lowest energy “eigenstate” of the effective Hamiltonian, then moves on to update the neighboring site. Usually one sweeps through the MPS multiple times until the energy converges. The accuracy of the ground state energy and MPS are determined by the bond dimension of the MPS. The cost of DMRG is linear in system size, compared to the exact diagonalization (ED) method which scales exponentially with system size \( L \).

For a given Hamiltonian \( H \) and a variational wave function \( | \psi \rangle \), one can drive \( | \psi \rangle \) towards the ground state wave function by minimizing the objective function,

\[
f = \langle \psi | H | \psi \rangle - \lambda (\langle \psi | \psi \rangle - 1)
\]

(2.30)
where $\lambda$ is a Lagrange multiplier to enforce the normalization condition.

One can assume that $|\psi\rangle$ is an MPS

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1}_{1}A^{\sigma_2}_{2} \cdots A^{\sigma_N}_{N} |\sigma_1\sigma_2 \cdots \sigma_n\rangle,$$  \hspace{1cm} (2.31)

where the matrices are the variational parameters, and the objective function $f$ is a quadratic function of the matrices $(A^{\sigma_i}_{i})$ for every $i$.

To optimize the MPS, one then takes the first order derivative of $f$ with respect to the matrices $(A^{\sigma_i}_{i})$ on site $i$,

$$\left(\frac{d}{d(A^{\sigma_i}_{i})^\dagger}\langle\psi|\right) H|\psi\rangle - \lambda \left(\frac{d}{d(A^{\sigma_i}_{i})^\dagger}\langle\psi|\right)|\psi\rangle = 0,$$  \hspace{1cm} (2.32)

which is linear in $(A^{\sigma_i}_{i})$. As shown in Fig. 2.6, the above prescription for updating the matrices $(A^{\sigma_i}_{i})$ is equivalent to an eigenvalue problem. To drive $|\psi\rangle$ closer to the ground state, one would replace $(A^{\sigma_i}_{i})$ with the “eigenvector” with the lowest eigenvalue of the above eigenvalue problem. Usually, one would sweep through all sites several times before the MPS converges to the ground state wave function.

As a side remark, the above is the skeleton of the one-site DMRG algorithm. The bond dimensions are usually preset in the one-site algorithm. One can optimize the matrices on two adjacent sites at a time, which allows one to dynamically tune the bond dimensions.
Chapter 3

Shift-and-invert Matrix product states

This chapter is mainly based on my project in Ref. [31]. We developed two efficient algorithms for obtaining highly excited states in the MBL phase using the matrix product state representation, and demonstrated their capability on large system sizes inaccessible to the exact diagonalization method.

3.1 Introduction

Obtaining the interior eigenstates of Hamiltonian models is a key step to studying the MBL phases and the transitions. It has been recently shown that the entire spectrum of eigenstates of a MBL system can be efficiently described by a matrix product operator (MPO) [26, 53]; currently the available algorithms for constructing this MPO is through quasi-Newton optimization [37, 57], which capture rough features of the entire spectrum but do not describe individual states to high fidelity. In this section, using the fact that eigenstates of many-body localized systems obey the area law [85, 105, 106] and can therefore be efficiently represented as a Matrix Product State (MPS), we develop two algorithms that generate excited states in the MPS representation, and use them to test the basic properties of MBL in the regime of large one-dimensional systems that were previously inaccessible due to the limitations of exact diagonalization (ED). Our algorithms bear close relations to the density matrix renormalization group (DMRG) [101]. We test our algorithms on the random field Heisenberg chain as in Eq. (1.13) with open boundary conditions.

3.1.1 ES-DMRG and SIMPS

Excited States DMRG (ES-DMRG) algorithm is simple to describe and has the advantage of requiring minimal modifications to a current DMRG code. As compared to the usual DMRG algorithm explained above, when updating the matrices on a particular site, instead of the replacing the matrices with the lowest energy eigenstate of the effective Hamiltonian, one considers the eigenstate with energy closest to the energy of the current MPS, in order to minimize the amount of change in the state as our algorithm progresses.

Given a MPO \( O = H - \lambda \), the key of shift-and-invert MPS (SIMPS) algorithm is to apply \( O^{-1} \) repeatedly
to a MPS $|\psi\rangle$. However, inverting a MPO directly is not practical as (1) there is no known efficient algorithm for accurately inverting a MPO and (2) the output MPO of such an algorithm would require a bond dimension significantly larger than what is required to describe a single eigenstate. The more efficient alternative is to minimize $\|O|\varphi\rangle - |\psi\rangle\|^2$, treating the matrices in $|\varphi\rangle$ as variational parameters. Specifically, we obtain the following fixed point equation

$$\frac{\partial}{\partial \varphi^*_{i,\sigma}} \langle \varphi | O^\dagger O | \varphi \rangle = \frac{\partial}{\partial \varphi^*_{i,\sigma}} \langle \varphi | O^\dagger | \psi \rangle,$$

(3.1)

where $\partial/\partial \varphi^*_{i,\sigma}$ indicates the matrix on site $i$ and spin $\sigma$. Eq. (3.1) is described in Fig. 3.1. To apply $(H - \lambda)^{-1}$ repeatedly, one can swap $|\psi\rangle$ with $|\varphi\rangle$ until $|\varphi\rangle$ is more or less converged to $(H - \lambda)^{-1}|\psi\rangle$ or after updating each site. The latter does not produce as accurate $(H - \lambda)^{-1}|\psi\rangle$ after every swap but moves in the right direction during the sweeping procedure. The convergence of the former is mathematically well controlled and the data presented here uses this version unless otherwise noted, but the latter is significantly faster.

The convergence of SIMPS is mostly controlled by the ratio of the second dominant eigenvalue to the first dominant eigenvalue present in the state

$$\rho = \left| \frac{(E_2 - \lambda)^{-1}}{(E_1 - \lambda)^{-1}} \right| = \left| \frac{E_1 - \lambda}{E_2 - \lambda} \right| < 1$$

(3.2)

where $E_1$ is the eigenvalue of $H$ closest to $\lambda$ and $E_2$ is the second closest to $\lambda$. As an example, given an MPS $|\psi\rangle = a|E_1\rangle + b|E_2\rangle + \cdots$ (where other states whose energies far away from $\lambda$ are left out), the MPS $|\varphi\rangle = (H - \lambda)^{-N}|\psi\rangle$ has an energy of

$$\langle E \rangle \approx \frac{E_1 + E_2 \frac{|b|^2}{|a|^2} \rho^{2N}}{1 + \frac{|b|^2}{|a|^2} \rho^{2N}}$$

(3.3)

Therefore, the energy of the MPS decays exponentially in $N$. To increase the convergence speed, one can fine tune $\lambda$ such that $\rho$ is much smaller than 1, by fitting the energy trace of $\langle E \rangle$ vs. $N$ accumulated during a particular run to Eq. (3.3). See fig. 3.2 for a prototypical example of SIMPS converging and an example
of this decay with a poorly chosen value of $\lambda$.

![Figure 3.2: A slow converging case of SIMPS for $L = 10$, $W = 8$ and $M = 12$ with a poorly chosen initial $\lambda$. After 240 power iterations, the MPS has not yet converged (only the last 120 iterations are shown and fitted). To fine tune $\lambda$, one can fit the energy versus number of iterations to a function taking the form of Eq. (3.3). The results in many cases are useful in learning how to tune $\lambda$ as the fitted targeted energy $E_1$ is an option. For the case displayed above, $E_1$ to high precision is already close to the ED eigenvalue 0.125020071154.](image)

A useful metric to quantify the quality of eigenstates found by our algorithms is $\sigma = \sqrt{\langle H \rangle^2 - \langle H^2 \rangle}$. Note that while a true eigenstate has $\sigma = 0$, numerically calculated standard deviations are limited by machine precision (due to the square root the limit is one part in $\sim 10^7$). We find that, using SIMPS at $M = 60$, we can obtain eigenstates of chains of length $L = 30, 40$ and $W = 8$ with values of $\langle \sigma \rangle$ peaked at machine precision (see fig. 3.4). These tests are conducted for the worst case scenario, with $\lambda$ targeted at the middle of the energy spectra where the density of states is near maximum. Running ES-DMRG at $M = 20$ for chains with $\{L = 30, W = 8\}$ and $\{L = 100, W = 10\}$, we find approximate eigenstates with $\langle \log_{10}(\sigma) \rangle$ somewhat larger than SIMPS.

### 3.1.2 Generating excited states

In order to compare with ED, we consider a fixed disorder sample with system size $L = 10$ and disorder strength $W = 8$, limiting the bond dimension to $M = 12$. Since ES-DMRG can’t target particular energies, we run the algorithm many times verifying that the energies it finds match those of the true Hamiltonian (see Fig. 3.3). In SIMPS, we have a tunable shift parameter $\lambda$ and focus on the energy window of $\lambda \in [-0.1, 0.1]$, within which there are 12 eigenstates as shown by ED. When running at a limited bond dimension with fixed initial conditions, the SIMPS algorithm does not always hit the targeted eigenstate. Remarkably, it does find an eigenstate near the desired energy with high fidelity; for $L = 10, M = 12$ we never see a situation
where the fidelity is less than $10^{-5}$. Fig. 3.3 shows the eigenvalues identified during a $\lambda$ sweep for different initial conditions and bond-dimensions of SIMPS.

We verify the found eigenstates aren’t biased toward low entanglement by comparing histograms of entanglement entropies for eigenstates generated using ED to those generated using SIMPS and ES-DMRG at artificially reduced bond-dimension $M=12$.

Another useful metric to quantify the quality of eigenstates is $\sigma = \sqrt{\langle H \rangle^2 - \langle H^2 \rangle}$. Note that while a true eigenstate has $\sigma = 0$, numerically calculated standard deviations are limited by machine precision (due to the square root the limit is one part in $\sim 10^7$).

We find that, using SIMPS at $M = 60$, we can obtain eigenstates of chains of length $L = 30, 40$ and $W = 8$ with values of $\langle \sigma \rangle$ peaked at machine precision (see fig. 3.3). These tests are conducted for the worst case scenario – we target $\lambda$ exactly to the middle of the energy spectra (lowest and highest energies calculated by DMRG) where the many-body density of states is near maximum. Running ES-DMRG at $M = 20$ for chains with $\{L = 30, W = 8\}$ and $\{L = 100, W = 10\}$, we find approximate eigenstates with $\langle \log_{10}(\sigma) \rangle$ somewhat larger than SIMPS. For long chains, the inter-level spacing is smaller than the $\sigma$ which can be resolved by machine precision, and we need to tune the target energy $\lambda$ and use fidelity to validate these states as shown in the right panel of Fig. 3.3.

### 3.1.3 Many-body localization in large systems

We now use the developed tools to test, in system sizes inaccessible to ED, three key properties of the MBL phase: failure to thermalize, low entanglement entropy of highly excited eigenstates, and the existence of a
The second key property that we investigate is the mid-bond entanglement entropy of highly excited states. The value of $\langle \log_{10}(\sigma) \rangle$ for chains of length $L$ lies in a narrow band, with the position of the maximum depending on the disorder strength $W$. Figure 3.4 shows that for $W \leq 5$ the values are not necessarily reliably converged. Green point is ES-DMRG at $M = 20$, blue line is $W = 10$, and the light blue line is SIMPS at $M = 20$, $L = 100$. The dark green point is SIMPS at $M = 20$, $L = 30$ showing that ES-DMRG and SIMPS agree to the same accuracy at the same bond dimension and chain length. Red line is SIMPS $M = 200$, $L = 30$ computed using the faster sweeping. Insets are distributions of $\sigma$ at the respective parameters.

Figure 3.5: **Left:** Value of $\langle S^z_0 \rangle$ as a function of energy at $L = 30$ for a fixed disorder configuration with disorder strength $W = 10$. Eigenstates are obtained using SIMPS, with $M = 40$. Note the small energy range. The energy scan was performed with 200 $\lambda$ evenly spaced in $[-0.1, 0.1]$. In the $S^z_0 = -3, -2, -1, 0$ sectors, a total of 74 distinct MPSs were found. **Right:** Value of $\langle S^z_0 \rangle$ for $L = 16, W = 0.8$ generated using ED.

We test the failure of ETH by computing the expectation value of a representative local observable $\langle S^z_0 \rangle$ for two chains: one with $L = 16$ at $W = 0.8$ (expected to obey ETH) and another with $L = 30$ at $W = 8$ (expected to violate ETH). As shown in Fig. 3.5, the corresponding $\langle S^z_0 \rangle$ vary wildly confirming the violation of ETH. On the other hand, for $W = 0.8$ ETH prevails – $\langle S^z_0 \rangle$ lies in a narrow band, with the position of the band depending on the global conserved quantity $S^z_0$.

The second key property that we investigate is the mid-bond entanglement entropy of highly excited eigenstates. In Fig. 3.5 we plot the mean mid-bond entanglement entropy as a function of disorder strength for chains of length $L = 14$ (ED) and $L = 30, 40$ (SIMPS). We observe that for $W > 4$ the mid-bond
entanglement entropy is essentially independent of system size, thus confirming the predicted saturation in the MBL phase. On the other hand for $W < 4$ the ED and SIMPS data strongly disagree. We attribute this disagreement to the failure of SIMPS to find high quality eigenstates in this near-ergodic and ergodic regime as demonstrated in Fig. 3.4.

The third property that we investigate is the existence of a large number of local excitations of the system. In Fig. 3.6 we show a spectrum of these local excitations constructed with respect to an eigenstate at $E = -15.002$. The local excitations on a given site are obtained by changing the matrices of a reference MPS with eigenstate of the effective Hamiltonian on that site.
Chapter 4

Efficient diagonalization of full MBL Hamiltonians using Wegner unitary gates

This chapter is mainly based on an unpublished project done in collaboration with David Pekker and Bryan Clark. An extension to continuous Wegner flow can be found in Appendix B.

4.1 Introduction

The many-body localized (MBL) phase is a dynamic phase of matter in which ergodicity breaks down. The system is called fully many-body localized (FMBL) if it is MBL at all energy densities.

There are three complementary ways to describe the FMBL phase. First, a Hamiltonian in the FMBL phase can be diagonalized by unitaries whose matrix-product operator (MPO) representation has small bond dimensions [26, 53]; equivalently this unitary can be represented by a small quantum circuit.

Secondly, the eigenstates of FMBL are area-law with a very special structure: all $2^n$ eigenstates are generated by building matrix product states from all combinatorial combinations of two sets of $n$ G and E tensors [26]. These eigenstates can be directly read off of the unitary MPO.

Finally, there are $n$ local Hermitian operators, called l-bits which commute with each other and the Hamiltonian. This latter fact is both implied by the existence of a small-bond dimension MPO [26] and implies [53] a small bond-dimension MPO. From the unitary MPO, the MPO for the $n$ l-bits can be constructed by computing $U\sigma_z U^\dagger$.

Therefore both all the eigenstates and l-bits are encoded in the unitary MPO. While Ref. [26] generated these matrix-product operators through an exponential $2^{3L}$ algorithm in system size $L$, they also suggested that the existence of these small MPO’s would make them an efficient variational basis for diagonalizing many-body localized Hamiltonians. Ref. [37] successfully carried out this program showing how to variationally generate the unitary MPO. This variational approach was able to produce some finite bond-dimension MPO at polynomial cost but still required $\exp[L]$ time for the general finite-bond dimension MPO. More recently, ref [57] has proposed an alternative approach to variationally generating MPO’s with smaller cost but that is still exponential for the general finite-bond dimension MPO.
Both of these latter works variationally optimize the MPO by explicitly defining an objective function over a quantum circuit and finding local extrema of this objective function by using conventional quasi-Newtonian optimization method. The necessary requirement for optimization is fast evaluation of the objective function and an optimization procedure. In ref. [37], the choice of the objective function is the average of the variance of all excited states of the Hamiltonian,

$$V \equiv \frac{1}{\dim(H)} \left( \Tr[H^2] - \sum_i E_i^2 \right) \quad (4.1)$$

where $E_i = \langle i | U H U^\dagger | i \rangle^2$, $U$ is the unitary matrix which is used to diagonalize the Hamiltonian and $|i\rangle$ is the $i$'th product state. For a single layer of quantum gates, the evaluation of $\Tr[H^2]$ as well as $E_i$ can be straightforwardly contracted (in time $M^3$ where $M$ is the bond-dimension of the unitary MPO). Ref. [37] developed an elegant $M^5$ algorithm for contracting a tensor network which represents $\sum_i E_i^2$. The work of ref. [57], uses a different objective function which can be evaluated, for a single layer, in time $M^3$. It is interesting to note the naive Monte Carlo algorithm can compute the variance in $O(M^3)$ time restoring many of the benefits of the alternative objective function of ref [57] for the variance.

Unfortunately, all previous algorithms have a computational complexity that is exponential in the number of layers of quantum gates and consequently requires exponential time in system size $L$ to optimize over arbitrary finite bond-dimension MPO. This latter fact follows from the existence of finite bond-dimension MPO which require circuits linear in system size to represent. While variational approaches are powerful, there has been recent interest in viewing the unitary matrix which diagonalizes Hamiltonians as a renormalization flow. Such a process is more naturally considered in the context of a constructive procedure which ‘flows’ the Hamiltonian from the local basis to the diagonal basis.

The primary contributions of this work are two-fold:

**Constructive quantum circuits:** We develop a constructive procedure for building finite-bond dimension MPO through the constructive generation of Wegner unitary gates. Each gate is considered once, and there is no optimization. This procedure is polynomial in circuit depth (for circuits which can be represented by a finite bond-dimension MPO throughout the constructive process). Unfortunately, while this procedure generates accurate MPO (competitive with those formed by variational optimization at the same depth), the accuracy as a function of circuit depth eventually plateaus. This actually is a previously unreported problem even with variational optimization of MPO. Our constructive approach allows gates of arbitrary length to be used (including non-local gates) with a cost that scales (for local gates) as $2^{3\ell}$ where $\ell$ is the length of a gate. We find, in the MBL phase (but not outside it), that the variance achieved decays
exponentially fast with gate length. Unfortunately, for reasonable MBL disorder strengths, the exponential cost rises faster than exponential increase in accuracy.

**Polynomial Time Variational Optimization:** In addition to the constructive approach, we consider again the approach of variational optimization; we develop the first polynomial (in system size) time scheme for diagonalizing MBL matrix-product operators. To accomplish this, we show how to compute each optimization step in time which doesn’t grow exponential in circuit depth (and hence system length $L$) for finite-bond-dimension MPO (obviously this is impossible for general linear-depth circuits). In the process we also show how to improve the single-layer computational complexity for the variance objective function from $M^5$ to $M^3$ allowing one to gain much of the benefit from variance optimization that using another objective function gains. Unfortunately, the optimization used in previous works which optimizes a single gate at a time appears to have a similar problem as our constructive approach; the accuracy as a function of circuit depth eventually plateaus. To resolve this, we develop a new approach to optimization which seems immune to this problem. We additionally demonstrate that, instead of working with quantum circuits, it is possible to directly optimize the MPO.

To benchmark our algorithm, we study the standard model of MBL – the Heisenberg chain with random magnetic fields.

$$H = \sum_i (S_i \cdot S_{i+1} + h_i S_i^z), \ h_i \in [-W, W], \ p(h_i) = \frac{1}{2W},$$  \hspace{1cm} (4.2)

with open boundary conditions. Notice with this Hamiltonian we can assume that all unitary matrices are real and hence orthogonal matrices.

### 4.2 Explanantion of the methods

#### 4.2.1 Unitary gates

We build a unitary MPO through the application of a number of unitary gates. Each gate will be a unitary which acts on $l$ nearest neighbor sites. When we build our circuit constructively we will generate one gate $G_i$ at a time, allowing our final unitary to be $U = \prod_i G_i$. Our algorithm’s efficiency depends on the number of gates but does not (explicitly) depend on the pattern of gates. This means that we can use, among others, gate patterns which consist of low-depth Suzuki-trotter gates (see fig. 6) as well as high depth (linear) staircase gates (see fig. 1)
4.2.2 Constructive unitary gates diagonalization procedure

Our algorithm for constructively generating a unitary MPO of a FMBL Hamiltonian \( H \) is summarized below. As input to our algorithm, we choose the length of each unitary gate \( \ell \). At each step \( T \) in the algorithm we have a Hamiltonian \( H(T) \) represented as a MPO which has a bond dimension \( M(T) \). The original Hamiltonian is \( H(0) \).

1. Given \( H(T) \) for a FMBL system of length \( L \), select a consecutive set of \( \ell \) sites. We will put our unitary gate on these \( \ell \) sites. Trace out the Hamiltonian on all other sites. This leaves an effective Hamiltonian in a Hilbert space of size \( 2^\ell \). This operation costs \( O(L M(T)^3) \).

2. Explicitly construct the effective \( 2^\ell \times 2^\ell \) Hamiltonian and diagonalize it using the Wegner flow equations (see below) constructing the unitary gate \( U_i \) (called Wegner unitary gate). The way the Wegner unitary gates are constructed is shown in Sec. 4.2.4. This step costs \( O(2^{3\ell}) \).

3. Compute the average variance \( V \) of the Hamiltonian \( U_i H(T) U_i^\dagger \). An efficient way of evaluating the average variance \( V \) is discussed in Sec. 4.2.5. In the tensor network language, the cost is equivalent to bringing the matrix product operator (MPO) of the transformed Hamiltonian into a canonical form. This costs \( O(M(T)^3) \). Accept this Wegner unitary gate if average variance \( V \) decreases, and reject it otherwise.

4. If it’s accepted, contract the unitary gate into the MPO \( H \). This costs \( O(M(T+1)^3) \), and changes the bond dimensions from \( M(T) \) to \( M(T+1) \).

5. Iterate this procedure until no gate decreases the variance.

An example of the above procedure using tensors diagram is shown in Fig. 4.1.

Notice that the cost of this algorithm is cubic in the largest bond-dimension reached of the effective Hamiltonian. We keep a small SVD cutoff of \( 10^{-12} \) while doing so and never notice any effect of this truncation on the average variance \( V \). As a practical matter, we usually repeat calculations with two different bond dimensions or truncation errors, and verify that the results don’t change.

Empirically, we found that diagonalizing FMBL Hamiltonians with Wegner unitary gates at small \( M \) did not stand as a problem at all. There are at least two reasons. Firstly, FMBL Hamiltonians have an extensive number of conserved quantities that are exponentially localized. This means that the systems favor the MPO representation which is very efficient for capturing short range interactions. Secondly, when one applies a unitary transformation to such Hamiltonians, if the transformation, just like a Wegner unitary transformation, does not scramble the local degrees of freedom, the resulting Hamiltonians will still be short.
Figure 4.1: This figure illustrates our scheme of tiling the FMBL Hamiltonian with Wegner unitary gates of length $\ell$ (here $\ell = 4$). The pink squares are the tensors of MPO $H$, the green boxes are Wegner unitary gates. The first Wegner unitary gate is placed at a sub-system that has the leading energy scale (maximum local energy gap). New gates are placed one after another at adjacent positions if they lower the average variance $V$ as defined in (4.1). This figure is produced for one sample with $L = 8, W = 8, \ell = 4$, whose other information are displayed in Fig. 4.3 and Fig. 4.4. The gates diagrams remain the same for two different maximum bond dimensions of $M = 30$ and $M = 48$.

ranged and a small bond dimension MPO will suffice. This is generally not achievable when working with random unitary gates, especially for longer gates.

A couple comments about our procedure are in order. To begin with, gates are never revisited. Second, because there is no optimization step there are no problems with local minima. Third, although we compute the variance so as to ensure monotonicity, it is not necessary and we can compute it less often.

4.2.3 Wegner flow equations

We use the Wegner flow equations to diagonalize the small effective Hamiltonian [107, 108]. This is a deterministic process which (heuristically) generates a short quantum circuit.

Wegner flow generates a continuous unitary transformation with flow equations

$$\frac{dH(\beta)}{d\beta} = [\eta(\beta), H(\beta)], \quad \frac{dU(\beta)}{d\beta} = \eta(\beta)U(\beta). \quad (4.3)$$

In the integral form, they can be rewritten as

$$H(\beta) = U(\beta)H(0)U^\dagger(\beta), \quad U(\beta) = Te^{\int_0^\beta \eta(\tau)d\tau}, \quad (4.4)$$

where the anti-Hermitian operator $\eta(\beta)$ is the generator of the one-parameter flow, and $T$ represents time.
ordering. For complete diagonalization, one often uses the canonical generator

$$\eta(\beta) = [H_0(\beta), H_1(\beta)],$$

(4.5)

where $H_0(\beta)$ and $H_1(\beta)$ are respectively the diagonal and off-diagonal parts of the Hamiltonian under a chosen set of basis vectors. For results and discussion below, we mainly use the $S_z$ basis, because the systems we study are dominated by the random fields in the $z$-direction at large disorder strength.

One can show that

$$\frac{dV}{d\beta} \equiv \frac{1}{\dim(H)} \frac{d}{d\beta} \text{Tr}(H^2_1) = -\frac{2}{\dim(H)} \text{Tr}(\eta^\dagger \eta) \leq 0,$$

(4.6)

which ensures that the off-diagonal term shrinks as long as the generator $\eta(\beta)$ does not vanish.

As shown above, the Wegner flow unitary matrix $U(\beta = \infty)$ diagonalizes the Hamiltonian, and is continuously connected to the identity. In the case of FMBL Hamiltonians, especially spin-$\frac{1}{2}$ models, this means that the bare spin basis $\{\sigma\}$ can be continuously tuned into the l-bit basis $\{\tau\}$, which suggests that the Wegner unitary transformation $U(\beta = \infty)$ is void of swapping and scrambling operations that may destroy the local properties of the systems, as compared to other unitary transformations that also diagonalize the same Hamiltonians. This might be the very reason that Wegner flow equations have been successfully applied to studying the l-bit structures in [50, 55, 109–111].

### 4.2.4 Construction of Wegner unitary gates

To obtain an effective Hamiltonian for a subsystem, one needs to trace out degrees of freedom not in the subsystem. In the MPO language, this operation is particularly simple, as shown in Fig. 4.2. Because of the small subsystem sizes that we are dealing with, the effective Hamiltonian can easily be stored as a dense matrix.

Once we have the effective Hamiltonian, we can numerically solve the flow equations in Eq. (4.3) using the Runge-Kutta-Fehlberg method (denoted RK45, or RKF45) [112], which is a method of order 4 and allows for adaptive step size control. At a first glance, to obtain the final unitary matrix $U(\beta = \infty)$ which diagonalizes the effective Hamiltonian, one would have to run the Wegner flow indefinitely. But it is obvious that if we diagonalize the small effective Hamiltonian using a dense direct solver, the obtained unitary matrix $\tilde{U}$ differs with $U(\beta = \infty)$ only by a permutation, and an unimportant phase factor. Therefore, in order to
terminate the flow at an intermediate $\beta$, one just need to check if

$$P \equiv U(\beta)^\dagger \tilde{U}$$

(4.7)

is close to a permutation matrix. To check this, for each row (or column) of $P$, one replaces the element with largest magnitude with $\pm 1$ depending on the sign, and the others with 0. This procedure will produce a new matrix $\tilde{P}$. If $\tilde{P}$ satisfies $\tilde{P}^\dagger \tilde{P} = I$, then

$$U(\beta = \infty) = \tilde{U} \tilde{P}^\dagger$$

(4.8)

Using this approach, the final unitary matrix $U(\beta = \infty)$ can be found very quickly. It is then converted to an MPO, or a Wegner gate, according to Eq. (2.26), by performing a series of singular value decomposition (SVD).

Figure 4.2: An example of obtaining a 4-site effective Hamiltonian from an 8-site Hamiltonian, in the MPO representation. Note the vertical indices stand for the actual physics degrees of freedom (spin up/down). The traced out sites have small loops connecting the upper and lower physical indices, which is usually called contraction. After all the contractions, we get an MPO that effectively looks like one with only 4 sites. To get the correct normalization, each traced out site should be accompanied by factor of $1/2$.

### 4.2.5 Evaluate average variance

At every step of the simulation, the MPOs of the real symmetric Hamiltonian $H$ and the real symmetric unitary gates (represented in whole as $U$) are compressed into a single MPO $\tilde{H}$, whose bond dimension is limited by $M$. So

$$\tilde{H} = U^\dagger HU$$

(4.9)

In the case of FMBL Hamiltonian and Wegner unitary gates, empirically we do not find any problem with using a small bond dimension $M$. When evaluating the average variance $V$ defined in Eq. (4.1), the expression we actually use is

$$V \equiv \frac{1}{2L} \sum_{\{\tau\}} \left[ \langle \{\tau\}|\tilde{H}^2|\{\tau\} \rangle - \langle \{\tau\}|\tilde{H}|\{\tau\} \rangle^2 \right]$$

(4.10)
Considering the MPO representation of \( \tilde{H} \) (of length \( L \)) as in Eq. (2.26), on site \( i \), there are 4 matrices (spin-\( \frac{1}{2} \) model), labeled by \( A_{i}^{[\tau_{i}, \tau'_{i}]} \), where \( \tau \) can be either up (+) or down (−).

For the first part of the summation,

\[
\sum_{\{\tau\}} \langle \{\tau\} | \tilde{H}^{2} | \{\tau\} \rangle = \sum_{\{\tau\}, \{\tau'\}} \left( A_{1}^{[\tau_{1}, \tau'_{1}]} A_{2}^{[\tau_{2}, \tau'_{2}]} \cdots A_{L}^{[\tau_{L}, \tau'_{L}]} \right)^{2}.
\] (4.11)

To better understand the above tensor expression, one may assume that there exists an MPS (or wave-function) \( |\phi\rangle \), whose physical degrees of freedom on each site are labeled by a pair of bits as \( (\tau, \tau') \), and

\[
|\phi\rangle = \sum_{\{\tau, \tau'\}} A_{1}^{[\tau_{1}, \tau'_{1}]} A_{2}^{[\tau_{2}, \tau'_{2}]} \cdots A_{L}^{[\tau_{L}, \tau'_{L}]} |(\tau_{1}, \tau'_{1})(\tau_{2}, \tau'_{2}) \cdots (\tau_{L}, \tau'_{L})\rangle
\] (4.12)

It is then clear that

\[
\sum_{\{\tau\}} \langle \{\tau\} | \tilde{H}^{2} | \{\tau\} \rangle = \langle \phi | \phi \rangle,
\] (4.13)

which is just the norm of the MPS \( |\phi\rangle \), and can be very efficiently calculated using tensor contractions at a cost of \( O(4LM^{3}) \), especially when \( M \) is small.

For the second part of the summation,

\[
\sum_{\{\tau\}} \langle \{\tau\} | \tilde{H} | \{\tau\} \rangle^{2} = \sum_{\{\tau\}} \left( A_{1}^{[\tau_{1}, \tau_{1}]} A_{2}^{[\tau_{2}, \tau_{2}]} \cdots A_{L}^{[\tau_{L}, \tau_{L}]} \right)^{2}.
\] (4.14)

In the above summation, on any site, only 2 out of 4 matrices are used. One can also make a MPS \( |\psi\rangle \), whose physical degrees of freedom on each site are labeled by \( \tau \),

\[
|\psi\rangle = \sum_{\{\tau\}} A_{1}^{[\tau_{1}, \tau_{1}]} A_{2}^{[\tau_{2}, \tau_{2}]} \cdots A_{L}^{[\tau_{L}, \tau_{L}]} |\tau_{1} \tau_{2} \cdots \tau_{L}\rangle
\] (4.15)

Similarly,

\[
\sum_{\{\tau\}} \langle \{\tau\} | \tilde{H} | \{\tau\} \rangle^{2} = \langle \psi | \psi \rangle,
\] (4.16)

which is just the norm of the MPS \( |\psi\rangle \), and can be very efficiently calculated at a cost of \( O(2LM^{3}) \).

The re-arrangement of the MPO \( \tilde{H} \) into the MPS \( |\phi\rangle \) or \( |\psi\rangle \) above does not take any extra effort, as the tensors involved are exactly the same.
4.3 Constructive generate unitary MPO

4.3.1 Proof of concept

As a proof of concept, we apply the diagonalization scheme, discussed in Sec. 4.2.2, to a disordered sample with system size of $L = 8$, disorder strength $W = 8$, and gate lengths $\ell = 2, 3, 4$. The resulting gate diagram, the convergence history, and the energy spectrum are shown in Fig. 4.1, Fig. 4.3, and Fig. 4.4, respectively. The gate diagram, Fig. 4.1 shows the ordering of gates that we applied for this example. Gates that are ‘missing’ are those that increased the variance and so we skipped; we find similar behavior independent of this step. From Fig. 4.4, one can directly see the effectiveness of using Wegner unitary gates, whose right panel is a zoomed-in view of the middle of the spectrum. As we increase the gate length, our accuracy goes up significantly. In Fig. 4.3 we see the variance decrease as a function of number of gates. Once the entire system is covered with gates, there is minimal decrease of variance as more gates are included. We find that this saturation is a consequence of optimizing one gate at a time and we see a similar problem using variance optimization. Notice, again that the quality as measured by variance increases significantly as the gate length increases.

There are a few things to notice. Firstly, for a fixed $\ell$, the average variance $V$ decreases rapidly with the number of Wegner unitary gates applied, until, empirically, the entire MPO $H$ is covered once by the unitaries. This can be seen by matching the gates in Fig. 4.1 with the green curve in Fig. 4.3. Applying more unitaries after that usually does not provide any significant benefits. We have also seen this behavior
in all other disorder samples at different system sizes, gate lengths, and disorder strengths. Secondly, the final, converged average variance decreases with \( \ell \), which serves as a control parameter to this algorithm. Thirdly, as in Fig. 4.4, the accuracy of diagonalization is inversely related to \( \ell \), or the average variance \( V \).

### 4.3.2 Systematic analysis

Besides this, we have done systematic simulations at system sizes of \( L = 12, 20, 40, 60, 80, 100 \), for \( W = 4, 6, 8, 10, 12, 14, 16 \) and \( \ell = 2, 3, 4 \). For each sample and each configuration, the algorithm is run with two different truncation errors to make sure the results are converged. The final disorder-averaged \( \log_{10} V \) and the disorder averaged bond dimension \( M \) are shown in Fig. 4.5. Interestingly, given a unitary gate’s length \( \ell \), the disorder averaged variance per site seems to saturate at large system size, as in Fig. 4.6.

As can be seen, although we have not used any quasi-Newton optimization methods, the Wegner unitary gates alone are already producing final average variances that are similar, or even better than the numbers previously reported in [37, 57], the latter of which, to be fair, uses a very similar indicator but not exactly the same as the average variance.

The only bottleneck of this method lies in the gate length \( \ell \), because the size of the unitary matrices grow exponentially with \( \ell \). This creates an exponential slowdown when building longer Wegner unitary gates. In the quasi-Newton optimization methods, this also means exponentially many variational parameters.
4.3.3 Comparison with Quasi-Newtonian method

In this section, we compare the performance of Wegner unitary gates diagonalization with quasi-Newton optimization method. The particular quasi-Newton method we use is the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm [113, 114]. The actual code is ported from a FORTRAN implementation by Jorge Nocedal.

For simplicity, we only look at system size of $L = 12$ and gate length of $\ell = 2$. For this case, each unitary gate is a $4 \times 4$ unitary matrix. Since we only consider real matrices, the unitary matrices are just orthogonal matrices, thus can be described by 6 rotational angles – each characterizing a rotation in a 2D plane. This is exactly the way we use to parametrize the unitary matrices for quasi-Newton optimization. The objective function for the quasi-Newton method is the average variance $V$.

The particular comparisons done are listed as follows.


2. Wegner unitary gates diagonalization plus quasi-Newton optimization versus pure quasi-Newton opti-
Figure 4.6: Disorder-averaged $V$ vs system size $L$, obtained from Wegner unitary gates diagonalization of 100 disorder samples with $W = 16$ and $\ell = 2, 3, 4$, with SVD cutoffs of $10^{-9}$ (black dots) and $10^{-11}$ (colored solid lines). It can be seen that $\log_{10} V$ obtained grows weakly with system size.

3. Wegner unitary gates diagonalization plus quasi-Newton optimization versus pure quasi-Newton optimization starting from unitaries that are identity matrices.

Especially, to better compare with previous studies [37, 57], we choose the gates arrangement as shown in Fig. 4.7.

With this setup, for each sample, pure Wegner unitary gates diagonalization usually take seconds to finish while the pure quasi-Newton methods take hours to converge. The results are shown in Fig. 4.8. Wegner unitary gates diagonalization usually stops improving the averaged variance after one layer. It can be seen that full optimization, where all parameters are optimized at the same time, has consistently the best performance, followed by sweeping optimization method, where the optimization is done gate by gate. Wegner unitary gates diagonalization method has the highest averaged variance, but the difference between it and the other two methods is much less than a factor of 2 (because $\log_{10} 2 \approx 0.3$). Additionally, we notice that the Wegner unitary diagonalization method produces averaged variances that are very similar to those produced by the end of the first sweep of the sweeping optimization. This is further illustrated in Fig. 4.9.

It is interesting to notice that the Wegner unitary gates diagonalization method and the sweeping optimization method during the first sweep (starting with all rotational parameters set to 0) produce almost the same variance at each gate applied. This has two implications: (1) The effect of Wegner unitary gates diagonalization is similar to the first sweep of the sweeping optimization, but much faster; (2) The remaining small improvement of the sweeping optimization comes from revisiting the inner gates optimized earlier,
Figure 4.7: This figure shows the Suzuki-Trotter-like gates arrangement we used for the comparison with the quasi-Newton method for $L = 12$ and $\ell = 2$, which is fixed across methods for more consistent comparison. The first unitary gate is always placed at the left-bottom of the inner most layer (the first layer). (1) For the case of pure Wegner unitary gates diagonalization, each green box is a Wegner Unitary matrix, denoted by $U_W$; (2) For the case of quasi-Newton optimization, each green box is equal to $U(\theta_1, \theta_2, \cdots, \theta_6)$, where $(\theta_1, \theta_2, \cdots, \theta_6)$ parametrize the 6 rotational degrees of freedom of a real $4 \times 4$ unitary matrix. The initial value of every angle $\theta$ is zero, making $U(\theta_1, \theta_2, \cdots, \theta_6) = I$ for every gate. In general we found that setting the initial values of $\theta$ to 0, other than randomly drawn from a uniform distribution, leads to much faster convergence, and is what we used if not stated otherwise.

which means that Wegner unitary gates optimization can serve as a very good starting point.

### 4.4 Extension to multi-scale entanglement renormalization ansatz (MERA)

The constructive method designed above can be conveniently modified to generate a multi-scale entanglement renormalization ansatz (MERA) network. Basically, one can extract the l-bits at different levels of the unitary gates because they usually involve different energy scales. As shown in Fig. 4.10, where we used a gate length of $\ell = 3$, at each Wegner unitary gate, a bit that maximally splits the local energy spectrum will be designated as the approximate l-bit (red dot in the figure), and one can choose the l-bit as being either $\uparrow$ or $\downarrow$, doing so will cut down the size of the Hilbert space by half. If one repeats this step of applying Wegner unitary gates and extracting approximate l-bit, this will generate a MERA tensor network that approximate an eigenstate of the MBL system.

### 4.5 Conclusion

The algorithm discussed above is very fast and efficient for several reasons. Firstly, working with small bond dimension $M$ allows for very fast evaluation of the average variance, as compared to previous methods.
Figure 4.8: Disorder-averaged $V$ obtained from different methods, for 100 disorder samples with $L = 12, W = 8, 10, 12, 14, 16$ and $\ell = 2$. SVD cutoff is set at $10^{-11}$. All these methods use 4 layers of Suzuki-Trotter gates (the definition of a layer is shown in Fig. 4.7). But Wegner unitary gates diagonalization usually stops improving the averaged variance after one layer. It can be seen that full optimization, where all parameters are optimized at the same time, has consistently the best performance, followed by sweeping optimization method, where the optimization is done gate by gate. Wegner unitary gates diagonalization method has the highest averaged variance, but the difference between it and the other two methods is much less than a factor of 2 (because $\log_{10} 2 \approx 0.3$). Additionally, we notice that the Wegner unitary diagonalization method produces averaged variances that are very similar to those produced by the end of the first sweep of the sweeping optimization. This is further illustrated in Fig. 4.9.

Secondly, the average variance in our scheme is more like an indicator of the performance, rather than an objective function in a quasi-Newton optimization method. Therefore, for each Wegner unitary gate, in the current scheme we just need to evaluate the average variance once. One can go even further by postponing the evaluation until covering the system once with Wegner unitary gates, thus saving more computation time. In contrast, for a quasi-Newton optimization method, when optimizing the parameters in each unitary gate, the objective function, usually average variance, needs to be evaluated multiple times, as the gradient-based optimizer finds its way down the variational landscape. Not to mention that one needs to sweep through all unitary gates multiple times to reach convergence. Thirdly, we have a very efficient way of constructing Wegner unitary gates. While the Wegner flow approach is highly effective at producing a unitary constructively it does not always produce the optimal circuit because of the greediness. We also showed that it is possible to construct a MERA tensor network that can represent a MBL eigenstate.
Figure 4.9: Average variance $V$ vs number of gates applied at each step of the Wegner unitary gates diagonalization and the sweeping optimization method, for 2 disorder samples (represented separately in the top and bottom panels) with $L = 12$, $W = 8$ and $\ell = 2$. SVD cutoff is set at $10^{-11}$. These two methods use 4 layers of Suzuki-Trotter gates (the definition of a layer is shown in Fig. 4.7), 44 of them in total. The Wegner unitary gates diagonalization method, and the sweeping optimization method during the first sweep (starting with all rotational parameters set to 0) produce almost the same variance at each gate applied.

Figure 4.10: (Left:) A diagrammatic illustration of using the Wegner unitary gates to produce a MERA. (Right:) A tensor network produced for a $L = 64$ disordered Heisenberg chain with disorder strength $W = 10$. 
Chapter 5

Bimodal entanglement entropy distribution in the many-body localization transition

This chapter is mainly based on my project in Ref. [32]. We developed a new metric for gauging the behaviors of the entanglement entropy based on the strong subadditivity theorem, and used it characterized the distribution of the entanglement entropy at the transition region.

5.1 Introduction

![Graph](image_url)

Figure 5.1: **Top:** von Neumann entanglement entropies ($S$) for different fixed left cut positions as a function of subsystem size $\ell$ of a single eigenstate for one sample with system size $L = 20$ and disorder strength $h = 3.0$. Notice that the $S(\ell)$ curves are in general not differentiable. However, the cut-averaged entanglement entropy (CAEE, defined in Eq. (CAEE)) is a smooth and concave function of $\ell$. **Bottom:** Typical CAEE (denoted as $\overline{S}(\ell)$) sampled from different disorder strengths, for periodic Heisenberg chains of length $L = 20$. Each curve is generated from a single eigenstate of one disorder realization. The slope of CAEE, abbreviated as SCAEE and defined in Eq. (SCAEE), can directly probe the volume law or area law scaling behavior of an eigenstate.
The many body localization (MBL) transition is a dynamical phase transition driven by the interplay of strong interactions and disorder[7, 8]. While disordered noninteracting systems in one dimension localize for arbitrarily small disorder[1], the presence of interactions thermalizes quantum systems up to a finite critical disorder strength. This thermalization is typically expected to occur through the eigenstate thermalization hypothesis[15, 17–19] (ETH), which states that local few-body observables become a smooth function of the energy. Furthermore, their canonical expectation values match those obtained from the mixed state thermal density matrix at inverse temperature $\beta$, chosen such that the thermal expectation value of the energy $\langle H \rangle_{\beta} = \frac{1}{Z} \text{Tr} \left( e^{-\beta H} H \right)$ is equal to the eigenenergy of the state. To satisfy this, the reduced density matrix of individual eigenstates at energy $E$ becomes equal to the thermal density matrix, leading to an extensive (volume law) entanglement entropy.

On the other hand, in the MBL phase at stronger disorder the ETH is no longer valid. While ETH is a consequence of quantum chaos (a generic feature of interacting nonintegrable systems[115]), the MBL phase shows features of integrability, most prominently signaled in a change of the spectral statistics that was explored in several pioneering works [64–66] and are now a standard measure for the detection of MBL [21, 24, 30, 67, 68]. The integrability in the MBL phase is due to an emergent extensive number of local conserved quantum operators [49–51], which prohibit thermalization and lead to a subextensive (area law) entanglement entropy; this has been numerically verified in many studies[30, 31, 38–40, 85]. In particular, after the transition to the full MBL regime, nearly all eigenstates exhibit area law entanglement[31, 38, 39, 85] at arbitrarily high energies.

While the ETH is typically only expected[116] to be valid for subsystems of size $\ell$ such that $\ell/L \rightarrow 0$, evidence for the MBL transition typically considers the average half-cut entanglement entropy averaged over the ensemble of disorder realizations, finding it to either follow a volume law (in the ergodic region) or an area law (in the MBL region). In this chapter, we will consider subsystem sizes which are a constant fraction ($< \frac{1}{2}$) of the entire system.

Although the many-body localized and ergodic phases have been heavily studied, the transition between them is still subject to debate. On general grounds, it has been argued that the scaling of the entanglement entropy at the critical point should follow a volume law [95], whereas phenomenological RG calculations point to a strongly fluctuating behavior [94]. Other studies point to strong multifractal behavior at the critical point [69, 117] and the possibility of a power law scaling of the entanglement entropy as $S \propto L^\alpha$ with an exponent $\alpha < 1$ (i.e. slower than volume law) [96].

In this chapter, we consider the properties of the transition (as well as the adjoining phases), by focusing on the cut-averaged entanglement entropy (CAEE) $\bar{S}(\ell)$ (as in Eq. (CAEE)) and its slope (SCAEE) (as in
Eq. (SCAEE)) of subsystems with size $\ell$ at a fixed ratio of $\ell/L$. Cut averaging here literally means averaging over all subsystems of a particular size $\ell$. The CAEE for any eigenstate of a periodic system is a concave function of $\ell$ (cf. lower panel of Fig. 5.1 as opposed to the upper panel for the entropy without cut average). We prove this using strong subadditivity (SSA) in Sec. 5.2. The CAEE and SCAEE can be used to directly identify the volume or area law scaling in single eigenstates.

Using these concepts, we study the distribution of the SCAEE over disorder realizations. This distribution appears Gaussian at weak disorder, while at moderate disorder in the ergodic region the distribution is generically non-Gaussian for system sizes we can access, a feature that has been observed also in the distributions of the diagonal [40] and off-diagonal [41] matrix elements of local operators in the eigenbasis of the Hamiltonian. On the MBL side, the distribution of the SCAEE is peaked at zero slope and has an exponential tail. In addition, in the MBL and ergodic phases the variance of this distribution gets smaller as a function of system size $L$, which naturally suggests that the variance approaches zero in the thermodynamic limit (TDL); this would leave all eigenstates to follow either an area law (SCAEE equal to 0) or a volume law (SCAEE close to $\ln(2)$).

In the transition region, we also find that as the system size grows, $\bar{S}/L$ at a fixed subsystem ratio of $\ell/L$ appears to approach a one-parameter family of curves, which can be parameterized by the value of the CAEE or the SCAEE at any $\ell/L$.

Most interestingly, in the critical regime we find that the distribution of the SCAEE is bimodal both over multiple disorder realizations as well as for single disorder realizations. The variance of the SCAEE distribution in the transition region seems to grow with system size when considered over disorder realizations. Our system sizes are too small to pin down its maximal value, but they are consistent with (among other possibilities) the maximal variance possible which would lead to half the states having zero SCAEE and half having maximal SCAEE. This scenario would lead to an entanglement entropy at the transition which scales as a volume law with half its thermal value.

5.2 Strong Subadditivity and Entanglement Entropy under Periodic Boundary Conditions

Strong subadditivity (SSA) is a theorem of entropy, applicable to both classical and quantum entropies\(^1\). SSA of the von Neumann entropy was proved by E.H. Lieb and M.B. Ruskai in 1973 [118], and can be formulated as many equivalent inequalities[118–121]. The von Neumann entanglement entropy $S(A)$ quantifies the

\(^1\)With Rényi index 1
entanglement of subsystem $A$ with the rest of the system and is obtained from the reduced density matrix, given by a partial trace of the degrees of freedom in the complement of subsystem $A$:

$$S = -\text{Tr}_A (\text{Tr}_B |\psi\rangle \langle \psi|) \ln (\text{Tr}_B |\psi\rangle \langle \psi|).$$

(5.1)

As recently pointed out by Tarun Grover\cite{95}, for MBL systems, SSA ensures that the disorder averaged von Neumann entanglement entropy at any energy density is concave, where $\bar{S}(l, e)$ is averaged over a tiny energy density window and all disorder configurations.

Unfortunately, without disorder averaging, the curve $S(\ell)$ for individual eigenstates obeys no concavity conditions showing essentially random behavior, which stems from the local entanglement structure (cf. Fig. 5.1 Top).

In this section, we show how to use SSA to derive constraints on $S(\ell)$ in the continuum for any individual state in a periodic one-dimensional system where the von Neumann entanglement entropy is averaged over all cuts with subsystem size $\ell$. This average over all subsystems of size $\ell$ is sufficient to restore concavity for individual states (see Eq. (CAEE)) and puts constraints on the sign of the slope at different $\ell$ (see Eq. (SCAEE)). This can be used to identify whether individual states separately obey an ‘area law’ or a ‘volume law’. We note that the result in Ref. [95] for periodic systems is a direct corollary of this result as the sum of concave functions is concave.

For the following, $x$ denotes the center position of a simply connected subsystem. We define the cut-averaged entanglement entropy (CAEE) as

$$\bar{S}(\ell) \equiv \frac{1}{L} \int_0^L dx \ S(x, \ell),$$

(CAEE)
and define the slope of the cut-averaged entanglement entropy (SCAEE) as

\[ \frac{\partial \bar{S}}{\partial \ell} \equiv \frac{1}{L} \frac{\partial}{\partial \ell} \int_0^L dx \, S(x, \ell). \]  

(SCAEE)

For a density matrix of any quantum state, according to SSA, the von Neumann entanglement entropy obeys

\[ S(A) + S(B) \geq S(A \cup B) + S(A \cap B). \]  

We apply this where \( A \) and \( B \) are subsystems of equal length, but slightly shifted apart as in Fig. 5.2. Translational invariance is not assumed due to the presence of disorder and we focus on single eigenstates of a particular disorder pattern from now on.

The inequality (5.2) is equivalent to

\[ S(x, \ell) + S(x + \epsilon, \ell) \geq S(x + \frac{\epsilon}{2}, \ell + \epsilon) + S(x + \frac{\epsilon}{2}, \ell - \epsilon). \]  

(5.3)

When expanded to second order in \( \epsilon \), it becomes

\[ \frac{\partial^2 S(x, \ell)}{\partial^2 \ell} \leq \frac{1}{4} \frac{\partial^2 S(x, \ell)}{\partial^2 x}. \]  

(5.4)

For a system with periodic boundary conditions, by integrating the above equation over the entire system, it is easy to see that

\[ \frac{\partial^2 \bar{S}(\ell)}{\partial^2 \ell} \leq 0, \]  

(5.5)

because the boundary terms at \( x = 0 \) and \( x = L \) cancel each other exactly. Eq. (5.5) puts a constraint on the concavity of \( \bar{S}(\ell) \) which holds for any given eigenstate of an arbitrary disorder configuration, because SSA is applicable to the density matrix of any quantum state.

Figure 5.3: A typical arrangement of the subsystems to apply the strong subadditivity (SSA) inequality \( S(A \cup B) + S(B \cup C) \geq S(A) + S(C) \). \( A \) and \( C \) are non-overlapping, which means \( l < L/2 \), where \( L \) is the length of the entire periodic system.
There exists an essentially equivalent constraint on the first derivative of $\bar{S}(\ell)$, based on an equivalent formulation of the SSA theorem as in Fig. 5.3.

\[ S(A \cup B) + S(B \cup C) \geq S(A) + S(C), \quad (5.6) \]

When written explicitly, it becomes

\[ S(x + \frac{\epsilon}{2}, \ell + \epsilon) + S(x + \ell + \frac{\epsilon}{2}, \ell + \epsilon) \geq S(x, \ell) + S(x + \ell + \epsilon, \ell). \quad (5.7) \]

One can expand it to the first order in $\epsilon$

\[ \frac{\partial S(x, \ell)}{\partial \ell} + \frac{\partial S(x + \ell, \ell)}{\partial \ell} \geq \frac{1}{2} \frac{\partial S(x + \ell, \ell)}{\partial x} - \frac{1}{2} \frac{\partial S(x, \ell)}{\partial x}. \quad (5.8) \]

Again, with periodic boundary conditions, integrating the above equation over the entire system reduces to

\[ \frac{\partial \bar{S}(\ell)}{\partial \ell} \geq 0. \quad (5.9) \]

where $\ell < L/2$.

One can also derive the lattice version of SSA constraints. In this scenario, the $x$ and $\epsilon$ in Eq. (5.3) and Eq. (5.7) are integers (assuming lattice constant is 1). For the following discussion, we set $\epsilon = 1$.

Summing over all $x$ on a periodic lattice for Eq. (5.3) and Eq. (5.7), one easily obtains

\[ 2\bar{S}(\ell) \geq \bar{S}(\ell + 1) + \bar{S}(\ell - 1), \quad (5.10) \]

and

\[ 2\bar{S}(\ell + 1) \geq 2\bar{S}(\ell), \quad \ell < L/2. \quad (5.11) \]

Usually, one defines first and second order discrete derivatives with respect to $\ell$ as follows.

\[ \Delta^+ \bar{S}(\ell) \equiv \bar{S}(\ell + 1) - \bar{S}(\ell). \quad (5.12) \]

\[ \Delta \bar{S}(\ell) \equiv \frac{\bar{S}(\ell + 1) - \bar{S}(\ell - 1)}{2}. \quad (5.13) \]
\[ \Delta^{-} \bar{S}(\ell) \equiv \bar{S}(\ell) - \bar{S}(\ell - 1). \] (5.14)

\[ \Delta^{2} \bar{S}(\ell) \equiv \bar{S}(\ell + 1) + \bar{S}(\ell - 1) - 2\bar{S}(\ell). \] (5.15)

Then we have the following SSA constraints concerning the discrete derivatives.

\[ \Delta^{2} \bar{S}(\ell) \leq 0. \] (5.16)

\[ \Delta^{+} \bar{S}(\ell) \geq 0, \Delta \bar{S}(\ell) \geq 0, \Delta^{-} \bar{S}(\ell) \geq 0, \quad \ell < L/2. \] (5.17)

In the present work, however, we use the continuum version of the SSA constraints by an analytic continuation of the \( \bar{S}(\ell) \) curve, because it allows us to study incommensurate subsystem sizes. This is important due to the serious constraints in available system sizes from exact diagonalization.

The two constraints (5.5) and (5.9) imply that the cut averaged entanglement entropy \( \bar{S}(\ell) \) is a concave function of subsystem size with positive slope for \( 0 \leq \ell \leq L/2 \) and negative slope for \( L/2 \leq \ell \leq L \). Its negative second derivative makes the slope of larger subsystems at most equal to or smaller than the slope of smaller subsystems. It should be emphasized that these considerations are only valid for the cut averaged entanglement entropy in periodic systems. Without this average, the ‘slope’ of the \( S(\ell) \) curve can become negative even for \( \ell < L/2 \), which we argue to be a sign for localized regions in the system (cf. Fig. 5.8).

### 5.3 Model and Method

We study the “standard model” of the MBL transition: The periodic random field Heisenberg chain (1.13).

Interior eigenpairs are obtained using a shift-invert technique, where the Hamiltonian is transformed to \((H - \sigma)^{-1}\), with a target energy \( \sigma \) inside the spectrum. The transformed problem is then amenable to standard Krylov space methods to obtain eigenpairs from the (upper and lower) edges of the transformed spectrum, reducing the computational difficulty virtually to the problem of applying the inverse of the shifted Hamiltonian to arbitrary vectors. This is a formidable task, due to the rapid growth of the problem dimension and high density of states in the middle of the spectrum. Currently, no more than \( L = 22 \) spins in the \( S_z = 0 \) sector of the random Heisenberg chain can be treated using the shift-invert methodology even when applied in a massively parallel way[30]. Throughout this chapter, we address eigenpairs in the
center of the spectrum at fixed energy density $\epsilon = (E - E_{\text{min}})/(E_{\text{max}} - E_{\text{min}}) = 0.5$, where the extensive target energy $E$ in each disorder configuration is determined by the corresponding groundstate ($E_{\text{min}}$) and antigroundstate ($E_{\text{max}}$) energies.

5.4 Cut averaged entanglement entropy (CAEE)

The considerations in Sec. 5.2 represent a strong constraint on the CAEE as a function of subsystem size. In particular, for $\ell \leq L/2$, the CAEE for larger subsystems always has to be larger than (or equal to) the ones for smaller subsystems. Note that, while this property holds for individual disorder realizations, the disorder average of the cut-averaged entanglement entropy is identical with the disorder average of the standard (single cut) entanglement entropy.

The bottom panel of Figure 5.1 shows typical CAEE curves as a function of subsystem size $\ell$ obtained from single (mid-spectrum) eigenstates of the Hamiltonian at various disorder strengths $h$. Due to the subadditivity constraints, the value of the CAEE at a given subsystem size has to be correlated with its values at other subsystem sizes. The CAEE curve is mirror symmetric around $\ell = L/2$ and finite size effects seem to be strongest in the region of the half cut, especially for the slope of the curve. We therefore primarily focus on the quarter cut $\ell = L/4$, where these effects are much less important. Notice that in the absence of cut averaging (cf. top panel of Figure 5.1), the entanglement entropy as a function of subsystem size is non-differentiable and therefore its slope is not well defined.

For each eigenstate, we calculate the reduced density matrix of all possible cuts of the system with a fixed subsystem length $\ell$ and average the von Neumann entropy over them. This is repeated for all subsystem sizes $\ell \in [1, L/2]$, yielding the CAEE $\bar{S}(\ell)$ as a function of the (integer) subsystem size $\ell$. In the next step, we interpolate this set of points (extended down to $\ell = 0$ and up to $\ell = L$ by the symmetry $S_\ell = S_{L-\ell}$) by a cubic spline, yielding a smooth and continuous function of $\bar{S}(\ell)$. The result for several typical states is depicted by the lines connecting the points of Fig. 5.1 for various values of the disorder strength. This allows us to look at derivatives of the entanglement entropy curve at fixed ratio $\ell/L$, which ensures the limit of an extensive subsystem size and can be estimated even for system sizes, where $\ell/L$ is incommensurate with the lattice. We have checked that using discrete derivatives (for the commensurate cases) yields virtually identical results and does not change the conclusions of this chapter.
5.4.1 Cut averaged entanglement entropy slope (SCAEE)

We calculate the CAEE \( \bar{S}(\ell) \) as a function of subsystem size for all eigenstates at fixed energy density \( \epsilon = 0.5 \) and determine the SCAEE \( \partial \bar{S}(\ell)/\partial \ell \). A fully ergodic eigenstate should have a SCAEE close to its maximal value: \( \ln 2 \). On the other hand, if the state is fully localized, the slope should be close to zero. In this section, we present detailed results on the SCAEE in different regimes; we consider its distribution over disorder realizations considering the first and second moment of the distribution as well as the entire distribution itself.

**Mean slope**

We begin with the mean of the SCAEE for subsystems of size \( \ell = L/4 \) for different system sizes. The top panel of Fig. 5.4 shows the result obtained from the disorder average over \( \approx 10^3 \) disorder configurations and \( \approx 50 \) eigenstates per realization as a function of disorder strength. The best estimate of the critical point in the center of the spectrum from Ref. [30] is indicated by the vertical dashed line.

![Figure 5.4: Disorder averaged mean entanglement entropy slope (top) and standard deviation of the mean entanglement entropy slope (bottom). The black dashed lines mark the rough intersecting positions of the curves of different system sizes. The red horizontal line for the bottom panel indicates the standard deviation of a uniform (box) distribution on the interval \([0, \ln 2]\), given by \( \sigma_{\Box} = \frac{\ln 2}{2\sqrt{3}} \). Note that the maximal variance of a bounded distribution on \([0, \ln 2]\) is given by a bimodal delta distribution, yielding \( \sigma_{\max} = \frac{\ln 2}{2} \approx .34657 \). The maximum can at most saturate at this value.

At weak disorder, the slope gets closer to its maximal value of \( \ln 2 \) for increasing system size. In addition,
Figure 5.5: Variance peak locations at different subsystem ratio $\ell/L$ for various system sizes. The variance peak locations are extracted from standard deviation plots as in Fig. 5.4, where the discrete $\bar{S}(\ell)$ are interpolated by cubic splines. The solid lines are linear fit curves to data points. The variance peak location $(h)$ rises with increasing system sizes. It is important to notice that for a particular $L$, the differences between the peak locations at different ratios becomes smaller, as $L$ increases, which is reflected by the decreasing slope of the lines connecting different subsystem sizes.

at larger system sizes, the ln 2 plateau extends to larger values of $h$ consistent with the idea of a sharp transition away from ln 2 in the TDL. Near the critical point, the average slope decreases rapidly to a smaller (near zero) value in the MBL phase. As the system size grows, the slope outside the critical region decreases as system size increases. These behaviors are fully consistent with the results obtained for other quantities and in particular the entanglement entropy density $S/L$, studied in Ref. [30], a quantity that is closely related to the SCAEE if averaged over disorder, as we shall see in Sec. 5.4.2.

In the critical region we see that the mean SCAEE for different system sizes generally intersect. While finite size effects will cause this crossing to drift with system size, we may treat it as a rough estimate for the critical point and find it consistent with the critical $h_c$ estimated by other approaches[24, 30].

It is interesting to note that the mean SCAEE is approximately 0.1 at this crossing point. Again, noting that there will be a drift of this value, a non-zero slope implies a non-area law value of the entanglement at the transition.

**Variance peak of the entanglement entropy slope**

Recently, it has been discovered that the variance of the distribution of the entanglement entropy in MBL systems exhibits a maximum close to the MBL transition[30, 62, 122]. In Fig. 5.4, we present results on the standard deviation of the SCAEE, std[$\partial S/\partial \ell$], for subsystem sizes $\ell = L/4$. This quantity also exhibits a maximum close to the transition and although the slope is an intensive quantity, the variance peak seems to
grow in amplitude for the accessible system sizes $L \leq 22$.

Because the cut-averaged entanglement entropy slope is strictly bounded by $0 \leq \partial \bar{S}/\partial \ell \leq \ln 2$, the peak of the standard deviation can not grow infinitely and can at most saturate\(^2\) at the maximal standard deviation given by a bimodal delta distribution $p(x) = \frac{1}{2} (\delta(x) + \delta(x - \ln 2))$.

We will discuss the origin of the variance peak of the entanglement entropy slope below, when we present the full probability distributions of this quantity and show that it becomes bimodal close to the transition. This is clear from the behavior of the standard deviation with system size in Fig. 5.4, which grows for the available size as a function of $L$ and exceeds the value obtained for a box distribution for system sizes larger or equal than $L = 20$. This bound is important as it represents the largest standard deviation of a unimodal distribution on $[0, \ln 2]$. Larger variances necessarily imply that the distribution has to be multimodal and the inspection of our histograms in Sec. 5.4.1 clearly points to a bimodal distribution with maxima close to 0 and $\ln 2$.

We attempted polynomial extrapolations of the maxima of the variance to the TDL. Given our system sizes and the lack of justification for the scaling ansatz, such an extrapolation is obviously unreliable but the results are not inconsistent with the maxima reaching the maximal possible variance ($\frac{\ln 2}{2}$) close to the critical point ($h_c = 3.7(1)$).

In Fig. 5.4 we have chosen a subsystem of size $\ell = L/4$ to mitigate strong finite size effects occurring at the half cut. The difference between the peak locations of various subsystem ratios becomes smaller as system size grows (cf. Fig. 5.5). This suggests that the transition, as identified by the variance peak, occurs at the same value of $h$ for all subsystem sizes in the TDL. This latter fact is a necessary condition if all states in the TDL have linear (possibly zero) SCAEE for all subsystem sizes.

**Slope histogram**

It is known from many studies [28, 29, 35, 40, 94, 123–125] that the surrounding of the MBL transition is dominated by rare region effects, responsible for subdiffusion [28, 29, 35, 124] on the thermal side of the transition. This is reflected in pathological (non-Gaussian) features of the probability distributions over disorder of various observables [40]. In particular the entanglement entropy [39, 40, 85] develops long tails down to zero entanglement, although the mean remains extensive and the weight of the tails is exponentially suppressed.

Here, we are interested in the SCAEE, which can be expected to wash out some of the rare region effects.

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\(^2\)We have tried a tentative extrapolation of the peak height to the thermodynamic limit using a polynomial ansatz as a function of $1/L$, pointing to a maximal variance of $\ln 2/2$, although this extrapolation is not reliable, as the extrapolation typically overshoots the theoretical maximum due to finite size effects.
while capturing the dominant scaling behavior of the entanglement entropy. As in the above discussion, we focus on extensive subsystems, where we expect that the localization length $\xi$ will be overcome at subsystem system sizes where $\ell \gg \xi$, thus providing a clear separation of dominant localized and delocalized behaviors for large system sizes.

Figure 5.6: Probability distribution of SCAEE evaluated at $\ell = L/4$, for systems of size $L = 20$ at various disorder strengths. The black vertical line indicates the maximal slope of $\ln 2$.

At weak disorder, the distribution of the SCAEE shown in Fig. 5.6 is close to a normal distribution with a mean close to the maximal slope at $\ln 2$, indicated by the vertical line. As also seen in the entanglement entropy presented in Ref. [40], there may be small deviations from the normal distribution, surviving in the thermodynamic limit but significant tails start to develop only at slightly larger disorder strengths around $h \gtrsim 0.8$. The weight in the tails reduces with system size as seen in Fig. 5.7 but the distributions remain generically non-Gaussian starting at relatively small disorder strengths of $h \approx 1$.

Near the critical point (middle panels of Fig. 5.7), the distribution becomes broad, giving rise to the maximal variance as discussed in the previous section. In fact, with growing system sizes, the distribution becomes increasingly bimodal, developing maxima close to zero (minimal) slope and $\ln 2$ (maximal) slope. As the position of the variance peak (lower panel of Fig. 5.1) moves towards the critical point for large systems and becomes sharp, we expect a bimodal distribution of the entanglement slope to be characteristic for the MBL transition. We show in Fig. 5.1 that the value of the variance at its maximum is already slightly larger than the value of a uniform distribution for systems of size $L = 20$ and is definitely larger than the uniform variance for larger system sizes (with growing tendency of the peak height for larger system sizes, possibly up to saturation at the theoretical maximum of the standard deviation at $\sigma_{\text{max}} = \frac{\ln 2}{2\sqrt{3}}$). This rules out the possibility of a flat or unimodal distribution, leaving as the only possibility consistent with
our results for the shapes of the distribution a bimodal distribution with maxima close to the minimal and maximal slope. Whether the weight between these maxima vanishes completely in the thermodynamic limit can not be definitely answered from our finite size results but this scenario is consistent with our data.

In the MBL phase, the maximum of the distribution of the SCAEE has clearly shifted towards very small slopes with an exponentially suppressed tail, extending up to the maximal slope. For the \( h = 8 \) plot, one observes a small weight for negative slopes, which are an artifact of our spline interpolation: For very low entanglement entropies, the spline tends to become oscillatory and leads to slightly negative slopes. This is not a problem for larger entanglement entropies.

![Figure 5.7: System size dependence of the probability distributions of SCAEE evaluated at \( \ell/L = 1/4 \). At weak disorder (\( h = 1 \) and \( h = 2 \)), the distribution approaches a Gaussian distribution for large system sizes. For our finite systems, the zone showing critical behaviour is roughly at \( h = 3.0 \) and drifts to larger disorder strength for larger systems. We observe a clear signature of an emerging bimodal distribution. In the MBL phase (\( h = 4 \) and \( h = 8 \)), the distribution is again unimodal and sharply peaked at zero slope. The black vertical line indicates the maximal slope of \( \ln 2 \). Note that the panels in the critical region are shown on a linear scale for clarity, while the other panels are on a logarithmic scale to exhibit the tails.](image)

While the SCAEE captures the \textit{dominant} scaling behavior of the entanglement entropy, it has a tendency to hide the effect of rare (localized and ergodic) regions. Therefore, we also study the distribution of the discrete entanglement entropy slope \( \Delta^- S(L/4) = S(L/4) - S(L/4 - 1) \text{ without averaging over cuts} \) in Fig. 5.8. The most striking difference to the cut averaged slope is the absence of the SSA constraints, allowing
for a decrease of the entanglement entropy with increasing system size, which can typically be expected if the boundary of the subsystem touches a localized part of the system as recently discussed in Ref. [40].

At weak disorder strength ($h \lesssim 0.8$), the histogram of $\Delta^- S$ approaches a Gaussian distribution for large system sizes, very similar to the cut averaged slope and no negative discrete slopes $\Delta^- S$ are observed. This changes significantly at intermediate disorder $h \gtrsim 2$, where more weight at negative discrete slopes is built up and a peak at 0 appears. We may speculate that this peak is caused by situations in which the changing subsystem boundary of the subsystems of length $L/4$ and $L/4 - 1$ both lie in a localized region, thus leading to a small change of the entanglement entropy and consequently $\Delta^- S = 0$. This peak becomes dominant in the MBL phase at $h \gtrsim 3.7$, where the distribution of $\Delta^- S$ becomes increasingly symmetric for larger system sizes with positive and negative discrete slopes being equally probable. The behaviour of these distributions is in very good agreement with the picture that rare localized regions of the system exist in the ergodic phase, while in the MBL phase the role of localized and delocalized regions switches and the latter become rare.

Figure 5.8: Discrete entanglement entropy “slope” $\Delta^- S(L/4) = S(L/4) - S(L/4 - 1)$ of the raw entanglement entropy without averaging over all subsystem cuts. The appearance of negative slopes is associated with localized regions[40].

Variance peak of the entanglement entropy slope of individual disorder realizations

In Sec. 5.4.1 we find a bimodal distribution of the SCAEE when sampled over eigenstates and disorder realizations. Here, we consider this distribution over single disorder realizations. In particular, we show that (i) eigenstates within a single sample can (but do not always) show bimodal behavior of the SCAEE (ii) partially contribute to the variance of the SCAEE seen in Sec. 5.4.1 and (iii) have values of the SCAEE
which are not independent of each other. This means that within one disorder realization some eigenstates show area law scaling of the entanglement entropy, while others scale by a volume law, at fixed energy density.

There are two extreme limits that can be considered in understanding the variance of the SCAEE. In one case, each disorder realization could individually contain eigenstates that all have (near) maximal or (near) zero SCAEE and hence individually have (near) zero variance. Then the entire variance results from a distribution over different disorder realizations. Alternatively, every eigenstate in a given disorder realization could be uncorrelated with each other. We can emulate this case by independently sampling states from the middle panels of fig. 5.7. Sampling groups of 50 eigenstates at $L = 20$ and $h = 2.8$ we see that the standard deviation of each group of 50 samples is a tight Gaussian centered around 0.2. We find our data is consistent with neither extreme. Instead, both effects seem to be relevant for the overall variance in Fig. 5.4.

Figure 5.9: Probability density of the standard deviation of the SCAEE $\partial \bar{S} / \partial \ell$ of eigenstates from the middle of the spectrum ($\epsilon = 0.5$) of one disorder realization with $\ell = L/4$. For each value of the disorder strength $h$, the distribution is sampled from $\approx 1000$ disorder realizations. Black curves indicate the mean of the distribution. Red dashed lines mark the largest standard deviations of the mean curves. A comparison of the results for system sizes $L = 20$ and $L = 12$ shows that for larger systems the states close to the critical point of one disorder realization become more diverse.

In order to understand if the large variance of the entanglement entropy and its slope can also be (partly) created by single disorder realizations, we calculate the standard deviation of the SCAEE for single disorder realizations at fixed energy density $\epsilon = 0.5$ from approximately 50 eigenstates per disorder configuration. Fig. 5.9 shows a two dimensional histogram of the per-sample standard deviation of the SCAEE $\text{std}[\partial \bar{S}(L/4)/\partial \ell]$
Figure 5.10: Histograms of horizontal slices \((h = 2.6 \text{ for } L = 12 \text{ and } h = 2.8 \text{ for } L = 20)\) through the mean curves’ largest standard deviation points of Fig. 5.9. In comparison, the one disorder realization distribution for a larger system size has more weight shifted towards higher standard deviation, which indicates a higher likelihood of finding bimodality in a single sample.

For different disorder strengths and system sizes \(L = 12\) and \(L = 20\). Most disorder realizations show a larger variance of the SCAEE close to the critical point at \(L = 12\) and the disorder averaged standard deviation (mean of the histogram) shown by the black line looks very similar to the overall variance peak shown in Fig. 5.4. For larger systems, we see the following two trends in the critical regime (cf. Fig. 5.10 for a cut through Fig. 5.9 in the critical regime). First, the distributions over a single sample span a wider range of standard deviations as the system size grows. There are therefore disorder realizations for which there is essentially no variance and disorder realizations for which there is large variance among the eigenstates. This is the opposite of what we would expect if these eigenstates were independent, implying significant correlation between them. Secondly, both the average per-sample standard deviation is larger and the plurality of samples lie at higher standard deviations. This can be seen in Fig. 5.9 where the red dashed lines correspond to the means of the distributions at their maxima. Note that the maximum of the distribution is actually larger than the mean close to the MBL transition, showing that typical realizations exhibit a mix of volume and area law states (increasingly diverse for larger systems).

If these trends continue this means that the bimodality of the SCAEE distribution would arise at a single disorder realization level, and become more and more common for increasing system sizes. To verify that bimodality is present for single disorder realizations, we numerically analyzed 500 disorder realizations of system size \(L = 16\) and a disorder strength \(h = 2.69\) that corresponds to the variance peak location of the SCAEE at \(\ell/L = 1/4\). Each sample has about 6000 eigenstates within the energy density window of \([0.45, 0.55]\). Among the 500 samples, the one with the largest standard deviation is shown in Fig. 5.11.
The distribution of the SCAEE for this sample is strikingly bimodal. Note that this is not a result of the curvature of the mobility edge, because the distribution of the SCAEE has no visible dependence on energy density as seen in the inset of Fig. 5.11. Especially, for this sample, the distributions of the SCAEE of the eigenstates within energy density windows of $[0.45, 0.50]$, $[0.50, 0.55]$, and $[0.45, 0.475] \cup [0.525, 0.55]$ are all bimodal and very similar to each other. Therefore, bimodality does indeed seem to be a generic feature of the SCAEE of individual disorder realizations.

We speculate that the mechanism for this bimodality may be caused by a mix of quasi-local and extended $\tau$ operators\cite{49, 50, 126} at the transition, where volume law states correspond to corresponding occupied extended orbitals and area law states are given by an occupation of only localized orbitals.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.11.png}
\caption{SCAEE distribution of a single disorder realization that has the largest standard deviation among the 500 samples at $L = 16$. Each sample contains 6000 eigenstates, with disorder strength $h$ corresponding to the variance peak location of SCAEE evaluated at $\ell/L = 1/4$ as in Fig. 5.4. The inset shows SCAE vs. energy density of each eigenstate of this disorder sample. Bimodality is clearly visible, and not likely due to the curvature of mobility edge.}
\end{figure}

### 5.4.2 Correlations between the entanglement entropy and its derivatives

In this section we show the nearly complete correlation between the CAEE density $\bar{S}/L$ and the SCAEE $\partial \bar{S}/\partial \ell$ and between $\partial \bar{S}/\partial \ell$ and $\partial^2 \bar{S}/\partial \ell^2$ at a fixed subsystem ratio $\ell/L$ (which we choose as 1/4), for various system sizes. These correlations are particularly compelling in the transition region, where, for finite system sizes, all accessible entropy densities are present (due to the wide and even bimodal distributions, depending on system size). This suggests that in the approach to the TDL there is a universal one-parameter family of curves $\bar{S}/L$ in the transition region parameterized by (for example) the value of the $\bar{S}/L$ at any fixed $\ell/L$. 

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Correlation between $\bar{S}/L$ and $\partial \bar{S}/\partial \ell$

We show two dimensional histograms of $\bar{S}/L$ vs. $\partial \bar{S}/\partial \ell$ at various disorder strengths in Fig. 5.12 for systems of size $L = 20$, together with the mean curves for $L = 12, 16, 20$ on the same plot. The color scale is logarithmic in the probability density.

The red lines are upper and lower bounds of $\bar{S}/L$ as a function of $\partial \bar{S}/\partial \ell$, that can be derived from the SSA constraints: Because of the SSA constraint and the fact that the slope is bounded from above by $\ln 2$, we have

$$
\int_{0}^{L/4} \frac{\partial \bar{S}(L/4)}{\partial \ell} d\ell \leq \int_{0}^{L/4} \frac{\partial \bar{S}(\ell)}{\partial \ell} d\ell \leq \int_{0}^{L/4} \ln 2 \, d\ell \leq \ln 2 \frac{L}{4}
$$

which reduces to

$$
\frac{1}{4} \frac{\partial \bar{S}(L/4)}{\partial \ell} \leq \frac{\bar{S}(L/4)}{L} \leq \frac{\ln 2}{4}
$$

Figure 5.12: Two dimensional histogram of CAEE vs. SCAEE for systems of size $L = 20$ and $\ell = L/4$, at disorder strength $h = 2.0, 3.0, 3.2, 4.0$. The mean curves for $L = 12, 16$ are also shown in the figure. The color bar indicates the bin counts on a logarithmic scale. The red straight lines indicate the upper ($\bar{S}/L \leq \ln 2/4$) and lower ($\bar{S}/L \geq \frac{1}{4}\partial \bar{S}/\partial \ell$) bounds of the entanglement entropy. The mean curves are nearly converged, indicating possible universal behavior.

At small disorder strength ($h = 2.0$), substantial weight is centered around $\partial \bar{S}/\partial \ell = \ln 2$ and $\bar{S}/L = \ln(2)/4$, indicating volume law entanglement. A light tail extending all the way to the MBL (low entanglement and low slope) region is visible.

At large disorder strength ($h = 4.8$), the weight is primarily around $\partial \bar{S}/\partial \ell = 0$ and $\bar{S}/L = 0$, indicating area law entanglement. Again, a light tail extends to the ergodic region. At intermediate disorder strengths, for $L = 20$, the weight spans from the ergodic to the MBL side.

Notice, that there appears to be significant correlation between the CAEE and SCAEE and that the
mean of these distributions seems to be largely independent of system size (at least from $L = 12$ to $L = 20$). In fact, even for different disorder distributions the banana-shaped histograms are located in the same region.

Besides, as discussed in Sec. 5.4.3, we show that the width of the ‘banana’ becomes narrower and more centered around the mean values for larger system sizes.

All these points above are strongly suggesting the existence a one-parameter family of curves of $\bar{S}/L$ in the transition region as a function of $\partial \bar{S}/\partial \ell$ in the approach to the TDL. We also observed that the weight in the middle of the ‘banana’ becomes diminished with increasing system sizes, consistent with the previously discussed bimodality.

**Correlation between $\partial \bar{S}/\partial \ell$ and $L(\partial^2 \bar{S}/\partial \ell^2)$**

We also consider the correlations between $\partial \bar{S}/\partial \ell$ and $L(\partial^2 \bar{S}/\partial \ell^2)$ again finding significant correlation between them. The two dimensional histograms of $\partial \bar{S}/\partial \ell$ vs. $L(\partial^2 \bar{S}/\partial \ell^2)$ at various disorder strengths are shown in Fig. 5.13 for systems of size $L = 20$, together with the mean curves for $L = 12, 16, 20$ on the same plot.

![Figure 5.13: Two dimensional histogram of 2nd order derivative of CAEE vs. SCAEE for systems of size $L = 20$ and $\ell = L/4$, at $h = 2.0, 3.0, 3.2, 4.0$. The mean curves for $L = 12, 16$ are also shown on the graphs. The color bar indicates the bin counts at a log scale. The mean curves are nearly converged, indicating possible universal behavior.](image)

Similarly, one can make the following observations. At small disorder strength, the distribution is centered around $\partial \bar{S}/\partial \ell = \ln 2$ and $L(\partial^2 \bar{S}/\partial \ell^2) = 0$, indicating volume law entanglement entropy. At large disorder strength, the distribution is centered around $\partial \bar{S}/\partial \ell = 0$ and $L(\partial^2 \bar{S}/\partial \ell^2) = 0$, indicating area law entanglement. At intermediate disorder strengths, the weights of the histograms span the high entanglement and low entanglement regions. In addition, the lack of weight with concavity zero at values distant from zero
or ln(2) slope indicates that we never see volume law (strictly linear) curves with non-thermal (non-ln(2)) or non-zero slope. Again, we find that curves of system sizes between $L = 12$ and $L = 20$ have nearly identical means, and the width of the ‘U’ shaped distribution becomes narrower and more centered around the mean values for larger system sizes, as discussed in Sec. 5.4.3.

### 5.4.3 Standard deviations of the correlations distributions

In Section 5.4.2, we discussed the correlations between the CAEE density $\bar{S}/L$ and the SCAEE $\partial \bar{S}/\partial \ell$ and between $\partial \bar{S}/\partial \ell$ and $\partial^2 \bar{S}/\partial \ell^2$ at a fixed subsystem ratio $\ell/L$ (which we choose as $1/4$), as shown in Fig 5.12 and 5.13. Here we further examine these distributions to establish the standard deviation, or spread, of each distribution around its mean, finding it narrower as the system size grows.

![Figure 5.14](image)

Figure 5.14: Standard deviation of vertical slices of CAEE vs. SCAEE histograms as in Fig. 5.12, for systems of size $L = 20$ and $\ell = L/4$, at $h = 2.0, 3.0, 3.2, 4.0$. The standard deviations decreases with system size. The 3rd and the 4th cumulants (not included) of the vertical slices of the histograms shows that the vertical distributions become more Gaussian with increasing system size.

For the 2D histograms of the CAEE density $\bar{S}/L$ and the SCAEE $\partial \bar{S}/\partial \ell$, we consider a slice of the two dimensional histograms vertically around a fixed value of $\partial \bar{S}/\partial \ell$. This vertical slice gives a distribution of different $\bar{S}/L$ values at some fixed value of $\partial \bar{S}/\partial \ell$. We calculated the third and fourth cumulants of these distributions, and find their absolute values to be less than $10^{-6}$ for $L = 12$ and even smaller for larger $L$; therefore these vertical slices are very likely Gaussian with well behaved mean and variances. The standard deviations of these vertical slices are shown in Fig. 5.14, which exhibit a slow decrease with system size. Similarly, for the 2D histograms of the $\partial \bar{S}/\partial \ell$ and $L\partial^2 \bar{S}/\partial \ell^2$, we also looked at the distribution of vertical slices of the two dimensional histograms. The standard deviations of these vertical slices are shown in Fig.
5.15, which exhibits a slow decrease with system size. Calculating the third and fourth cumulants also suggests that these distributions become more and more Gaussian with increasing system sizes.

5.5 Conclusion

We have presented an analysis of the scaling of the entanglement entropy up to the largest accessible system sizes in state of the art exact diagonalization and introduced the cut averaged entanglement entropy (CAEE) as well as its derivatives (SCAEE, etc.) with respect to subsystem size $\ell$ in periodic chains. We anticipate that the CAEE and SCAEE will be useful quantities to study the scaling behavior of the entanglement entropy of single eigenstates in other inhomogeneous systems.

We find that the slope of the cut averaged entanglement entropy (SCAEE) reproduces perfectly the volume law to area law transition associated with the MBL transition. We have also studied the slope without performing the cut average and observe increasing weight at negative slopes, which we argue to be associated with rare localized regions, which appear already in the ergodic phase and are believed to be responsible for subdiffusion.

More interestingly, the probability distribution of the cut averaged entanglement entropy slope becomes sharply bimodal for large system sizes in the transition region, leading to eigenstates which have near zero and near maximal slope. The variance of this distribution in the critical regime grows with system size, already exceeding the largest variance possible for a unimodal distribution at $L = 20$. In addition, we find
that the scaling of the CAEE is mostly linear in subsystem size at the variance peak with either maximal \((\ln 2)\) or minimal \((0)\) slope, but no state displays an intermediate value of the SCAEE and zero curvature. At the variance peak this implies that the scaling of the disorder averaged entanglement entropy is a volume law with a coefficient below its thermal value. We want to emphasize that due to the bimodal distribution, almost no state will show this behavior.

An extrapolation of the current trend is not inconsistent with the scenario that the variance peak would reach the largest possible variance in the TDL, which would lead to a coefficient of the volume law at half the thermal value of \(\ln(2)\) (in the disorder average).

An important finding of our work is that this mixture of states is intrinsic and occurs in single disorder realizations. Interestingly enough, it seems that there is significant correlation between eigenstates in a disorder realization and some such realizations actually have essentially no variance in their SCAEE of states within a tiny energy window. This mixture of states is potentially connected to the important open question on the nature of the local integrals of motion at the transition. In addition, at the system sizes we can access, we see a clear distinction between the standard deviations of SCAEE of the inter and intra disordered samples (comparing bottom panel of Fig. 5.4 and black curves of Fig. 5.9). If this difference survives to the TDL, this suggests a breakdown of self averaging.

In the final part of this chapter, we discussed the correlation between the cut averaged entanglement entropy slope and the entropy itself and find that for large systems the value of the slope is a strong predictor of the value of the entropy suggesting a one-parameter family of curves for the CAEE in the critical region in the approach to TDL. In particular, this observation allows us to draw conclusions on the behavior of the cut averaged entanglement entropy itself, which has to become bimodal, just as its slope.

On a more speculative note, the observed bimodal features of the distributions could be connected to the strong fluctuations of the entanglement entropy at the critical point in RG calculations \([92, 94]\) and possibly to multifractal features\([117]\).
Chapter 6

Pseudo spin symmetry and absence of full many-body localization in spin-disordered Hubbard model

This chapter is mainly based on an unpublished project done in collaboration with Di Luo and Bryan Clark.

6.1 Introduction

Fully many-body localized systems are characterized by the area-law entanglement entropy of excited states and the existence of a complete set of local integrals of motion, or l-bits. Typical MBL models are disordered spin chains and spinless fermion chains, where the spin or the charge degrees of freedom become localized in the MBL phase. Non-ergodic systems beyond the l-bit picture are considered controversial. As shown in Ref. [87, 88], spin chains with continuous non-Abelian symmetry are impossible to have a complete set of integrals of motion, and forbid the existence of a typical MBL phase, which provide a starting point for finding non-ergodic, non-MBL phases.

In this chapter, we consider the strongly disordered one-dimensional Hubbard model with spin disorder, which, as we will show, cannot be categorized as a conventional MBL phase. Though the spin rotation \( SU(2) \) symmetry is broken by the spin disorder, this model still preserves the pseudo-spin \( SU(2) \) symmetry under periodic boundary conditions. On the theoretical side, using the pseudo-spin algebra we showed that a significant number of the excited states at any disorder strength have logarithmic correction to their von Neumann entanglement entropy, which violates the area-law entanglement for a typical MBL phase. A common feature of this group of excited states is that they usually have far more double occupancies than single occupancies. On the numerical side, we studied the time evolution after quantum quench from two extreme cases of product states – all single occupancies at quarter filling, and all double occupancies at half filling. We found in the former case entanglement entropy behaves as in a typical MBL system, while the latter is clearly delocalized, which suggests the existence of incomplete set of local integrals of motion.
6.2 Model and pseudo-spin algebra

Disordered Hubbard models have been very popular in cold-atom experiments to study the MBL transition [74, 76, 127]. Usually disorder is added to the hopping parameters and the on-site potentials independently for spin up and spin down. A recent numerical study explored the case where only charge disorder that does not discriminate spins degrees of freedom are added to the one-dimensional Hubbard model [128]. By studying the spin and charge correlation functions, they demonstrated numerically that at large disorder strength the spin degrees of freedom remain ergodic while the charge degrees of freedom are localized, resulting in dynamical spin-charge separation. The authors also showed that the entanglement entropy after a quantum quench grows in a power-law fashion instead of logarithmically, which further indicated that this model does not become fully many-body localized at large disorder.

In the following, we focus on a model with spin disorder

\[
H = -t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) + \sum_i U_{i\uparrow} n_{i\uparrow} + \sum_i h_i S_i^z,
\]

where \(S_i^z = (n_{i\uparrow} - n_{i\downarrow})/2\), \(U > 0\), and the disordered Zeeman field \(h_i \in [-W, W]\) is sampled uniformly. We will mainly use \(t = 1\) and \(U = 1\) unless stated otherwise. This model bears close resemblance to that in Ref. [128]. At large disorders, the Zeeman terms dominate. It is reasonable to expect the \(S_i^z\) to be localized. However for spins \(S_i^z = \pm \frac{1}{2}\) to be localized, it also pins exactly one electron to site \(i\). When \(S_i^z = 0\), there is an ambiguity as to whether the site is empty or fully occupied. Intuitively, this means there is a qualitative difference between eigenstates mostly with single occupancies and eigenstates mostly with double occupancies. As we will show below, this model fails to settle into a full many-body localized phase as a direct result of the pseudo-spin \(SU(2)\) symmetry.

It is easy to see that the spin disorder breaks the spin rotation symmetry of \(H\). To prove that the pseudo-spin \(SU(2)\) symmetry is intact, one can introduce the eta-pairing operators [129, 130]

\[
\eta_- = \sum_r e^{i r \pi} c_{r\uparrow} c_{r\downarrow}, \quad \eta_+ = \eta_-^\dagger, \quad \eta_0 = \frac{1}{2} (\hat{N} - M),
\]

where \(M\) is the number of sites, and \(\hat{N}\) is the operator for total number of electrons in the system. The eta-pairing operators generate a \(SU(2)\) algebra because

\[
[\eta_0, \eta_{\pm}] = \pm \eta_{\pm}, \quad [\eta_+, \eta_-] = 2 \eta_0.
\]
To prove that pseudo-spin symmetry is preserved, one can straightforwardly check that

\[ [H, \eta_{\pm}] = \pm U \eta_{\pm}, \quad [H, \eta_0] = 0, \quad [H, \eta^2] = 0, \tag{6.4} \]

where the total pseudo-spin operator \( \eta^2 \) is

\[ \eta^2 = \frac{1}{2} (\eta_+ \eta_- + \eta_- \eta_+) + \eta_0^2. \tag{6.5} \]

As a result, \( \eta_{\pm} \) are a pair of ladder operators for the Hamiltonian, and \( \{H, \eta^2, \eta_0\} \) compose a complete set of commuting observables. As a side note, Eq. (6.4) requires the number of sites \( M \) in every spatial dimension to be even. Otherwise the \( \pi \) point in the Brillouin zone cannot be accessed.

### 6.3 Entanglement entropy of excited states

The pseudo-spin \( SU(2) \) symmetry has subtle influence on the entanglement entropy of a significant number of eigenstates. Because of Eq. 6.4, one can see that applying \( \eta_+ \) to an arbitrary eigenstate will result in another eigenstate of \( H \) (if not annihilated completely), whose energy is higher by \( U \). Given an reference eigenstate \( |\psi\rangle \) of \( H \), we can therefore build a tower of excited states

\[ |\psi_N\rangle = A_N \eta_+^N |\psi_{\text{ref}}\rangle, \quad N \in \mathbb{N}, \tag{6.6} \]

where \( A_N \) is the normalization factor. From here on, these excited states will be called the eta-pairing states. Similar to the approach used in Ref. [131], one can write down the reduced density matrix of the eta-pairing states by expressing the eta-pairing states as contour integrals.

Interestingly, in Ref. [131], the authors showed that for clean Hubbard model the entanglement entropies of eta-pairing states built from vacuum and fully polarized Slater determinants are always accompanied by a logarithmic correction. Here we will extend this claim to the spin-disordered case, and go beyond the vacuum and fully polarized reference states, proving that the logarithmic correction is universal for eta-pairing states which are dominated by double occupancies, with arbitrary disorder strength.

With this in mind, we will start with a simpler reference state where there are two interacting particles, which is a easier case to check concretely.
6.3.1 Two interacting particles reference state

For simplicity, let’s first consider the two-interacting-particle (TIP) eigenstates of the Hamiltonian defined in Eq. (6.1). A general normalized TIP reference eigenstate can be written as

\[ |\psi_{\text{ref}}\rangle = \sum_{ij} \alpha_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger |0\rangle, \tag{6.7} \]

Since this is intended to be an eigenstate, it obeys the time independent Schrödinger equation

\[ -t(\alpha_{i-1,j} + \alpha_{i+1,j} + \alpha_{i,j-1} + \alpha_{i,j+1}) = (E - U\delta_{ij} - \frac{\hbar_i - \hbar_j}{2})\alpha_{ij}, \tag{6.8} \]

where \( E \) is the eigenvalue. For \( |\psi_{\text{ref}}\rangle \) to be normalized eigenstate satisfying the above equation, one can show that the coefficients \( \alpha_{ij} \) must satisfy these constraints

\[ \sum_{ij} |\alpha_{ij}|^2 = 1, \quad \sum_{j} (-1)^j \alpha_{jj} = 0. \tag{6.9} \]

Upon this TIP reference state, one can build a tower of eta-pairing eigenstates as

\[ |\psi_N\rangle = A_N \eta_+^N \sum_{ij} \alpha_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger |0\rangle, \tag{6.10} \]

where the normalization factor \( A_N \) is given by

\[ \frac{1}{A_N^2} = \sum_{ijkl} \alpha_{ij} \alpha_{kl}^* \langle 0|c_{i\downarrow} c_{k\uparrow} \eta_+^N \eta_-^N c_{l\uparrow}^\dagger c_{j\downarrow}^\dagger |0\rangle. \tag{6.11} \]

Note that \( \eta_{\pm} \) only creates/annihilates double occupancy. The summation above can be naturally split into three cases – (1) when \( i \neq j, k \neq l \); (2) when \( i = j, k = l, i \neq k \); (3) when \( i = j = k = l \).

It is then easy to see that

\[ \frac{1}{A_N^2} = \sum_{i \neq j} |\alpha_{ij}|^2 C_{M-2}^N(N!)^2 + \sum_{i \neq k} (-1)^{i+k} \alpha_{ii} \alpha_{kk}^* C_{M-2}^{N-1}(N!)^2 + \sum_{i} |\alpha_{ii}|^2 C_{M-1}^N(N!)^2. \tag{6.12} \]

where we used the combinatorial number \( C_n^k = n!/[ (n-k)! k! ] \). Using the equality \( C_n^k = C_{n-1}^k + C_{n-1}^{k-1} \), we can decompose the last term of the equation above and show that

\[ \frac{1}{A_N^2} = (N!)^2 \sum_{ij} (|\alpha_{ij}|^2 C_{M-2}^N + (-1)^{i+j} \alpha_{ii} \alpha_{jj}^* C_{M-2}^{N-1}). \tag{6.13} \]
Because of Eq. (6.9), we finally get

$$\frac{1}{A_N^2} = (N!)^2 C_M^N,$$

(6.14)

or equivalently

$$A_N = \sqrt{\frac{(M - N - 2)!}{(M - 2)!N!}}.$$  

(6.15)

As in Ref. [131], the normalized eta-pairing states can be re-written as

$$|\psi_N\rangle = A_N N! \oint_o \oint_o dz \frac{e^{z\eta_{+,B}}}{2\pi i z^{N+1}} \sum_{ij} \alpha_{ij} c_i^\dagger c_j^\dagger |0\rangle,$$

where the contour must enclose the origin.

Now let’s partition the system into region $A$ and $B$, where $A$ has $M_A$ sites and $B$ has $M_B$ sites. The reduced density matrix of region $A$ is

$$\rho_A = tr_B (|\psi_N\rangle\langle\psi_N|).$$

(6.17)

In general this reduced density is complicated to diagonalized analytically. Some simplification can be achieved by putting it in a block-diagonal form. Note that $\eta_{\pm}$ only creates/annihilates double occupancy, so single occupancies can only come from the original reference state $|\psi_{\text{ref}}\rangle$. Therefore, after tracing out region $B$, the reduced density matrix $\rho_A$ can be split into a block diagonal form according to the number of single occupancies left in region $A$. For the case of TIP reference state, there are clearly three sectors – (1) two single occupancies in $A$; (2) one single occupancy in $A$; (3) No single occupancy in $A$. As the reference state gets more and more complicated, the number of sectors would grow quickly. It is not practical to calculate the contributions of all block to the von Neumann entanglement entropy. But luckily, for the purpose of showing there is at least logarithmic corrections, one can focus on the block with the maximum number of single occupancies in region $A$, which is proved below.

The reduced density matrix in this block can be written as

$$\rho_A^{\text{single}} = (A_N N!)^2 \oint_o \oint_o \frac{dz_1 dz_2}{(2\pi)^2} \langle 0_B | \frac{e^{z_1\eta_{-,B}}}{z_1^{N+1}} \frac{e^{z_2\eta_{+,B}}}{z_2^{N+1}} |0_B \rangle \sum_{i \neq j, k \neq l, i, j, k, l \in A} e^{z_j\eta_{+,A}} \alpha_{ij} c_i^\dagger c_j^\dagger |0_A \rangle \alpha_{kl}^* c_k^\dagger c_l^\dagger e^{z_k\eta_{-,A}}$$

(6.18)

where

$$\eta_{-,A/B} = \sum_{r \in A/B} e^{i r \pi} c_r^\dagger c_r^\dagger, \quad \eta_{+,A/B} = \eta_{-,A/B}^\dagger.$$  

(6.19)
After carrying out the contour integrals, we get

$$\rho_{\text{single}}^A = \sum_n \frac{\beta_A}{C_{M-2}^N} C_{M_B}^n C_{M_A-2}^{N-n} |\phi_n^A\rangle \langle \phi_n^A|$$  \hspace{1cm} (6.20)

where

$$\beta_A = \sum_{i \neq j, i, j \in A} |\alpha_{ij}|^2,$$  \hspace{1cm} (6.21)

and $|\phi_n^A\rangle$ is a normalized state defined in region $A$ as

$$|\phi_n^A\rangle = \sqrt{\frac{(M_A - 2 - N + n)!}{\beta_A(M_A - 2)!(N-n)!}} \sum_{i \neq j, i, j \in A} \eta_{i+,i,j}^{N-n} \alpha_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger |0_A\rangle.$$  \hspace{1cm} (6.22)

The reduced density matrix $\rho_{\text{single}}^A$ is already completely diagonalized, because $|\phi_n^A\rangle$ for different $n$ have different number of particles, so they are all orthonormal to each other. As a results, for each $n$, $|\phi_n^A\rangle$ is a Schmidt vector for region $A$, with Schmidt coefficient

$$\lambda_n = \sqrt{\frac{\beta_A C_{M_B}^n C_{M_A-2}^{N-n}}{C_{M-2}^N}}.$$  \hspace{1cm} (6.23)

So the von Neumann entanglement entropy contributed by $\rho_{\text{single}}^A$ is

$$S_{\text{single}} = -\sum_n \frac{\beta_A}{C_{M-2}^N} C_{M_B}^n C_{M_A-2}^{N-n} \ln \left[ \frac{\beta_A C_{M_B}^n C_{M_A-2}^{N-n}}{C_{M-2}^N} \right].$$  \hspace{1cm} (6.24)

Naturally, we are interested in highly excited states, large total system size and large heat bath size. So we will take the limit of $M_B > M_A$, $N - M_A \gg 1$, and $M_A \gg 1$. In this case, one can simplify $S_{\text{single}}$ using the Stirling approximation $\ln n! = n \ln n - n + \frac{1}{2} \ln 2\pi n$. Then the summation over $n$ can be replaced by a Gaussian integral using a saddle point approximation, which finally leads us to

$$S_{\text{single}} \approx \frac{\beta_A}{2} (1 + \ln[2\pi\nu(1-\nu)\beta_A(M_A - 2)]).$$  \hspace{1cm} (6.25)

where $\nu = N/(M-2)$ indicates the portion of available sites taken by double occupancies. We can clearly see the logarithmic contribution of $\ln (M_A - 2)$ to the total von Neumann entanglement entropy, where $M_A$ is the subsystem size.

An example can be found in Fig. 6.1. The reference state is the ground state obtained using DMRG from a spin-disordered Hubbard chain with open boundary conditions, where the system size is $M = 400$, and has disorder strength of $W = 4$. As $\eta_+$ is applied more and more times, we can clearly see the entanglement...
Figure 6.1: **Top:** Entanglement entropy \( S \) of eta-pairing states built on a TIP reference state vs. subsystem size \( M_A \). The bottom curve represents the entanglement entropy of the reference state. From there on, every curve above is the result of applying one more \( \eta_+ \). The reference state is an eigenstate obtained using DMRG from one spin-disordered Hubbard chain with open boundary conditions, system size \( M = 400 \), disorder strength \( W = 4 \), \( t = 1 \), \( U = 1 \). **Bottom:** Difference between the entanglement entropy \( S \) of eta-pairing states and the entanglement entropy \( S_{\text{ref}} \) of the reference state. It is easy to see that the difference becomes more and more linear with respect to \( \ln M_A \), which reveals the logarithmic corrections. Strictly speaking, under open boundary conditions, pseudo-spin symmetry is no longer exact, but this does not seem to be a problem at large system sizes.

entropy becomes linear in \( \ln t \), even though the open boundary conditions does not preserve the pseudo-spin symmetry exactly.

### 6.3.2 Many interacting particles reference state

The above discussion can be generalized to the many-interacting-particle case with some mild modifications. Assume that we have a \( K \)-particle eigenstate of the spin-disordered Hubbard model as

\[
|\psi_{\text{ref}}\rangle = \sum_{(i_1,\sigma_1),\ldots,(i_K,\sigma_K)} \alpha_{(i_1,\sigma_1),\ldots,(i_K,\sigma_K)} c^\dagger_{i_1,\sigma_1} c^\dagger_{i_K,\sigma_K} |0\rangle,
\]

(6.26)

On top of this eigenstate, one can also build a tower of eta-pairing states as

\[
|\psi_N\rangle = A_N \eta_N^N \sum_{(i_1,\sigma_1),\ldots,(i_K,\sigma_K)} \alpha_{(i_1,\sigma_1),\ldots,(i_K,\sigma_K)} c^\dagger_{i_1,\sigma_1} c^\dagger_{i_K,\sigma_K} |0\rangle.
\]

(6.27)

Now it becomes too complicated to calculate the normalization factor directly.
To move forward, it is important to realize that $|\psi_{\text{ref}}\rangle$ is an eigenstate of both the Hamiltonian $H$ and the total pseudo-spin operator $\eta^2$. Because of Eq. (6.3), one can rewrite $\eta^2$ as
\[
\eta^2 = \eta_- \eta_+ + \eta_0 + \eta_0^2 = \eta_- \eta_+ - \eta_0 + \eta_0^2.
\]

Since any state with fixed number of electron is an eigenstate of $\eta_0$, $|\psi_{\text{ref}}\rangle$ has to be an eigenstate of $\eta_- \eta_+$ and $\eta_+ \eta_-$ as well. Using mathematical induction, one can prove that $|\psi_{\text{ref}}\rangle$ has to be an eigenstate of $\eta_-^N \eta_+^N$, as long as $\eta_+^N$ does not completely destroy the state.

Therefore, when $K + N < M$, one can assume that
\[
\eta_-^N \eta_+^N |\psi_{\text{ref}}\rangle = \lambda |\psi_{\text{ref}}\rangle.
\]

To figure out the eigenvalue $\lambda$, one should make use of the fact that $\eta_\pm$ does not affect single occupancies. So if one splits $|\psi_{\text{ref}}\rangle$ according to the number of single occupancies $s_i$ as in
\[
|\psi_{\text{ref}}\rangle = \sum_i |\psi_{\text{ref},s_i}\rangle,
\]
then applying $\eta_-^N$ and $\eta_+^N$ will never mix $|\psi_{\text{ref},s_i}\rangle$ and $|\psi_{\text{ref},s_j}\rangle$.

As a result, for every individual $|\psi_{\text{ref},s_i}\rangle$, it also satisfies
\[
\eta_-^N \eta_+^N |\psi_{\text{ref},s_i}\rangle = \lambda |\psi_{\text{ref},s_i}\rangle.
\]

In order to have a tall tower of eta-pairing states, we only consider the case where $K \ll N$, $K \ll M$, and $K + N < M$. And to make the discussion simpler, we will assume that the maximum number of single occupancy among all configurations of is equal to total number of electrons $K$. In this case, it is quite easy to show that
\[
\eta_-^N \eta_+^N |\psi_{\text{ref},s_K}\rangle = C_{M-K}^N (N!)^2 |\psi_{\text{ref},s_K}\rangle,
\]
which means that
\[
\frac{1}{A_N^2} = \langle |\psi_{\text{ref}}| \eta_-^N \eta_+^N |\psi_{\text{ref}}\rangle = C_{M-K}^N (N!)^2.
\]

So we finally arrive at
\[
A_N = \sqrt{\frac{(M-N-K)!}{(M-K)!N!}}.
\]

From here, by focusing on the block of the maximum number of single occupancies of the reduced density
matrix, it is straightforward to show that

\[ S^{\text{single}} \approx \frac{\beta_A}{2} (1 + \ln[2\pi \nu (1 - \nu) \beta_A (M_A - K)]). \]  

(6.35)

where \( \beta_A \) is some constant, and \( \nu = N/(M - K) \) indicates the portion of available sites taken by double occupancies. In the proper limit of \( M_B > M_A \), \( N - M_A \gg 1 \), \( M_A \gg K \), and \( N + K < M \), the above expression is valid and again shows that there is logarithmic correction to the entanglement entropy.

The above analysis of logarithmic correction is independent of disorder strength, and can be readily extended to higher dimensions. It seems to be a universal feature of the pseudo-spin \( SU(2) \) symmetry, and affects a significant amount of the eigen spectrum. These eigenstates strongly violate the area-law entanglement, thus making full MBL phase not likely. However, this is not to say that any localized behavior is impossible. In the proper limit that we work with, the eta-pairing states with logarithmic corrections to the entanglement entropy all have far greater numbers of double occupancies than single occupancies. And as we mentioned before, in the large disorder limit, single occupancies will be pinned to sites because they have \( S_i^z = \pm \frac{1}{2} \). But for \( S_i^z = 0 \), as long as the two electrons in a double occupancy move coherently, they are not affected by the disorders. This apparently shows a qualitative difference between eigenstates mostly made by single occupancies and mostly made by double occupancies.

### 6.4 Time evolution after quantum quench

To demonstrate the possible existence of a non-ergodic, non-MBL phase in one-dimensional spin disordered Hubbard model, we perform numerical simulation in a quantum quench setup, especially focusing on the qualitative differences between the single occupancies and double occupancies.

(A) Quarter filling

(B) Half filling

Figure 6.2: A: A schematic diagram for quarter filling initial state used in unitary time evolution. It has \( M = 12 \) and only single occupancies. B: A schematic diagram for half filling initial state used in unitary time evolution. It has \( M = 12 \) and only double occupancies. Both states have a charge imbalance of 1.

Here are two basic settings in our numerical simulation. The first setting is a quarter filled initial state
alternating between spin up and spin down. The second setting is a half filled initial state with all double occupancies in odd sites. The two settings are presented in the schematic diagrams in Fig. 6.2. They serve as two extreme limits where the first case starts with single occupancies only and the latter case starts with double occupancies only. Both of them start with zero entanglement entropy, and highly imbalanced charge distributions on even and odd sites.

With these two initial product states, we investigate the time evolution of von Neumann entanglement entropy, and charge imbalance

\[ I = \sum_{j=1}^{n} (-1)^j (n_{j\uparrow} + n_{j\downarrow}) \sum_{j=1}^{n} (n_{j\uparrow} + n_{j\downarrow}). \] (6.36)

The main goal is to check how fast the entanglement entropy grows, whether or how fast the the charge imbalance relaxes.

The real time evolution simulations are carried out separately for \( L = 8 \), which uses the exact diagonalization (ED) method, and for \( L = 12, 24 \), which uses the time-evolving block decimation (TEBD) method based on the open source ITensor library [132]. We mainly use two large disorder strengths \( W = 14 \) and \( W = 24 \). The hopping term \( t \) and the repulsive potential \( U \) are chosen to be 1 for the Hamiltonian in Eq. (6.1). Under each simulation, the entanglement entropy, and charge imbalance are averaged over disorder realizations.

![Figure 6.3: Growth of entanglement entropy \( S \) over time \( t \) obtained using ED, for the quarter filling (blue) and half filling (red) cases, with \( L = 8, W = 14 \), and periodic boundary conditions. For each case, \( S \) is averaged over 200 disorder realizations to \( t = 100 \). The same set of data for the two cases are plotted in three columns with different scales. Left column: This is \( S \) vs \( t \) plotted in the linear scale for \( S \) and \( t \). It is clear that the half filling case grows faster than the quarter filling case, and looks qualitatively different from it. Middle column: This is \( S \) vs \( t \) plotted in the linear scale for \( S \) and logarithmic scale for \( t \). For the quarter filling case, the entanglement entropy looks linear with respect to ln \( t \). But for the half filling case, the entanglement entropy curve clearly curves up. Right column: This is \( S \) vs \( t \) plotted in the logarithmic scale for \( S \) and \( t \). For the quarter filling case, the entanglement entropy curve slightly curves downward. For for the half filling case, the curve now look linear at large \( t \).]
6.4.1 Growth of entanglement entropy

In the fully MBL phase the entanglement entropy $S$ after a quantum quench grows logarithmically in time $t$, while the entanglement entropy in the ergodic phase grows linearly. For the spin-disordered Hubbard model, however, neither case alone can explain our observation.

From the ED results plotted in Fig. 6.3, based on the linearity of the curves, one can say that for the quarter filling case $S$ most likely grows linearly with respect to $\ln t$, while for the half filling case $S$ most likely grows in a power-law fashion with respect to $t$. Similar results are observed in $L = 12$ as well, as shown in Fig. 6.4.

![Graph showing growth of entanglement entropy]

Figure 6.4: Growth of entanglement entropy $S$ over time $t$ obtained using TEBD, for the quarter filling (blue) and half filling (red) cases, with $L = 12$, $W = 14$, SVD cutoff of $10^{-13}$, and open boundary conditions. For each case, $S$ is averaged over 200 disorder realizations. With a fixed amount of wall clock time, we have quarter filling data up to $t = 55$, and half filling data up to $t = 9$, because the latter has larger average entanglement entropy. For the quarter filling case, the entanglement entropy $S$ looks linear with respect to $\ln t$. For the half filling case, $S$ grows faster than the previous case. But because of the shorter time series, it almost looks linear with respect to $t$.

6.4.2 Relaxation of charge imbalance

The other characteristics of MBL phase is the lack of transport. As defined in Eq. (6.36), the charge imbalance $I$ measures the bias of charge distribution. For both the quarter filling and half filling cases, they
initially start with all charges on the odd sites, or, in other words, the maximum charge imbalance of 1. As the charge distribution evolves over time, for an ergodic system, one would expect $I$ to relax towards zero because charges are allowed to propagate through the systems, and spend equal amount of time on even sites and odd sites. But for a system in the MBL phase, one would instead expect $I$ to be stuck close to the initial value. As we can see in Fig. 6.5 and Fig. 6.6,

![Graph showing relaxation of charge imbalance $I$ over time $t$ obtained using ED, for the quarter filling (blue) and half filling (red) cases, with $L = 8$, $W = 14$, and periodic boundary conditions. For the quarter filling case, the charge imbalance clearly stabilizes towards a large non-zero value, which means in the long time limit, the charge distribution cannot relax completely, which is likely due to localization. For the half filling case, the charge imbalance clearly relaxes towards zero, which does not seem to suffer from localization effects as compared to the quarter filling case.](image)

**6.4.3 Number of double occupancies**

As pointed out earlier, the differences between the quarter filling case and the half filling case comes from the qualitative differences between single occupancies and double occupancies. As in Fig. 6.7, we can see the disorder averaged number of double occupancies obtained from the ED calculations for $L = 8$. For both cases, the number of doublons quickly stabilizes. The half filling case keeps more doublons than the quarter filling case does.
Figure 6.6: Relaxation of charge imbalance $I$ over time $t$ obtained using TEBD, for the quarter filling (blue) and half filling (red) cases, with $L = 12$, $W = 14$, SVD cutoff of $10^{-13}$, and open boundary conditions. For each case, $S$ is averaged over 200 disorder realizations. With a fixed amount of wall clock time, we have quarter filling data up to $t = 55$, and half filling data up to $t = 9$, because the latter has larger average entanglement entropy. For the quarter filling case, the charge imbalance clearly stabilizes towards a large non-zero value, which means in the long time limit, the charge distribution cannot relax completely, which is likely due to localization. For the half filling case, the charge imbalance clearly relaxes towards zero, which does not seem to suffer from localization effects as compared to the quarter filling case.

6.5 Conclusion

With the spin disordered Hubbard chains, we demonstrate an interesting interplay between spin and charge degrees of freedom, and between non-Abelian symmetry and MBL phase. Despite the similarity of our model to that in Ref. [128], our results in comparison are directly related to the pseudo-spin $SU(2)$ symmetry, and cannot be explained with spin-charge separation.

It is clear that in the spin disordered case, the outcome of unitary time evolution in the long time limit strongly depends on whether the initial state is dominated by double occupancies or single occupancies, which aligns well with our analytical analysis on eigenstates’ entanglement entropy. Although we mainly focus on the two extreme limits of product states made up of all double occupancies and all single occupancies, in the large disorder limit, it is easy to describe the outcome of unitary time evolution of a more general product state. Basically, the single occupancies will be pinned around their initial positions, while doublons can roam between two positions pinned by the single occupancy, forming a small bubble with higher entanglement
entropy. As long as the initial number of doublons are far greater than the number of single occupancies, most certainly there will be a large bubble with many doublons in it. Then one may still expect the entanglement entropy to grow in a power-law fashion.

To summarize, our results support the claims of logarithmic entanglement entropy and incomplete set of local integrals of motion in Ref. [88], and demonstrates the possibility of a non-ergodic, non-MBL phase in the one-dimensional spin-disordered Hubbard model.
This chapter is mainly based on the project as in Ref. [133].

7.1 Introduction

Non-abelian anyons, such as Ising and Fibonacci anyons have non-abelian braiding statistics and can store quantum information non-locally.[134–138] Such a state can be used as quantum memory and have promising application in topological quantum computing. These non-abelian anyons are expected to exist in a non-abelian fractional quantum Hall liquid.[139–141]

Recently, topological defects with non-abelian braiding statistics have been predicted in the abelian topological phases.[142–154] These topological defects are present at the heterostructures and dislocations in some abelian topological states.[151, 155–162] They can carry (fractional) Majorana-like characteristics and are manifested as the twist defects in topological phases with global symmetries, such as Kitaev toric code, the Bombin-Martin color code and its $Z_k$ generalization.[142–153, 163–166] There has been theoretical proposals for their realization in superconductor (SC)– (anti)ferromagnet (FM) – (fractional) topological insulator (TI) heterostructures, where Majorana zero modes or parafermions for the fractional case are bounded at the point defect interfaces.[151, 154, 157–162, 167–175]

For example, in the Kitaev’s toric code model [176], the twofold twist defect [142, 144] that associates with the electric-magnetic duality symmetry changes the $Z_2$ gauge charge $e$ into the gauge flux $m$, or vice versa, when the quasiparticle orbits around the defect (fig. 7.1). Due to the non-local twisting structure, the topological defect carries a non-trivial quantum dimension $d = \sqrt{2}$, and the defect system can be physically mapped [177] on to the SC-FM-TI heterostructure [157] that supports Majorana zero mode. In general, twist defects are extrinsic classical point defects in topological phases associating with a global anyonic symmetry $g$.[149, 152, 154] The twist defect permutes the anyon labels of orbiting quasiparticles and acts as fluxes of anyonic symmetry. They are non-abelian objects and their fusion and braiding properties can be systematically described by a defect fusion category or a $G$-crossed tensor category.[147, 154, 164–166]
In this chapter, we will consider one dimensional chains of twist defects and study the critical point of these chain modes. These twist defects are embedded in the background of a \( D(\mathbb{Z}_k) \) quantum double model, which is a \( \mathbb{Z}_k \) generalization of Kitaev \( \mathbb{Z}_2 \) toric code model, and can also be understood as a discrete \( \mathbb{Z}_k \) gauge theory in its deconfined phase.\[136, 176, 178–183\] The twist defects here are non-abelian defects and carry zero modes of \( \mathbb{Z}_k \) parafermions.\[184–187\] These are twofold defects in the sense that the corresponding anyonic symmetry operation is of order two, and that a pair of defects associates to a \( k \)-dimensional Hilbert space. We introduce pairwise interaction between twist defects and construct the defect chain Hamiltonian. Similar ideas have been used before to construct the non-abelian anyonic chain models and study the phase diagram in them.\[188–192\]

In our model, the pairwise interaction can be represented by the Wilson loop operator around the neighboring twist defects\[147, 193\] that separates the \( k \) quantum states. Based on the algebra of Wilson loop operators, we will show that the twist defect chain model with periodic boundary condition can be mapped to the \( \mathbb{Z}_k \) clock model with various boundary conditions. For even number of twist defects, the corresponding \( \mathbb{Z}_k \) clock model has periodic boundary condition (up to a phase for the boundary term), while for odd number of twist defects, after mapping to \( \mathbb{Z}_k \) clock model, this requires the introduction of a new type of boundary condition. This boundary term was studied in the \( k \)-state Potts model (\( k \leq 4 \)) using the language of Temperley-Lieb algebra and was called a duality twisted boundary condition.\[194\] In both even and odd cases, we will show that at critical point, the twist defect chain model preserves translational symmetry, which is identical to the Kramers-Wannier duality symmetry in the clock model setting. We will show that the translational symmetry operator has a simple physics interpretation and can be understood as a product of braiding operators which exchanges the positions of neighboring twist defects.

The critical point of the lattice models in 1 + 1 dimensions can be described by rational conformal field theory (CFT), which has finite number of primary fields.\[195, 196\] For an even chain, it corresponds to the \( \mathbb{Z}_k \) clock model at criticality and the structure of the CFT is well known.\[197, 198\] The simplest example is \( k = 2 \) case, which is the critical transverse field Ising model with central charge \( c = 1/2 \). For an odd chain, the underlying CFT is not well-studied in the literature in general when \( k \neq 2 \). For \( k = 2 \), the odd chain corresponds to the transverse field Ising model with a duality twisted boundary condition. This model can be mapped to a free fermion chain under Jordan-Wigner transformation and can been calculated analytically. Under this twisted boundary condition, the partition function takes a non-diagonal form in terms of characters, in which the holomorphic or anti-holomorphic character (depending on the phase of the boundary term) has conformal dimension \( h = 1/16 \).\[199, 200\]

For \( k > 2 \) cases with duality twisted boundary condition, the model is not interaction-free anymore and
therefore an analytical result is absent. In the present article, we will numerically study the energy spectra of these models for \( k = 3, 4, 5, 6 \) at criticality and extract the conformal scaling dimensions for the primary fields of the underlying CFT. Based on these result, we will demonstrate that when \( k \neq 4 \), as a CFT, the odd-chain models can simply be related to the even-chain models with some additional twofold twist field operators. However, special care is needed for \( k = 4 \), where we find that new excitations are consistent with some fourfold twist field operators in the \( SU(2)_1/D_4 \) CFT. Such kind of CFT is the so-called orbifold CFT and has been extensively studied in the literature.[201–204] We summarize the main results in Table 7.1.

<table>
<thead>
<tr>
<th>( k )</th>
<th>coupling</th>
<th>Even-chain</th>
<th>Odd-chain</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>F</td>
<td>three-state Potts</td>
<td>( \mathcal{M}(5,6) )</td>
</tr>
<tr>
<td>4</td>
<td>F/AF</td>
<td>( U(1)_3 )</td>
<td>( U(1)_3/\mathbb{Z}_2 )</td>
</tr>
<tr>
<td>( k &gt; 4 )</td>
<td>F/AF</td>
<td>( U(1)_k )</td>
<td>( U(1)_k/\mathbb{Z}_2 )</td>
</tr>
</tbody>
</table>

Table 7.1: The underlying CFT for chains with even number of defects (the third column) and the underlying CFT for chains with odd number of defects (the fourth column). \( U(1)_k \) refers to the K-matrix \( K = 2k \) in the boson Lagrangian density \( \mathcal{L} = (K/2\pi)\partial_t \phi \partial_x \phi \). For the odd-chain with \( k = 4 \), the numerical results show certain similarities with the \( SU(2)_1/D_4 \) orbifold CFT.

The rest of this chapter is as follows. In Sec. 7.2, we first briefly review the twist defect in topological phase and then we construct the Wilson loop Hamiltonian with even number and odd number of twist defects. We also discuss the translational symmetry in both cases. In Sec. 7.3, we first explain our numerical method and then calculate the primary fields for even number case. We further study the odd number case and extract the conformal dimension for the twist field operator. We summarize and conclude in Sec. 7.4. The appendices are devoted to details of the calculations and techniques used in this chapter.

### 7.2 Twist defect chain model

#### 7.2.1 Review of twist defect

The \( D(\mathbb{Z}_k) \) quantum double model in \( 2 + 1 \) dimensions is the \( \mathbb{Z}_k \) lattice gauge theory in the deconfined limit and is an abelian topological phase. It has two fundamental excitations the gauge charge \( \mathbf{e} = (1,0) \) and the gauge flux \( \mathbf{m} = (0,1) \) and all the \( k^2 \) quasi-particle excitations can be written as \( \mathbf{a} = \mathbf{e}^s \mathbf{m}^t \) with \( 0 \leq s, t \leq k \). The braiding phase between \( \mathbf{e} \) and \( \mathbf{m} \) is \( e^{2\pi i/k} \). For the \( \mathbb{Z}_2 \) case, the toric code is related to the s-wave superconductor with a deconfined \( \mathbb{Z}_2 \) fermion parity symmetry by identifying \( \mathbf{m} \) with the the \( hc/2e \) flux vortex, \( \mathbf{em} \) with the BdG fermion, and \( \mathbf{e} \) with an excited vortex.[165, 177, 205]

The \( D(\mathbb{Z}_k) \) quantum double model has the global duality symmetry operation, which will interchange \( \mathbf{e} \) and \( \mathbf{m} \) excitations. As shown in Fig.7.1, in the lattice model (Wen’s plaquette model [206]), the global
duality symmetry operation corresponds to the half lattice translation and will interchange the $e$ and $m$ particles which live on blue and red plaquettes respectively. In this sense, the topological phase weakly breaks the global duality/half lattice translation symmetry. The duality symmetry can be partially restored by introducing twofold twist defect, which is the dislocation on the lattice model as shown in Fig. 7.1.[142–151, 164] The twist defect can be pictorially represented by a cross attached with a branch cut. After crossing the branch cut, the $e$ particle and the $m$ particle will be interchanged. The twist defects are semi-classical non-abelian defects and each pair of them can form a $k$-level system. When $k = 2$, the twist defect corresponds to the more familiar Majorana zero mode.[155, 156] In our previous work, we systematically studied the fusion rule and F-symbols for basis transformation in a multi-defect system.[147, 148] The fusion between the twofold defects and abelian anyon are given by

\[
\sigma \times \sigma_{\lambda} = \sigma_{\lambda + s + t},
\]

\[
\sigma_{\lambda_2} \times \sigma_{\lambda_1} = \sum_{\lambda_1 + \lambda_2 = s + t} a
\]

where $\lambda$ runs from 0 to $k - 1 \ mod \ k$ and is the species label for the twist defect and $a = e^s m^t$ is the abelian anyon. The unitary braiding operator for twist defects projectively represents the sphere braid group.

### 7.2.2 Wilson loop Hamiltonian

In this chapter, we will use the bare twofold defect in the $D(\mathbb{Z}_k)$ quantum double model to construct some one dimensional chain models and in particular, we will focus on their critical behavior. The setup is like this, we first create $M$ bare twist defects in the background of $D(\mathbb{Z}_k)$ quantum double model and align them
in a line. Each twist defect is attached with a branch cut and two of them can pair up by gluing the branch cut together. This pairing procedure is arbitrary and for simplicity, we connect $\sigma_{2j+1}$ and $\sigma_{2j+2}$ by the branch cut as shown in Fig.7.2. For the even case with $M = 2N$, all twist defects can pair up and there are no branch cut left. While for the odd case with $M = 2N - 1$, the last twist defect $\sigma_{2N-1}$ cannot find twist defect to pair up with and has a dangling branch cut left behind. The quantum dimension for the total Hilbert space is $k^{M/2}$. For convenience, we will denote the bare twofold defect at site $a$ as $\sigma_a$. We use the Wilson loop operators to construct a one dimensional Hamiltonian (Fig.7.2 (a))

$$H = - \sum_{a=1}^{M} J_a (W_a + W^\dagger_a)$$

(7.2)

where each Wilson loop operator is generated by dragging an $e$ particle around two neighboring twist defects. The Wilson operator is also dyon tunneling (fermion tunneling for the $\mathbb{Z}_2$ case) between neighboring twist defects. When $1 \leq a < M$, $W_a$ is the Wilson loop circling around $\sigma_a$ and $\sigma_{a+1}$, and the boundary term $W_M$ is the Wilson loop circling around $\sigma_M$ and $\sigma_1$. For $\mathbb{Z}_2$ case, this is just the Majorana chain.[134] We are interested in constructing the translational invariant model for the bare twist defects. This requires that in Eq.(7.2), all the $J_a$ are equal up to a phase. The detail for this phase will be explained later in Sec.7.2.3 and Sec.7.2.4.

According to the fusion rule in Eq.(7.1), the two neighboring twist defects can fuse into an abelian anyon, the Wilson loop operator around these two twist defects can be used to detect the fusion channel of the two twist defects. The Wilson loop operator has eigenvalue equal to $e^{2\pi in/k}$ with $n = 0,\ldots, k-1$ and satisfies $W_a^k = 1$. The commutation relationship between different Wilson loop operators are determined by the intersection between them,

$$[W_a, W_b] = 0, \quad \text{when } |a - b| > 1$$

$$W_a W_{a+1} = \omega W_{a+1} W_a$$

$$W^\dagger_{a+1} W_a = \omega W_a W^\dagger_{a+1}$$

(7.3)

where $\omega = e^{2\pi i/k}$.

This model in Eq.(7.2) is invariant under translation symmetry operator and under this symmetry, $T W_a T^{-1} = W_{a+1}$. $T$ operator can be realized by moving the last defect $\sigma_M$ all the way back to the first and can be represented by a sequence of braiding operators

$$T = B_1 B_2 \ldots B_{M-1}$$

(7.4)
Figure 7.2: (a) Twist defect chain with six (even number) twofold defects. The twist defect at site $a$ is labelled as $\sigma_a$. $W_a$ is the Wilson loop operator around $\sigma_a$ and $\sigma_{a+1}$. In terms of $\mathbb{Z}_k$ clock variable, $W_{2j-1}$ (solid blue curve) corresponds to the term $\tau_j$, while $W_{2j}$ (dashed red curve) represents the term $\sigma_j^\dagger \sigma_{j+1}$. The Wilson loop Hamiltonian has periodic boundary condition here. (b) Twist defect chain with five (odd number) twofold defects, with $\sigma_6$ pulled away far from the defect chain. The branch cut connecting $\sigma_5$ is left behind. The boundary term $W_5$ (with green solid curve) is the boundary term and corresponds to the duality twisted boundary condition in the $\mathbb{Z}_k$ clock model. (c) The Hamiltonian of Wilson loop operator only at even site. Here we choose open boundary condition and therefore $\sigma_1$ and $\sigma_6$ do not show up in the Hamiltonian. In terms of $\mathbb{Z}_k$ clock variable, this Hamiltonian is the same as Eq.(7.9) with $J_2 = 0$ and no boundary term. (d) The Hamiltonian with Wilson loop operator only at odd site. It also corresponds to Eq.(7.9) with $J_1 = 0$.

where the braiding operator $B_i$ denotes a counter-clockwise permutation of a pair of adjacent defects at position $i$ and $i + 1$. We will show the translational symmetry operator $T$ is the Kramers-Wannier duality symmetry and guarantees that the model is at the critical point.

According to the definition of Wilson loop algebra in Eq.(7.3), the Wilson loop operator can be denoted as a $\mathbb{Z}_k$ clock variable with $W_{2j-1} = \sigma_j$ ($\sigma$ here does not mean the twist defect) and $W_{2j} = \tau_j \tau_{j+1}^\dagger$, where $\tau$ and $\sigma$ are both $k$-dimensional matrices

$$
\sigma = \begin{pmatrix}
1 & 0 & \cdots & 0 \\
0 & \omega & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \omega^{k-1}
\end{pmatrix}, \quad \tau = \begin{pmatrix}
0 & \cdots & 0 & 1 \\
1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 1 & 0
\end{pmatrix}
$$

(7.5)

with $\omega = e^{2\pi i/k}$. $\sigma$ and $\tau$ satisfy $\sigma^k = 1$, $\tau^k = 1$ and $\sigma \tau = \omega \tau \sigma$. The $\sigma$ operator here is a measurement of the quantum state (or $\mathbb{Z}_k$ parafermion parity) associates to the defect pair joined by a branch cut. The $\tau$ operator is a parafermion parity flip and the Wilson operator $W_{2j}$ flips the $\mathbb{Z}_k$ parity of the two pairs of defects next to it. The Hamiltonian in terms of $\mathbb{Z}_k$ clock variables takes this form (up to some boundary
This is quantum $Z_k$ clock model at critical point and there has been a long history of studying this model.[184–186, 192] Notice that there is a subtle difference between twist defect chain and $Z_k$ clock model. The single-site translation operation in $Z_k$ model actually corresponds to two-site translation operator $T^2$ in the twist defect chain model. This indicates that in the $Z_k$ clock model, the unit cell is doubled. The $T$ symmetry operator corresponds to the famous Kramers-Wannier duality symmetry operator in $Z_k$ clock model,[185]

$$D\sigma_a\sigma_{a+1}D^{-1} = \tau_{a+1}, \quad D\tau_aD^{-1} = \sigma_a\sigma_{a+1}$$

(7.7)

Since the unit cell is doubled, the ordinary quantum $Z_k$ clock model always corresponds to the twist defect chain with even number of twist defects $2N$. For the defect chain with odd number of twist defect $2N − 1$, if it is written in terms of $Z_k$ clock model, the boundary term will be modified. We will explain these two different cases in the following subsections.

### 7.2.3 Wilson loop Hamiltonian with $2N$ twist defects

For the Wilson loop Hamiltonian with $2N$ number of twist defects and with periodic boundary condition shown in Eq.(7.2), the corresponding $Z_k$ clock model also has periodic boundary condition. The Hamiltonian in terms of $Z_k$ variables takes this form

$$H = -J \sum_{j=1}^{N-1} (\sigma_j + \tau_j^\dagger \tau_{j+1} + h.c.) - J (\sigma_N + \tau_1^\dagger \tau_N + h.c.)$$

(7.8)

This is the $Z_k$ clock model at the critical point. If not at the critical point, the translational invariant $Z_k$ clock model with periodic boundary condition is

$$H = -J_2 \sum_{j=1}^{N} (\sigma_j + \sigma_j^\dagger) - J_1 \sum_{j=1}^{N-1} (\tau_j^\dagger \tau_{j+1} + \tau_j \tau_{j+1}^\dagger) - J_1 (\tau_N^\dagger \tau_1 + \tau_1 \tau_N^\dagger)$$

$$= -J_2 \sum_{j=1}^{N} (W_{2j-1} + W_{2j-1}^\dagger) - J_1 \sum_{j=1}^{N} (W_{2j} + W_{2j}^\dagger)$$

(7.9)
The above model has a global \( Z_k \) symmetry and therefore we can define a global \( Z_k \) charge operator

\[
Q = \prod_{j=1}^{N} \sigma_j
\]  

(7.10)

We briefly explain the phases for Eq.(7.9) here. For the \( Z_k \) clock model, there are two limits, one is \(|J_2| < |J_1|\) limit, which corresponds to the ferromagnetic or antiferromagnetic phase depending on the sign of \( J_1 \). This model can be re-written in terms of parafermions after performing a non-local Fradkin-Kadanoff transformation.[185, 186] The parafermion with \( k > 2 \) can be considered as a generalization of Majorana fermion for the transverse field Ising model (\( Z_2 \) clock model).[185, 186] For this model with open boundary condition, after performing a non-local Fradkin-Kadanoff transformation, there will be a parafermion zero mode left on the edge. As shown in Fig.7.2 (c), in terms of twist defect chain model, this zero mode actually corresponds to the unpaired twist defect left on the boundary. Another limit is when \(|J_1| < |J_2|\), this is the disordered paramagnetic phase without any parafermion zero mode left on the boundary (Fig.7.2 (d)).

For the \( Z_k \) clock model, the Kramers-Wannier duality transformation in Eq.(7.7) exchanges the disordered paramagnetic phase and ordered phase. Under this duality transformation \( D \),

\[
DH(J_1,J_2)D^{-1} = H(J_2,J_1)
\]

(7.11)

The Hamiltonian Eq.(7.9) has an ordered ferromagnetic / anti-ferromagnetic phase and a disordered paramagnetic phase and both of them are gapped phases. At the self-dual point, it turns out to be a gapless critical point protected by the additional duality symmetry. The low energy excitation of this model is described by a conformal field theory (CFT) and is closely related with the self-dual Sine-Gordon model,[208]

\[
S = \int d^2x \frac{1}{2} (\partial\mu \Phi)^2 + g \cos(\sqrt{2\pi k}\Phi) + g \cos(\sqrt{2\pi k}\Theta)
\]

(7.12)

where \( \Phi \) is the bosonic field and \( \Theta \) is the dual field. This model is invariant under the dual transformation \( \Phi \leftrightarrow \Theta \) transformation and is always critical. In the renormalization group (RG) language, the two cosine terms are irrelevant when \( k > 4 \) and therefore the self-dual Sine-Gordon model is the same as the Luttinger liquid at infrared (IR) limit with the central charge \( c = 1 \). When \( k = 4 \), the cosine terms are marginal, and the interaction will only change the compactification radius for the compact boson field. When \( k < 4 \), the cosine terms are relevant, according to Zamolodchikov’s \( c \)-theorem, the relevant perturbation will drive the model from the ultraviolet (UV) \( c = 1 \) fixed point to the IR fixed point with \( c < 1 \).[209] When \( k = 2 \), the self-dual Sine-Gordon model can be refermionized by introducing two Majorana fields. One of them will be
gapped and the other one remains gapless with $c = 1/2$. This is the Ising CFT and is the effective theory for critical $Z_2$ clock model (transverse field Ising model). When $k = 3$, it corresponds to the three-state Potts CFT with $c = 4/5$, and is identical to the critical $Z_3$ clock model with ferromagnetic coupling.[203] The three-state Potts CFT can be considered as the deformation of $Z_4$ parafermion CFT, which has $c = 1$ and is the effective theory for the critical $Z_3$ clock model with antiferromagnetic coupling.

**7.2.4 Wilson loop Hamiltonian with $2N – 1$ twist defects**

For the Wilson loop Hamiltonian with $2N – 1$ number of twist defects defined in Eq.(7.2), the Hamiltonian can still be written in terms of $Z_k$ clock models with some twisted boundary term,

$$H = -J \sum_{j=1}^{N-1} (\tau_j^+ \tau_{j+1}^- + \sigma_j + h.c.) - H_B$$

(7.13)

The boundary term $W_{2N-1}$ [Fig. 7.2(b)] can be derived by computing the intersection with the neighboring Wilson loop and is proportional to $\sigma_N \tau_N^+ \tau_1^-$. The coefficient in front of the boundary term depends on whether $k$ is even or odd and is fixed by the translational symmetry. The detail of the coefficient will be discussed in Sec. 7.2.5.

The Wilson loop Hamiltonian is translational invariant and thus the twisted $Z_k$ clock model is still invariant under the Kramers-Wannier duality transformation. In this sense, this symmetry protects the criticality of the model. Since there are odd number of twist defects, the dimension of the total Hilbert space is equal to $k^{N-1/2}$ and the effective length for the twisted $Z_k$ clock model is $L = N - 1/2$. This will be useful in the numerical calculation later. The correspondence between the twist defect chain and the quantum $Z_k$ clock model is summarized in Table.7.2.

<table>
<thead>
<tr>
<th>$Z_k$ clock model</th>
<th>Twofold defect chain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Periodic boundary term</td>
<td>Even number of $\sigma_a$</td>
</tr>
<tr>
<td>Duality twisted boundary term</td>
<td>Odd number of $\sigma_a$</td>
</tr>
<tr>
<td>Duality symmetry (D)</td>
<td>$T$</td>
</tr>
<tr>
<td>Translation symmetry</td>
<td>$T^2$</td>
</tr>
</tbody>
</table>

Table 7.2: Comparison between the $Z_k$ clock model and the twofold twist defect chain.

Actually, similar boundary condition has already been explored in the quantum $k$-state Potts model in Refs. [194] and [210]. The $k$-state Potts model with $k \leq 4$ can be constructed in terms of Temperley-Lieb Hamiltonian and can be exactly solved. At the critical point (with $k \leq 4$), the model is invariant under the Kramers-Wannier duality transformation. By constructing the duality symmetry operator in terms of Temperley-Lieb algebra generators, Schütz noticed that there are two different kinds of duality symmetry
operators which correspond to two classes of toroidal boundary terms [194]. The first one is the traditional periodic boundary term in Eq.(7.8) and the second one is duality twisted boundary term in Eq.(7.13).

In fact, in our twist defect chain, there is a simple way to interpret this duality symmetry operator in terms of twist defect, which is equivalent to the translation symmetry operator $T$ for the Wilson loop. As we mentioned in Eq.(7.4), it can be realized by a sequence of braiding operators. This is also illustrated in Fig. 7.4, in the defect chain with $2N$ twist defects, the translation operator involves $2N - 1$ braiding moves, while for the $2N - 1$ twist defects (shown in Fig.7.5), $T$ involves $2N - 2$ braiding moves. In the next section, we will use the braiding operators to explicitly construct the $T$ operator/D operator.

### 7.2.5 Translational symmetry $T$

As shown in Eq.(7.4), the $T/D$ operator in the twist defect chain/$\mathbb{Z}_k$ clock model can be realized by a product of braiding operators. At critical point, the Hamiltonian is invariant under $T$ operator. In this section, we will use the braiding operator to construct $T$ operator explicitly for the twist defect chain and will also use the $T$ operator to fix the coefficient of the boundary term.

The duality transformation operator for $k$-state Potts model (with two different boundary conditions) has already been constructed using Temperley-Lieb algebra [194]. Although the $k$-state Potts model and $\mathbb{Z}_k$ clock model are equivalent for $k = 2, 3$, these two types of models are different for higher $k$ values. Therefore it is interesting to construct $T$ operator systematically for $\mathbb{Z}_k$ clock models and compare the result with that for $k$-state Potts model.

#### Diagrammatical construction

![Diagram](image)

Figure 7.3: A quantum state in a system with 6 defects labeled by the internal fusion channels $a_1, a_2, a_3$. The collection of quantum states $|a_j\rangle$ forms an orthonormal basis of the Hilbert space.

According to our results in previous paper,[147] the braiding operator for twofold twist defect takes this
Figure 7.4: A schematic diagram for the translational operator $\mathcal{T} = B_1 B_2 B_3$ in a defect chain model with four twofold defects. After performing $\mathcal{T}$ operator on this chain, every defect moves one site to the right. The defect $\sigma_4$ on the right boundary moves to the left front. The Wilson loop operator is also shifted by one site.

form

$$B_{2j-1}^{(a_j,a_j-1)} = e^{\frac{\pi i}{4} (a_j,2-a_j-1,2)[\frac{j}{2} - \frac{1}{2} (a_j,2-a_j-1,2)]}$$

$$[B_{2j}^{(\sigma_j+1,\sigma_j)}]^{a_j}_{a_j'} = e^{\frac{\pi i (k-1)}{\sqrt{k}}} e^{\frac{2\pi i}{4} (a_j'-a_2)[\frac{j}{2} + \frac{1}{2} (a_2'-a_2)]}$$

(7.14)

where $B_p$ is the braiding operator for two neighboring twist defects at position $p$ and $p+1$. For $B_{2j-1}$, it has the input and output channel fixed as abelian anyon $a_j$ and $a_{j+1}$ (Fig. 7.3), while $B_{2j}$ has the input and output channel as both twist defects. The superscript $a_j$ and subscript $a_j'$ in Eq.(7.14) are the internal channels and a braid operation can flip the anyon type of the internal channel. This braiding operator can be rewritten in the basis of $\mathbb{Z}_k$ rotors. When $k = 2$, the braiding operator is equal to

$$B_{2j-1} = e^{\frac{\pi i}{2}} (\sigma_j^z + e^{\frac{\pi i}{2}})$$

$$B_{2j} = e^{\frac{-\pi i}{2}} (\sigma_j^x a_{j+1}^x + e^{\frac{\pi i}{2}})$$
It is easy to check that

\[ B_{2j} \sigma_j^x B_{2j}^{-1} = -i \sigma_j^x \sigma_{j+1}^z \sigma_{j+1}^x \]
\[ B_{2j-1} (-i \sigma_j^x \sigma_{j+1}^z \sigma_{j+1}^x) B_{2j-1}^{-1} = \sigma_j^x \sigma_{j+1}^x \]  

(7.15)

Combining these, we get the transformation \( T \sigma_j^x T^{-1} = \sigma_j^x \sigma_{j+1}^x \). This can also be pictorially understood in Fig. 7.4 and Fig. 7.5 which show \( TW_j T^{-1} = W_{j+1} \). Similarly, this also shows that \( T \sigma_{j+1}^x \sigma_j^x T^{-1} = \sigma_{j+1}^x \). This relation can be generalized to \( k > 2 \) and we have

\[ T T^\dagger = \mathbb{I} \]
\[ T \sigma_j T^{-1} = \tau_j \tau_{j+1}^\dagger, \quad (1 \leq i \leq N - 1) \]
\[ T \tau_j \tau_{j+1}^\dagger T^{-1} = \sigma_{j+1}, \quad (1 \leq i \leq N - 1) \]

(7.16)

Therefore \( T \) transformation shifts the Wilson loop Hamiltonian by one lattice spacing and corresponds to the duality transformation \( D \) in \( \mathbb{Z}_k \) clock model.
For $k = 3$,

$$B_{2j-1} = \frac{1}{\sqrt{3}}[(\sigma_j + \sigma_j^\dagger) + \omega]$$  \hspace{1cm} (7.17)

$$B_{2j} = \frac{1}{\sqrt{3}}[(\tau_j \tau_{j+1}^\dagger + \tau_j^\dagger \tau_{j+1}) + \omega]$$  \hspace{1cm} (7.18)

For $k = 4$,

$$B_{2j-1} = \frac{1}{\sqrt{4}}[(\sigma_j + \sigma_j^\dagger) + \omega^2 \sigma_j^2 + \omega^{-\frac{1}{2}}]$$  \hspace{1cm} (7.19)

$$B_{2j} = \frac{1}{\sqrt{4}}[(\tau_j \tau_{j+1}^\dagger + \tau_j^\dagger \tau_{j+1}) + \omega^2 \tau_j^2 \tau_{j+1}^2 + \omega^{-\frac{1}{2}}]$$  \hspace{1cm} (7.20)

For $k = 5$,

$$B_{2j-1} = \frac{1}{\sqrt{5}}[(\sigma_j + \sigma_j^\dagger) + \omega^4(\sigma_j^2 + \sigma_j^1 \sigma_j^2) + \omega^2]$$  \hspace{1cm} (7.21)

$$B_{2j} = \frac{1}{\sqrt{5}}[(\tau_j \tau_{j+1}^\dagger + \tau_j^\dagger \tau_{j+1}) + \omega^4(\tau_j^2 \tau_{j+1}^2 + \tau_j^1 \tau_{j+1}) + \omega^2]$$  \hspace{1cm} (7.22)

For $k = 6$,

$$B_{2j-1} = \frac{1}{\sqrt{6}}[(\sigma_j + h.c.) + \omega^2(\sigma_j^2 + h.c.) + \omega^4 \sigma_j^3 + \omega^{-\frac{1}{2}}]$$  \hspace{1cm} (7.23)

$$B_{2j} = \frac{1}{\sqrt{6}}[(\tau_j \tau_{j+1}^\dagger + h.c.) + \omega^2(\tau_j^2 \tau_{j+1}^2 + h.c.) + \omega^4 \tau_j^3 \tau_{j+1}^3 + \omega^{-\frac{1}{2}}]$$  \hspace{1cm} (7.24)

Notice all $B$-operators defined above satisfy $BB^\dagger = I$, and commute with the charge operator $Q$.

However, the above relation only holds for $\mathbb{Z}_k$ variables in the bulk and may not work for the boundary term, i.e. the last term of Eq.(7.8). This is because on the boundary,

$$\mathcal{T} \sigma_N \mathcal{T}^\dagger = Q \tau_N \tau_1^\dagger,$$

$$\mathcal{T} Q \tau_N \tau_1^\dagger \mathcal{T}^\dagger = \sigma_1.$$  \hspace{1cm} (7.25)

There is an additional charge operator $Q$. Only when $Q$ takes a trivial value, i.e., $Q = 1$, the above relation works for the boundary condition. For a general charge $Q$, when the $\mathcal{T}$ operator moves the twist defect along the chain, the charge $Q$ is also shifted with the twist defect, therefore, this model is not translational invariant under $\mathcal{T}$ operator. One needs to carefully include boundary correction to $\mathcal{T}$, and define $\tilde{\mathcal{T}} = \mathcal{T} X$ (to be discussed below), so that $\tilde{\mathcal{T}}$ is an exact symmetry of the Hamiltonian.[194]

**Even number of twist defects**

For the case with even number of twist defects, one normally considers the periodic Hamiltonian as defined in Eq. (7.8), which amounts to choosing the boundary condition as $\tau_{N+1} = \tau_1$. More generally, one can
consider boundary conditions with

$$\tau_{N+1} = \omega^{-n} \tau_1, \ n = 0, 1, \cdots, k - 1.$$  \hspace{1cm} (7.26)

which leads to a large set of Hamiltonians with different boundary conditions

$$H^{(n)} = -J \sum_{i=1}^{N-1} (\sigma_i + \tau_i \tau_{i+1}^\dagger + h.c.)$$

$$- J (\sigma_N + \omega^n \tau_N \tau_1^\dagger + h.c.),$$  \hspace{1cm} (7.27)

Define projection operator $P^{(n)}$ as

$$P^{(n)} = \frac{1}{k} \left( \sum_{i=0}^{k-1} \omega^{-ni} Q^i \right).$$  \hspace{1cm} (7.28)

It is easy to check that $P^{(n)}$ is a projection into the $Q = \omega^n$ sector. For instance, one can write $Q = \sum_{n=0}^{k-1} \omega^n P^{(n)}$. Mixed sector Hamiltonians are produced by mixing in one charge sector of every $H^{(n)}$, and defined as

$$\widetilde{H}^{(n)} = \sum_{m=0}^{k-1} P^{(m+n)} H^{(m)} P^{(m+n)}.$$  \hspace{1cm} (7.29)

So all charge sectors of the normal periodic Hamiltonian in Eq. (7.8) are embedded into this set. Expanding the above equation, one gets

$$\widetilde{H}^{(n)} = -J \sum_{i=1}^{N-1} (\sigma_i + \tau_i \tau_{i+1}^\dagger + h.c.)$$

$$- J (\sigma_N + \omega^{-n} Q \tau_N \tau_1^\dagger + h.c.)$$  \hspace{1cm} (7.30)

If not for the additional phase factors of $\omega^{-n}$, the operator $T$ would be an exact symmetry of $\widetilde{H}^{(n)}$. To take into account that phase factor, following Ref. [194], one could choose a boundary correction term $X = \tau_N^\dagger V$, where the global operator $V$ is defined through its action on the $Z_k$ variables,

$$V^2 = \mathbb{I}$$

$$V \sigma_i V = \sigma_i^\dagger$$

$$V \tau_i V = \tau_i^\dagger$$  \hspace{1cm} (7.31)

Actually, there is an explicit matrix representation for $V$. First, we consider $V_i$ which only acts on the $\sigma_i$, $\tau_i$ sector. Let $V_i = (v_{ab})$ where $a, b = 0, 1, \cdots, k - 1$. Take $v_{ab} = 1$ for $a + b = 0 \mod k$ and 0 otherwise. In
other words, \( V_i \) is the matrix

\[
\begin{pmatrix}
1 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 1 \\
0 & 0 & 0 & \cdots & 1 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 1 & \cdots & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0
\end{pmatrix}
\]

(7.32)

Finally we can take the tensor product \( V = V_1 \otimes \ldots \otimes V_N \) which satisfies Eq.(7.31).

For \( \tilde{T} = T \tau_N^N \), now it is easy to check that

\[
\tilde{T} \sigma_i^\dagger \tilde{T}^{-1} = \tau_i \tau_{i+1}^\dagger \quad (1 \leq i \leq N - 1),
\]

(7.33)

\[
\tilde{T} \tau_i \tau_{i+1}^\dagger \tilde{T}^{-1} = \sigma_{i+1}^\dagger \quad (1 \leq i \leq N - 1),
\]

(7.34)

\[
\tilde{T} \sigma_N^\dagger \tilde{T}^{-1} = \omega^{-n} Q \tau_N \tau_1^\dagger,
\]

(7.35)

\[
\tilde{T} \omega^{-n} Q \tau_N \tau_1^\dagger \tilde{T}^{-1} = \sigma_1^\dagger.
\]

(7.36)

Therefore, we have \( \tilde{T} \tilde{H}^{(n)} \tilde{T}^{-1} = \tilde{H}^{(n)} \), which means \( \tilde{T} \) is an exact duality symmetry of mixed sector Hamiltonian \( \tilde{H}^{(n)} \), and \( \tilde{T}^2 \) is a translational operator in the \( \mathbb{Z}_k \) clock model.

**Odd Number of twist defects**

The construction of \( \tilde{T} \) is very similar to the previous case. Define \( T = B_1 B_2 \cdots B_{2N-2} \), and \( \tilde{T} = TX \), where \( X \) is a boundary correction to be clarified. Using the braiding operators \( B \), one can show that

\[
T \sigma_i T^\dagger = \tau_i \tau_{i+1}^\dagger \quad (1 \leq i \leq N - 1),
\]

(7.37)

\[
T \tau_i \tau_{i+1}^\dagger T^\dagger = \sigma_{i+1} \quad (1 \leq i \leq N - 2),
\]

(7.38)

\[
T \tau_{N-1} \tau_N^\dagger T^\dagger = e^{i\phi_k} Q^\dagger \tau_N \tau_1^\dagger \sigma_N,
\]

(7.39)

\[
T e^{i\phi_k} Q^\dagger \tau_N \tau_1^\dagger \sigma_N T^\dagger = \sigma_1^\dagger.
\]

(7.40)

where \( \phi_k \) is a phase determined by Eq. (7.39) and is equal to \( \phi_3 = 2\pi/3, \phi_4 = -\pi/4, \phi_5 = 4\pi/5, \) and \( \phi_6 = -\pi/6. \) Once again, the additional terms in the last two lines need to be matched with a properly chosen \( H_B \), so that \( \tilde{T} \) is an exact symmetry of the Hamiltonian.

In order to construct the mixed sector Hamiltonians that commute with \( \tilde{T} \), we consider the following
duality twisted Hamiltonians with different boundary conditions

\[ H^{(m)} = -J \sum_{i=1}^{N-1} (\sigma_i + \tau_i \tau_{i+1}^\dagger + h.c.) - J(\omega^m e^{-i\phi_k} \sigma_N^\dagger \tau_N \tau_1^\dagger + h.c.). \]  

(7.41)

where \( m = 0, 1, \cdots, k - 1 \). Unlike the even number case, here the Hamiltonians \( H^{(m)} \) are not actually independent, as they are related by a local unitary transformation

\[ H^{(m+1)} = \tau_N H^{(m)} \tau_N^\dagger, \quad Q = \omega \tau_N Q \tau_N^\dagger. \]  

(7.42)

To elaborate on its meaning, let’s assume that we have an eigenstate \( |\alpha, q\rangle \) of \( H^{(m)} \) and \( Q \), which satisfies

\[ H^{(m)} |\alpha, q\rangle = E_\alpha |\alpha, q\rangle \quad \text{and} \quad Q |\alpha, q\rangle = q |\alpha, q\rangle. \]

Then Eq. (7.42) says that \( \tau_N |\alpha, q\rangle \) is an eigenstate of \( H^{(m+1)} \) and \( Q \), since \( H^{(m+1)} \tau_N |\alpha, q\rangle = E_\alpha \tau_N |\alpha, q\rangle \) and \( Q \tau_N |\alpha, q\rangle = \omega^m q \tau_N |\alpha, q\rangle \). This essentially means Hamiltonians \( H^{(m)} \) of different \( m \) are all equivalent, up to some changes to the charge sector labels.

We define the mixed sector Hamiltonians as

\[ \tilde{H}^{(m)} = \sum_{l=0}^{k-1} P^{(l+m)} H^{(l)} P^{(l+m)} . \]  

(7.43)

which expands to

\[ \tilde{H}^{(m)} = -J \sum_{i=1}^{N-1} (\sigma_i + \tau_i \tau_{i+1}^\dagger + h.c.) - J(\omega^m e^{-i\phi_k} \sigma_N^\dagger \tau_N \tau_1^\dagger + h.c.). \]  

(7.44)

Similarly, one can show that for \( \tilde{T} = T(\sigma_N^\dagger)^m V, \)

\[ \tilde{T} \sigma_i^\dagger \tilde{T}^{-1} = \tau_i \tau_{i+1}^\dagger \quad (1 \leq i \leq N - 1), \]  

(7.45)

\[ \tilde{T} \tau_i \tau_{i+1}^\dagger \tilde{T}^{-1} = \sigma_i^\dagger \quad (1 \leq i \leq N - 2), \]  

(7.46)

\[ \tilde{T} \tau_N \tau_{N-1}^\dagger \tilde{T}^{-1} = \omega^{-m} e^{-i\phi_k} \sigma_N^\dagger \tau_N \tau_1^\dagger, \]  

(7.47)

\[ \tilde{T} \omega^{-m} e^{-i\phi_k} \sigma_N^\dagger \tau_N \tau_1^\dagger \tilde{T}^{-1} = \sigma_1^\dagger. \]  

(7.48)

Therefore, we have \( \tilde{T} \tilde{H}^{(m)} \tilde{T}^{-1} = \tilde{H}^{(m)} \), which means \( \tilde{T} \) is an exact duality symmetry of \( \tilde{H}^{(m)} \). \( \tilde{T}^2 \) can also be interpreted as a special “translational operator”, in the sense that it correctly translates a local term which is far from the boundary, and applying it \((N - 1/2)\) number of times on a local term will return it back.
to itself, where the 1/2 factor comes from the twisted boundary condition. Notice that $\hat{T}$ does not commute with $Q$.

Numerically, we are interested in the CFT content of $H^{(0)}$, but since $H^{(0)}$ does not commute with $\hat{T}$, it is more favorable to work with $\tilde{H}^{(m)}$, from which we can extract the “momentum” eigenvalues of $\hat{T}^2$ as well. Due to Eq. (7.42), for $\tilde{H}^{(m)}$ with a fixed $m$, all these $k$ different charge sectors (labelled by charge operator $Q$ ) have the same energy spectrum. However, $\tilde{H}^{(m)}$ with different $m$ can have different energy spectrum and corresponds to different charge sector in $H^{(0)}$. Therefore, to obtain the low lying energy levels of all the charge sectors of $H^{(0)}$, we need to solve for the low lying energy levels of $k$ different $\tilde{H}^{(m)}$. To distinguish the results from the even-defect chains, when summarizing the conformal dimensions into tables, we describe the charge sectors using label $m$, in correspondence to the fact that we are using mixed sector Hamiltonians $\tilde{H}^{(m)}$.

7.3 Numerical methods and numerical results

To determine the properties of the CFTs underlying the Wilson loop Hamiltonian in Eq.(2.2), we extract the conformal dimensions $\tilde{h}$ and $\bar{h}$ using finite and infinite density matrix renormalization group (DMRG/iDMRG) [101], and exact diagonalization (ED) methods. The DMRG calculations are based on the open-source C++ library ITensor [132].

**Wilson loop Hamiltonian with 2N twist defects**

Twist defect chains with 2N twist defects in Eq. (7.8) correspond to critical $\mathbb{Z}_k$ clock models with length $L = N$, and have difference CFTs at criticality. In order to uncover the contents of the CFTs, except for a few cases which allow analytical solutions, one needs to perform numerical calculations on the energy spectrum of the critical system as explained below.

It has been shown that the energy spectrum of a critical chain with finite length $L$ with periodic boundary conditions obeys [211–213]

$$
E = \epsilon_\infty L - \frac{\pi \nu c}{6L} + \frac{2\pi \nu}{L} (\tilde{h} + \bar{h} + n + \bar{n}) + O(L^{-2})
$$

$$
= E_0 + \frac{2\pi \nu}{L} (\tilde{h} + \bar{h} + n + \bar{n}) + O(L^{-2})
$$

(7.49)

where $\epsilon_\infty$ is the energy density of the ground state in the limit of $L \to \infty$; $\nu$ is the sound velocity; $c$ is the central charge. These three parameters can be pinned down by using DMRG method with high accuracy. The details for the numerical calculation is explained below.
The central charge $c$ can be obtained by fitting to the scaling form of the entanglement entropy. Given the ground state of a $1+1d$ critical chain of length $L$ with open boundary conditions, if we consider a consecutive block of size $L_A$ starting from the left (or right) edge, the von Neumann entanglement entropy of that block has been shown to exhibit the following scaling behavior [214]

$$S(L_A) = \frac{c}{6} \log \left( \frac{L}{\pi \sin \frac{\pi L_A}{L}} \right) + S_0$$

(7.50)

where $S_0$ is a constant piece. Numerically, we use DMRG to obtain the ground state wave function of a finite chain with length $L$ and open boundary conditions, and determine the central charge $c$ by fitting the numerical results of $S(L_A)$ onto Eq. (7.50). Finally, we can extract the sound velocity $v$ based on the ground state energy $E_0 = \epsilon_\infty L - \pi c v/6L + O(L^{-2})$ (obtained by ED). Polynomial extrapolation in terms of $1/L$ is used to mitigate the finite size correction ($O(L^{-2})$).

As an example, in the following we demonstrate how we obtain $\epsilon_\infty$, $c$, and $v$ for the critical $\mathbb{Z}_4$ clock model. $k = 4$ is a special case where the anti-ferromagnetic and ferromagnetic critical clock models are related by using $\sigma \tau = \omega \tau \sigma$. First of all, through iDMRG we find $\epsilon_\infty = 2.54647904$, which agrees with the exact value of $8/\pi$ up to very high precision.[215] Secondly, DMRG calculations, as can be see in Fig. 7.6, show that $c = 1$. Then, using the ED calculations for lengths $L = 6, 7, 8, 9, 10, 11, 12, 13$, we calculate the sound velocity, and extrapolate it to $v = 2.0000$ in the $1/L \to 0$ limit as in Fig. 7.7, compared to the exact value of $v = 2$. [215] All the parameters above are obtained to high accuracy.

![Figure 7.6: Entanglement entropy $S$ vs. subsystem size $L_A$, for a open boundary $\mathbb{Z}_4$ critical chain with $L = 250$. The central charge $c = 1$ can be read off from the linear fit in the inset, which is based on Eq. (7.50).](image)

The parameters of $\epsilon_\infty$, $c$ and $v$ for $\mathbb{Z}_3$, $\mathbb{Z}_4$, $\mathbb{Z}_5$, and $\mathbb{Z}_6$ clock models are listed in Table 7.3. In addition to
the comparison between the numerical and exact results for the $k = 4$ case, our results for the ferromagnetic
and antiferromagnetic $k = 3$ cases also match up extremely well with previous numerical results [192],
and the Bethe ansatz solutions [216] of $\epsilon_\infty = -2\sqrt{3}/\pi - 4/3$, $v = 3\sqrt{3}/2$ (ferromagnetic), and $\epsilon_\infty = -\sqrt{3}/\pi - 3\sqrt{3}/2 + 4/3$, $v = 3\sqrt{3}/4$ (anti-ferromagnetic).

The expression $E_0 = \epsilon_\infty L - \pi vc/6L$, up to small correction in order of $O(L^{-2})$, is the ground state energy;
$h$ is the holomorphic conformal dimension of the primary field and $\bar{h}$ is the anti-holomorphic counterpart;
and $n$ and $\bar{n}$ are non-negative integers marking the energy levels. Besides, the momentum quantum numbers
are related to the conformal dimensions of the primary (and descendant) fields as

$$P = \frac{2\pi}{L}(h + \bar{h} + n + \bar{n}). \quad (7.51)$$

As a side note, in ED calculations, $P$ can be trivially obtained through the eigenvalues of the translation
operator. One usually shifts the eigenstates by one site, and the resulting phase factors would lead to
the quantized momenta. The only complication arises because of the even and odd pattern of the critical
anti-ferromagnetic $Z_3$ and $Z_5$ clock models.[192] For these cases with different system sizes, the eigenstates’
momenta are only consistent if one calculates the phase factors through a translation by two sites, while
translation by one site does not produce meaningful results.

Once we have all the necessary parameters, we can calculate the conformal dimensions based on the
rescaled energy

$$E_R \equiv (h + \bar{h} + n + \bar{n}) = \frac{L}{2\pi v}(E - E_0) + O(L^{-1}), \quad (7.52)$$
Because of the finite size correction at the order of $O(L^{-1})$, polynomial extrapolation in terms of $1/L \to 0$ is often needed for small system sizes. We extrapolate the conformal dimensions at different system sizes using polynomials of various orders of $1/L$, and check whether consistent results can be obtained in the limit of $1/L \to 0$. Reliable results are then listed in the tables.

In particular, we show several figures (Fig. 7.8 for $Z_4$ clock models below to illustrate this idea.

![Figure 7.8: Polynomial extrapolation of the first 4 excited states’ rescaled energy for the critical $Z_4$ clock model with even (left four) and odd (right four) number of twist defects. The black dots are ED data points. There are three polynomial fit curves, at 2nd, 3rd, and 4th order respectively. One can see that for all cases, all three polynomial fit curves have nearly the same y-intercept.]

In the Table 7.4,7.5,7.6,7.7,7.8, we show the results for the $k = 3, 4, 5, 6$ critical chain with even number of twist defects with both ferromagnetic/antiferromagnetic coupling. $h$ and $\tilde{h}$ extracted from energy spectrum match up with the known CFT results for critical $Z_k$ clock models and are summarized in Table 7.1. In the following section, we will study the energy spectrum for the odd number of twist defects and compare the...
results with the even case.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$E_R$</th>
<th>$\frac{L_p}{2\pi P}$</th>
<th>$(h + n, \bar{h} + \bar{n})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$(0, 0)$</td>
</tr>
<tr>
<td>0</td>
<td>0.80304</td>
<td>0</td>
<td>$(\frac{2}{7}, \frac{2}{7})$</td>
</tr>
<tr>
<td>0</td>
<td>1.79620</td>
<td>±1</td>
<td>$(\frac{2}{7}, \frac{2}{7}), (\frac{7}{2}, \frac{2}{7})$</td>
</tr>
<tr>
<td>0</td>
<td>1.80524</td>
<td>±1</td>
<td>$(\frac{7}{2}, \frac{7}{2}), (\frac{7}{2}, \frac{7}{2})$</td>
</tr>
<tr>
<td>0</td>
<td>1.99987</td>
<td>±2</td>
<td>$(2, 0), (0, 2)$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.13341</td>
<td>0</td>
<td>$(\frac{1}{2}, \frac{1}{7})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>1.13378</td>
<td>±1</td>
<td>$(\frac{1}{2}, \frac{1}{7}), (\frac{16}{17}, \frac{1}{17})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>1.33391</td>
<td>0</td>
<td>$(\frac{2}{5}, \frac{2}{3})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>2.13351</td>
<td>±2</td>
<td>$(\frac{1}{17}, \frac{25}{17}, \frac{17}{17})$</td>
</tr>
</tbody>
</table>

Table 7.4: Conformal dimensions of primary and descendant fields of the ferromagnetic $Z_3$ clock model with even number of twist defects. $q$ above is a label for the charge sector, with $\epsilon^{2q\pi i/k}$ as the eigenvalue of $Q$. The results shown above are obtained using ED for $N = 5, 6, 7, 8, 9, 10, 11, 12, 13, 14$. Rescaled energies higher than 2.13351 are not well resolved for the system sizes available.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$E_R$</th>
<th>$\frac{L_p}{2\pi P}$</th>
<th>$(h + n, \bar{h} + \bar{n})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$(0, 0)$</td>
</tr>
<tr>
<td>0</td>
<td>1.00027</td>
<td>±1</td>
<td>$(1, 0), (0, 1)$</td>
</tr>
<tr>
<td>0</td>
<td>1.49975</td>
<td>0</td>
<td>$(\frac{3}{7}, \frac{2}{7})$</td>
</tr>
<tr>
<td>0</td>
<td>1.50268</td>
<td>0</td>
<td>$(\frac{3}{4}, \frac{3}{4})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.16667</td>
<td>0</td>
<td>$(\frac{1}{17}, \frac{17}{17})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.66675</td>
<td>0</td>
<td>$(\frac{3}{7}, \frac{7}{7})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>1.16728</td>
<td>±1</td>
<td>$(\frac{13}{17}, \frac{13}{17}), (\frac{13}{17}, \frac{2}{17})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>1.67321</td>
<td>±1</td>
<td>$(\frac{3}{7}, \frac{3}{7}), (\frac{3}{7}, \frac{5}{7})$</td>
</tr>
</tbody>
</table>

Table 7.5: Conformal dimensions of primary and descendant fields of the anti-ferromagnetic $Z_3$ clock model with even number of twist defects. $q$ above is a label for the charge sector, with $\epsilon^{2q\pi i/k}$ as the eigenvalue of $Q$. Here we only show the lowest 10 excitations. The results shown above are obtained using ED for $N = 6, 8, 10, 12, 14$.

Wilson loop Hamiltonian with $2N − 1$ twist defects

The Wilson loop Hamiltonian with $2N − 1$ twist defects corresponds to the twisted $Z_k$ clock model in Eq.(7.44). Although the twisted $Z_k$ clock model still has $N$ sites, the effective length is $L = N − 1/2$ and the energy spectra of the twisted $Z_k$ clock model is described by Eq.(7.49), where the parameters $\epsilon_\infty$, $c$ and $v$ are the same as in the even number case.

As with the previous case, $(h + \bar{h} + n + \bar{n})$ can be obtained by calculating the rescaled energy $E_R$, which is now defined in this way,

$$E_R \equiv (h + \bar{h} + n + \bar{n})$$

$$= (N - \frac{1}{2})^2 (\frac{E}{N - \frac{1}{2}} - \epsilon_\infty) + \frac{\pi \epsilon c}{6} + O(N^{-1})$$

(7.54)
Table 7.6: Conformal dimensions of primary and descendant fields of the ferromagnetic/antiferromagnetic $Z_4$ clock model with even number of twist defects. $q$ above is a label for the charge sector, with $e^{2q\pi i/k}$ as the eigenvalue of $Q$. The results shown above are obtained using ED for $N = 5, 6, 7, 8, 9, 10, 11, 12$.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$E_R$</th>
<th>$\frac{L}{2\pi} P$</th>
<th>$(h + n, \bar{h} + \bar{n})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$(0, 0)$</td>
</tr>
<tr>
<td>0</td>
<td>0.99999</td>
<td>0</td>
<td>$(\frac{1}{5}, \frac{1}{2})$</td>
</tr>
<tr>
<td>0</td>
<td>1.24986</td>
<td>$\pm 1$</td>
<td>$(\frac{7}{10}, \frac{7}{10}), (\frac{1}{2}, \frac{1}{2})$</td>
</tr>
<tr>
<td>0</td>
<td>1.99896</td>
<td>$\pm 1, \pm 2$</td>
<td>$(\frac{7}{10}, \frac{7}{10}), (\frac{1}{2}, \frac{1}{2}), (0, 0)$</td>
</tr>
<tr>
<td>1, 3</td>
<td>0.12500</td>
<td>0</td>
<td>$(\frac{9}{16}, \frac{9}{16}), (\frac{1}{16}, \frac{1}{16})$</td>
</tr>
<tr>
<td>1, 3</td>
<td>1.12485</td>
<td>$0, \pm 1$</td>
<td>$(\frac{9}{16}, \frac{9}{16}), (\frac{1}{16}, \frac{1}{16})$</td>
</tr>
<tr>
<td>2</td>
<td>0.25000</td>
<td>0</td>
<td>$(\frac{1}{5}, \frac{1}{2})$</td>
</tr>
<tr>
<td>2</td>
<td>0.99999</td>
<td>0</td>
<td>$(\frac{7}{10}, \frac{7}{10})$</td>
</tr>
<tr>
<td>2</td>
<td>1.24986</td>
<td>$\pm 1$</td>
<td>$(\frac{7}{10}, \frac{7}{10}), (\frac{1}{2}, \frac{1}{2})$</td>
</tr>
<tr>
<td>2</td>
<td>1.99896</td>
<td>$\pm 1, \pm 2$</td>
<td>$(\frac{7}{10}, \frac{7}{10}), (\frac{1}{2}, \frac{1}{2}), (0, 0)$</td>
</tr>
</tbody>
</table>

Table 7.7: Conformal dimensions of the primary and descendant fields of ferromagnetic (F) and antiferromagnetic (AF) $Z_5$ clock models. $q$ above is a label for the charge sector, with $e^{2q\pi i/k}$ as the eigenvalue of $Q$. The ferromagnetic results shown above are obtained using ED for $N = 5, 6, 7, 8, 9, 10, 11, 12$, while the anti-ferromagnetic results are obtained using ED for $N = 4, 6, 8, 10, 12$. Notice that the conformal dimensions for F and AF cases are identical.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$E_R^F$</th>
<th>$E_R^A$</th>
<th>$\frac{L}{2\pi} P^{F/AF}$</th>
<th>$(h + n, \bar{h} + \bar{n})^{F/AF}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$(0, 0)$</td>
</tr>
<tr>
<td>0</td>
<td>1.0014</td>
<td>1.0004</td>
<td>$\pm 1$</td>
<td>$(1, 0), (0, 1)$</td>
</tr>
<tr>
<td>1, 4</td>
<td>0.0998</td>
<td>0.1001</td>
<td>0</td>
<td>$(\frac{1}{20}, \frac{1}{20})$</td>
</tr>
<tr>
<td>1, 4</td>
<td>1.0959</td>
<td>1.1050</td>
<td>$\pm 1$</td>
<td>$(\frac{1}{20}, \frac{1}{20}), (\frac{9}{20}, \frac{9}{20})$</td>
</tr>
<tr>
<td>2, 3</td>
<td>0.3939</td>
<td>0.4010</td>
<td>0</td>
<td>$(\frac{3}{20}, \frac{3}{20})$</td>
</tr>
<tr>
<td>2, 3</td>
<td>0.8930</td>
<td>0.8979</td>
<td>0</td>
<td>$(\frac{9}{20}, \frac{9}{20})$</td>
</tr>
</tbody>
</table>

Table 7.8: Conformal dimensions of primary and descendant fields of the ferromagnetic/antiferromagnetic $Z_6$ clock model with even number of twist defects. $q$ above is a label for the charge sector, with $e^{2q\pi i/k}$ as the eigenvalue of $Q$. The results shown above are obtained from ED results of $N = 4, 5, 6, 7, 8, 9, 10$. |
However complication arises for the calculation of \((h + n - \bar{h} - \bar{n})\). First of all, under the duality twist boundary conditions, it is not known a priori whether there exists a relation between the momenta and \((h + n - \bar{h} - \bar{n})\) as in Eq. (7.51). Secondly, assuming the same relations holds, there no longer exists a simple translation operator, where one can shift the eigenstates by one or two sites in ED, and find the momenta through the phase factors. The system as defined in Eq. (7.13) has a translational operation given by \(\tilde{T}\), which is built by consecutive multiplication of \(B\)-operators and commutes with the Hamiltonian. We will calculate the eigenvalues of \(\tilde{T}\) and extract the “momenta” of a system of length \(N - 1/2\). However, since there is an overall phase ambiguity in the definition of \(\tilde{T}\), the “momentum” quantum numbers are quantized up to an unknown additive constant which changes in each charge sector and also depends on each system size. Therefore we can only fix the difference of the “momentum” quantum numbers of \(\tilde{T}\) (denoted as \(\Delta P\)) between any excited state and the lowest energy eigenstate in identical charge sector and of the same system size. Due to this overall phase ambiguity, it is not possible to pin down a unique combination of \((h + n, \bar{h} + \bar{n})\).

However, in most of the cases, it turns out the decomposition into \((h + n, \bar{h} + \bar{n})\) is quite simple. We will show that when \(k \neq 4\), in each charge sectors, only the holomorphic part \((h)\) or the anti-holomorphic part \((\bar{h})\) has a twist with the rest part remains the same. This result matches up with the \(Z_2\) orbifold CFT. The \(k = 4\) case is more complicated since we don’t find any known orbifold CFT which precisely has the same excitation spectrum. Nevertheless, we still manage to show that these new excitations in \(k = 4\) case should be related with \(Z_4\) twist fields.

### 7.3.1 \(k = 3\), Ferromagnetic

The \(Z_3\) clock model with ferromagnetic coupling at critical point can be described by the three-state Potts CFT. It has a block-diagonal modular invariant partition function, \([217, 218]\)

\[
Z = |\chi_0 + \chi_3|^2 + |\chi_{\frac{5}{2}} + \chi_{\frac{7}{2}}|^2 + 2|\chi_{\frac{1}{4}}|^2 + 2|\chi_{\frac{3}{4}}|^2
\]  
(7.55)

where \(\chi_h\) denotes the character for each primary field with conformal dimension \(h\). As shown in Table 7.4, \(h\) obtained from the energy spectrum difference is consistent with the CFT prediction.

Once we consider odd-defect chain at critical point, there will be some new excitations in the low energy spectrum. In Table 7.9, we present the rescaled energy spectrum and momentum difference. From these numerical data, we can calculate the possible combination \((h + n, \bar{h} + \bar{n})\) and we find two new excitations with conformal dimensions equal to 1/40 and 1/8. They are not in the original three-state Potts CFT but can be found in \(\mathcal{M}(5, 6)\) minimal model.
Actually, the three-state Potts CFT can be considered as a subset of $\mathcal{M}(5,6)$ minimal model (tetracritical Ising CFT), which includes all the ten primary fields and has a diagonal modular invariant partition function $Z = \sum_{i=1}^{10} |\chi_i|^2$. These ten primary fields have conformal dimension $h = 0, \frac{1}{5}, \frac{2}{5}, \frac{13}{20}, \frac{2}{5}, \frac{1}{10}, \frac{24}{40}, \frac{7}{10}, \frac{3}{5}, 3$ (see Ref. [196, 217, 218]). The two CFTs are connected through $\mathbb{Z}_2$ orbifolding and the $\mathcal{M}(5,6)$ minimal model involves some new twist field operators. There is a simple way to understand this $\mathbb{Z}_2$ orbifold:[203] the three-state Potts CFT ($\mathbb{Z}_3$ parafermion CFT) is defined by the coset,

$$SU(2)_3/U(1)_3 = (G_2)_1 \times SU(3)_1 = (1, \tau) \times (1, \bar{s}, s^2)$$

where $(G_2)_1$ refers to the exceptional Lie group $G_2$ at level 1 and it contains 1 and the Fibonacci anyon $\tau$ with conformal dimension $h_{\tau} = 2/5$. Here $SU(3)_1$ means the time reversal or anti-holomorphic part of $SU(3)$ with the reverse propagating direction. Notice that $SU(3)_1$ CFT contains three primary fields $1, s$ and $s^2$ with $h_{s,s^2} = 1/3$. Therefore, the three-state Potts CFT can be understood as the tensor product between $(G_2)_1$ and $SU(3)_1$ with $2 \times 3 = 6$ primary fields and has central charge $c = 14/5 - 2 = 4/5$.

The abelian $SU(3)_1$ CFT has $\mathbb{Z}_2$ symmetry. After orbifolding this $\mathbb{Z}_2$ symmetry, it becomes $SU(2)_4$ CFT which has five primary fields with conformal dimension $h = 0, 1/8, 1/3, 5/8, 1$.[164, 165, 204] Among them, there are two $\mathbb{Z}_2$ twist fields with $h = 1/8, 5/8$. Combined with $(G_2)_1$ sector, this new CFT has ten primary fields and has similar structure as the $\mathcal{M}(5,6)$ minimal model.

Coming back to Table 7.9, we observe that $\tilde{h}$ is still the same as the original three-state Potts CFT, while $h$ is new and comes from the $\mathbb{Z}_2$ twist fields in $\mathcal{M}(5,6)$ minimal model. We will show that similar behavior occurs for other cases except $k = 4$ model.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$E_R$</th>
<th>$L^{-1/2} \Delta P$</th>
<th>$(h + n, \bar{n} + \bar{n})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.12499</td>
<td>$-\frac{1}{4}$</td>
<td>$(\frac{1}{5}, 0)$</td>
</tr>
<tr>
<td>0</td>
<td>0.42533</td>
<td>$\frac{1}{2}$</td>
<td>$(\frac{7}{10}, \frac{2}{5})$</td>
</tr>
<tr>
<td>0</td>
<td>0.92317</td>
<td>0</td>
<td>$(\frac{11}{20}, \frac{7}{5})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.09161</td>
<td>$-\frac{1}{2}$</td>
<td>$(\frac{1}{5}, \frac{1}{5})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.59202</td>
<td>$\frac{1}{2}$</td>
<td>$(\frac{1}{10}, \frac{1}{10})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.79175</td>
<td>$-\frac{1}{2}$</td>
<td>$(\frac{1}{5}, \frac{1}{5})$</td>
</tr>
</tbody>
</table>

Table 7.9: Conformal dimensions of primary fields of the ferromagnetic $\mathbb{Z}_3$ clock model with odd number of twist defects. $m$ above is a label for the mixed sector Hamiltonian $H^{(m)}$, or the $Q = e^{2\pi i/k}$ charge sector for $H^{(0)}$. $\Delta P$ is the difference of the “momentum” quantum numbers between any excited eigenstate and the lowest energy eigenstate in the same charge sector and of the same system size. The results shown above are obtained using ED for $N = 7, 8, 9, 10, 11, 12, 13, 14$. 

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7.3.2 $k = 3$, Anti-Ferromagnetic & $k \geq 5$

For the even-defect chain with $k = 3$, i.e., $\mathbb{Z}_3$ clock model, if the coupling is antiferromagnetic, the critical point is described by $U(1)_3$ CFT with $\mathbb{Z}_2$ charge-conjugation symmetry. The conformal dimension for this CFT is equal to $r^2/12$ with $0 \leq r < 6$ and $r \in \mathbb{Z}$. In Table 7.5, we present the numerical results for $h$ and $\bar{h}$. For each excited state, $h$ and $\bar{h}$ are always the same, suggesting that the partition function takes a diagonal form.

For the odd-defect chain shown in Table 7.10, we observe that the ground state has energy shifted by $1/16$, which is the same as the conformal dimension for $\mathbb{Z}_2$ twist field in $U(1)_3/\mathbb{Z}_2$ CFT (for more details see [196, 203]). Moreover, $h$ and $\bar{h}$ do not come in pairs. $h$ is still the same as the original $U(1)_3$ CFT, while $\bar{h}$ is coming from the $\mathbb{Z}_2$ twist field.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$E_R$</th>
<th>$\Delta P$</th>
<th>$(h+n, \bar{h}+\bar{n})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.06250</td>
<td>$-\frac{1}{2}$</td>
<td>$(0, \frac{1}{16})$</td>
</tr>
<tr>
<td>0</td>
<td>0.56249</td>
<td>$-\frac{1}{2}$</td>
<td>$(0, \frac{5}{16})$</td>
</tr>
<tr>
<td>0</td>
<td>0.81244</td>
<td>$\frac{1}{2}$</td>
<td>$(\frac{3}{16}, \frac{1}{16})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.14583</td>
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<td>$(\frac{15}{16}, \frac{1}{16})$</td>
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<td>$(\frac{11}{16}, \frac{5}{16})$</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.64581</td>
<td>$-\frac{1}{2}$</td>
<td>$(\frac{11}{16}, \frac{1}{16})$</td>
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</tbody>
</table>

Table 7.10: Conformal dimensions of primary fields of the anti-ferromagnetic $\mathbb{Z}_3$ clock model with odd number of twist defects. $m$ above is a label for the mixed sector Hamiltonian $H^{(m)}$, or the $Q = \epsilon^{2m \pi i/k}$ charge sector of $H^{(0)}$. $\Delta P$ is the difference of the “momentum” quantum numbers between any excited eigenstate and the lowest energy eigenstate in the same charge sector and of the same system size. The results shown above are obtained using ED for $N = 6, 8, 10, 12, 14$.

Similar rules apply when $k \geq 5$. For $\mathbb{Z}_k$ clock model, the critical point is described by $U(1)_k$ CFT. In Table 7.7 and 7.8, we present the numerical results of conformal dimensions for $k = 5, 6$ with both ferromagnetic and antiferromagnetic coupling in even number twist defect chain. In all of these cases, $h$ and $\bar{h}$ are consistent with the result for $U(1)_k$ CFT. Moreover, they always come in pairs, suggesting the partition function takes a diagonal form.

When $k = 6$, if we consider odd-defect chain (Table 7.12), for both ferromagnetic and antiferromagnetic coupling, the lowest several excitations have $E_R = 1/16 + r^2/4k$, where $1/16$ is coming from the $\mathbb{Z}_2$ twist field operator and $r^2/24$ corresponds to the excitation in the original $U(1)_6$ CFT. When $k = 5$, for the odd-defect chain, if the coupling is antiferromagnetic, as shown in Table 7.11, the lowest several excitations are still equal to $1/16 + r^2/4k$. For the ferromagnetic coupling, the quality of the numerical result is not fine enough due to strong finite size effect and we cannot extract meaningful $h$ and $\bar{h}$. Nevertheless, these results suggest that for $k \neq 4$, the underlying CFT for odd-defect chain and even-defect chain are related through $\mathbb{Z}_2$ orbifolding and the extra twist defect in the odd-chain effectively introduces a $\mathbb{Z}_2$ twist field in
the original CFT.

\[
\begin{array}{|c|c|c|c|}
\hline
m & E_R & \frac{L-1/2}{2\pi} \Delta P & (h + n + \bar{h} + \bar{n}) \\
\hline
0 & 0.0625 & - & (0, \frac{1}{16}) \\
0 & 0.563 & -\frac{1}{2} & (0, \frac{1}{16}) \\
1, 4 & 0.1125 & - & \left(\frac{1}{16}, \frac{17}{16}\right) \\
1, 4 & 0.614 & -\frac{1}{7} & \left(\frac{1}{7}, \frac{17}{16}\right) \\
2, 3 & 0.2628 & - & \left(\frac{3}{16}, \frac{17}{16}\right) \\
2, 3 & 0.513 & \frac{1}{4} & \left(\frac{5}{16}, \frac{17}{16}\right) \\
\hline
\end{array}
\]

Table 7.11: Conformal dimensions of primary fields of anti-ferromagnetic $Z_5$ clock model with odd number of twist defects. $n$ above is a label for the mixed sector Hamiltonian $\tilde{H}^{(m)}$, or the $Q = e^{2m\pi i/k}$ charge sector of $H^{(0)}$. $\Delta P$ is the difference of the “momentum” quantum numbers between any excited eigenstate and the lowest energy eigenstate in the same charge sector and of the same system size. The results shown above are obtained from ED results of $N = 4, 6, 8, 10, 12$.

\[
\begin{array}{|c|c|c|c|}
\hline
m & E_R & \frac{L-1/2}{2\pi} \Delta P & (h + n + \bar{h} + \bar{n}) \\
\hline
0 & 0.0625 & - & (0, \frac{1}{16}) \\
1, 5 & 0.1042 & - & \left(\frac{1}{16}, \frac{17}{16}\right) \\
1, 5 & 0.6047 & -\frac{1}{2} & \left(\frac{1}{7}, \frac{17}{16}\right) \\
2, 4 & 0.2295 & - & \left(\frac{1}{6}, \frac{17}{16}\right) \\
3 & 0.438 & - & \left(\frac{9}{16}, \frac{17}{16}\right) \\
\hline
\end{array}
\]

Table 7.12: Conformal dimensions of primary fields of ferromagnetic/anti-ferromagnetic $Z_6$ clock model with odd number of twist defects. $n$ above is a label for the mixed sector Hamiltonian $\tilde{H}^{(m)}$, or the $Q = e^{2m\pi i/k}$ charge sector of $H^{(0)}$. $\Delta P$ is the difference of the “momentum” quantum numbers between any excited eigenstate and the lowest energy eigenstate in the same charge sector and of the same system size. The results shown above are obtained from ED results of $N = 4, 5, 6, 7, 8, 9, 10$.

### 7.3.3 $k = 4$

The $k = 4$ odd-chain is much more complicated than $k > 5$ cases. This is because when the chain consists of even number of defects, the $Z_4$ clock model is already described by the $U(1)_2/Z_2$ orbifold CFT, which is equivalent to the Ising\(^2\) CFT.[165, 202] As shown in Table 7.6, there are already some excitations with conformal dimension $h = \bar{h} = 1/16$. For the odd number twist defect chain, we find that this model cannot be described by further orbifolding $Z_2$ symmetry. We list the rescaled excitation energy $E_R$ shown in the second column of Table 7.14. Notice that the ground state has $E_R = 1/16 + 1/64$, where the new $1/64$ excitation is smaller than $h = 1/32$ of the twist field in Ising\(^2\)/$Z_2$ CFT.[219] This suggests that the odd-defect chain cannot be described by the $Z_2$ orbifold CFT like other $k \neq 4$ cases. We further observe that for the excitations in $m = 0, 2$ sectors, apart from $1/16$ part, the rest part of $E_R$ fits well with $t^2/64 + n$ or $t^2/64 + n + 1/2$, where $t = 1, 3, 5, 7$. Surprisingly, this $1/64$ excitation also shows up in the $SU(2)_1/D_4$ CFT ($D_4 = Z_4 \rtimes Z_2$ is the dihedral group at order 8) and is the conformal dimension for the four-fold symmetry sector.[165] This coincidence
motivates us to propose that the odd defect chain might be related with some $\mathbb{Z}_4$ orbifold CFT.

Here we briefly explain the physics in $SU(2)_1/D_4$ CFT and its connection with four-state Potts CFT. The self-dual Ashkin-Teller quantum chain model, in terms of $\mathbb{Z}_4$ clock variable, has the following Hamiltonian,[220]

$$\begin{align*}
H &= -\sum_i \left[ \sigma_i + \sigma_i^\dagger + \lambda(\sigma_i)^2 \\
&\quad + \tau_i \overline{\tau}_{i+1} + \tau_i^\dagger \overline{\tau}_{i+1} + \lambda(\tau_i)^2(\overline{\tau}_{i+1})^2 \right].
\end{align*}$$

For this model, as we vary $\lambda$ from 0 to 1, the model changes from $\mathbb{Z}_4$ clock model to four-state Potts model and remains critical for the whole regime for $\lambda$ between 0 and 1. This critical line is the famous Ashkin-Teller line and can be described by $U(1)/\mathbb{Z}_2$ orbifold CFT, where the compactification radius of $U(1)$ CFT changes as we vary $\lambda$.[221] For four-state Potts CFT, it corresponds to $U(1)_4/\mathbb{Z}_4$ CFT, which is also equivalent to $SU(2)_1/D_2$ CFT, where $D_2$ is the dihedral group at order 4 and is the double-cover of the 180° rotations about the $x$, $y$, $z$-axes.[201, 202] Actually, starting from the $SU(2)_1$ CFT, we can get a family of orbifold CFTs by modding out the subgroup of $SU(2)$ (or called ADE classification).[165, 201, 202, 222] For $SU(2)_1/D_2$ CFT, it lies in the middle of this interesting series orbifold CFTs and has eleven characters which are reorganized in Table (7.13) in a more symmetric way. There exists a $S_3 = \mathbb{Z}_3 \rtimes \mathbb{Z}_2$ symmetry for $SU(2)_1/D_2$ CFT, which shuffles the twist fields $J_a$, $\sigma_a$ and $\tau_a$ ($a = 1, 2, 3$) separately. In principle, we can orbifold the full $S_3$ symmetry and obtain $SU(2)_1/O$ CFT, where $O$ represents the octahedral group.[165, 201, 202, 222] However for our purpose in this chapter, we only need to orbifold the two-fold symmetry and we obtain $SU(2)_1/D_4$ CFT which is equivalent to $U(1)_4/\mathbb{Z}_4$ CFT. This CFT has eight primary fields from the four-fold symmetry sector with conformal dimension $h = 1/64 + s(2s - 1)/8$ or $h = 33/64 + s(2s - 1)/8$ with $s = 0, 1, 2, 3$.[165] These values actually are the same as $t^2/64$ or $t^2/64 + 1/2$ for $m = 0, 2$ sectors in the second column of Table 7.14.

We also compute the momentum by diagonalizing $\tilde{T}$ operator and show $\Delta P$ in the third column of Table 7.14. Based on $E_R$ and $\Delta P$, we list one possible decomposition $(h + n, \overline{h} + \overline{n})$ in the fourth column of Table 7.14. We compare this $\#/64$ in $h$ or $\overline{h}$ in $m = 0, 2$ sectors with conformal dimension for primary fields in four-fold symmetry sector in $SU(2)_1/D_4$ CFT and we find that they can partially match up. Moreover, $SU(2)_1/D_4$ CFT also has two-fold symmetry sector corresponding to twofold rotation about a diagonal axis like (110) which actually has $h = 1/16, 9/16$ and is consistent with $m = 1, 3$ sectors. At this moment, it is unclear why there is connection between odd number twist defect chain and $SU(2)_1/D_4$ ($U(1)_4/\mathbb{Z}_4$) CFT. What is puzzling is that the even chain and odd chain are not seemingly related by orbifold. The even chain has an Ising$^2$ CFT with the compactification radius $R = 1$, but the odd chain is suggestively $SU(2)_1/D_4$
which has a larger radius $R = \sqrt{2}$. We leave this disagreement for future studies.

<table>
<thead>
<tr>
<th>$d_\chi$</th>
<th>$h_\chi$</th>
<th>$\chi$</th>
<th>$\chi_l$</th>
<th>$\chi^a$</th>
<th>$\chi^a_l$</th>
<th>$\chi^a$</th>
<th>$\chi^a_l$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 7.13: The quantum dimensions $d_\chi$, conformal dimension $h_\chi$ of characters for chiral $U(1)_4/\mathbb{Z}_2$ CFT, where $a = 1, 2, 3$.

The table below shows the results for the mixed sector Hamiltonian $\hat{H}^{(m)}$, and for the odd number of twist defects, $\Delta P$ is the difference of the "momentum" quantum numbers between any excited eigenstate and the lowest energy eigenstate in the same charge sector and of the same system size. The results shown above are obtained from ED results of $N = 6, 7, 8, 9, 10, 11, 12, 13$.

### 7.4 Conclusion

In the first part of the chapter, we study the twofold twist defect chain at critical point. We demonstrate that for even number of twist defects, it maps to the $\mathbb{Z}_k$ clock model with periodic boundary condition (up to some phase factor), while for the odd number case, it is equivalent to the $\mathbb{Z}_k$ clock model with a duality twisted boundary condition. The translation symmetry in the twist defect chain model becomes the Kramers-Wannier duality symmetry in the $\mathbb{Z}_k$ clock model. This symmetry operator can be generated by a
series of braiding operators for twist defects, and is discussed in section 7.2.5.

In the second part of the chapter, we numerically investigate the defect chain model at its self-dual critical point. We first extract the conformal dimensions for the primary fields in the even-defect chain model and find that they match up with that of the $Z_k$ clock CFT. We then turn to study the underlying CFT for odd-defect chains and we observe the energy spectrum is shifted, where the energy difference is caused by the twist field in the orbifold CFT. We find that when $k \neq 4$, the odd-defect chain is described by orbifolding the $Z_2$ symmetry in the even-defect chain CFT. On the other hand, when $k = 4$, there is a mysterious $1/64$ excitation in the spectrum of odd-defect chain which turns out to be related with the $Z_4$ twist field in the $SU(2)_1/D_4$ orbifold CFT. Our model can be generalized to twist defect with other symmetries and can be used to realize more complicated orbifold CFTs.
References


Appendix A: Stochastic imaginary time evolution with matrix product states

This is a side project that I explored in collaboration with Bryan Clark.

DMRG has been a very powerful numerical method to solve for low lying eigenstates of 1D gapped systems. It can also be applied to quasi-1D systems that look like a thin strip as in Fig. A.1, the only downside is that the bond dimension of the MPS usually has to grow exponentially with the width of the strip. Often one will find him or herself in a situation where it is unfordable to run DMRG at such a large bond dimension, but if a smaller bond dimensions is used, then the MPS cannot converge to the true ground state, and may likely be stuck at a meta-stable state. Here we describe a simple Monte Carlo technique that may help with this issue. We call it Stochastic imaginary time Evolution with Matrix Product States (SEMPs).

![Figure A.1: A diagram showing a “snake” shape MPS on a $4 \times 8$ lattice with open boundary conditions, where the orange bonds represent the physical degrees of freedom, while the black bonds represent the virtual degrees of freedom. Notice that the MPS does not allow direct connection between nearest neighbor pairs on the horizontal direction. Instead, it makes these nearest neighbor pairs 4 sites apart on the MPS. In general, MPS is not efficient for 2D simulations, as the the bond dimensions will grow exponentially with the number of legs (4 here).](image)

Given a not converged MPS $|\psi\rangle$, the skeleton of the SEMPS algorithm is as follows.
1. Choose an orthonormal product states basis \( \{ |c_i\rangle \} \), theoretically one can expand \( |\psi\rangle \) as

\[
|\psi\rangle = \sum_i \alpha_i |c_i\rangle.
\] (A.1)

With the MPS representation of \( |\psi\rangle \), it is easy to sample \( |c_i\rangle \) according to its probability \( p_i = |\alpha_i|^2 \). So one may sample a large set of product states \( |c_i\rangle \) from \( |\psi\rangle \), which will be called \( S_{\text{sampled}} \), and record the coefficients \( \alpha_i \). So the original wave function can be reconstructed as

\[
|\tilde{\psi}\rangle = \sum_{i \in S_{\text{sampled}}} \frac{1}{\alpha_i} |c_i\rangle.
\] (A.2)

as each \( |c_i\rangle \) is added into \( S_{\text{sampled}} \) with probability \( p_i = |\alpha_i|^2 \). If one has sufficient number of product states in \( S_{\text{sampled}} \), then \( |\tilde{\psi}\rangle \) is a close approximation to \( |\psi\rangle \).

2. To drive \( |\psi\rangle \) closer to the ground state, theoretically one could directly perform imaginary time evolution as

\[
|\psi(\beta)\rangle = \frac{1}{\sqrt{\langle \psi|e^{-2\beta H}|\psi\rangle}} e^{-\beta H} |\psi\rangle.
\] (A.3)

But because time evolution of MPS usually increases its bond dimension over time, which is already a bottleneck for quasi-1D systems, so it is better to do

\[
|\tilde{\psi}(\beta)\rangle = \frac{1}{\sqrt{\sum_j \sum_i \frac{1}{\alpha_i} \langle \psi|e^{-2\beta H}|c_j\rangle \frac{1}{\alpha_j} \langle c_j|e^{-\beta H}|c_i\rangle}} \sum_i \sum_j \frac{1}{\alpha_i} e^{-\beta H} |c_i\rangle.
\] (A.4)

And we can evaluate the energy expectation value at imaginary time \( \beta \) according to

\[
E(\beta) = \frac{1}{\sum_j \sum_i \frac{1}{\alpha_i} \langle \psi|e^{-2\beta H}|c_j\rangle} \sum_i \sum_j \frac{1}{\alpha_i} \langle c_j|H e^{-2\beta H}|c_i\rangle.
\] (A.5)

It is clear that instead of directly time evolving a already complicated MPS \( |\psi\rangle \), now the basic operation is to time evolve product states according to \( e^{-2\beta H} |c_i\rangle \). Since the product states have bond dimension 1, they are far easier to time evolve in the MPS format. For other observables that may not commute with \( H \), one can generally evaluate them in a slightly different way

\[
\langle O \rangle(\beta) = \frac{1}{\sum_k \sum_i \frac{1}{\alpha_k} \langle \psi|e^{-2\beta H}|c_k\rangle} \sum_i \sum_j \frac{1}{\alpha_i \alpha_j} \langle c_j|e^{-\beta H} O e^{-\beta H}|c_i\rangle.
\] (A.6)
where one also need to keep track of $e^{-\beta H}|c_i\rangle$, which can be obtained as one is on the way of getting $e^{-2\beta H}|c_i\rangle$.

3. When even the bond dimensions of $e^{-2\beta H}|c_i\rangle$ becomes unfordable, one can once again sample it with product states. So instead of a single wave function, we now have many sets of product states that approximates the original wave functions, where the time evolution of every product state is easily tractable.

![Energy estimate](image.png)

Figure A.2: Energy estimate calculated using Eq. (A.5) for a $4 \times 8$ Hubbard ladder. 2048 product states are sampled from a not converged MPS with a bond dimension of $M = 100$. The $M$ in the legend corresponds to the maximum bond dimension allowed for the product states during imaginary time evolution. One can see that before $\beta = 0.2$, the time evolutions for different cases follow the same trajectory. After $\beta = 0.2$, however, the larger the $M$ allowed, the lower the energy decays to. This divergence suggests that after $\beta = 0.2$ one should re-sample the time evolved states using product states again.

The above method basically allows one to time evolve the wave function stochastically and more efficiently. An example is given in Fig. A.2. With the time evolution, one can clearly see that the energy decays fast from the energy of the original MPS obtained from DMRG.
Appendix B: Exploring distance measures in constructive unitary tensor networks for MBL systems

This appendix is mainly based on an unpublished project explored in collaboration with David Pekker and Bryan Clark, which is an extension of Chapter 4.

B.1 Introduction

Unitary tensor networks (UTN) play important roles in fields ranging from many-body localization (MBL) to holography. In both cases, unitary tensor networks are used to transform between two complementary descriptions of the physical system. In the case of holography, UTN are used as models of the bulk/boundary correspondence mapping boundary states to bulk states. This idea was partially inspired by the fact that both the “vertical” direction in a multi-scale entanglement renormalization ansatz (MERA) tensor network and the radial direction of the holographic bulk can be thought of as a renormalization flow. Tensor network models often capture many important aspects of the holographic correspondence including obeying the Ryu-Takayanagi formula [93, 223–242].

In this work, we generate UTN which diagonalizes MBL Hamiltonians and can be treated holographically using continuous Wegner flow equations. With the canonical generator, the Wegner flow performs a continuous unitary transformation that incrementally diagonalizes the Hamiltonian by removing off-diagonal terms which couple the largest difference in energies. For more details, please see the discussion in Chapter 4. In contrast to previous approaches to finding unitary tensor networks for MBL, our approach is both constructive (without optimization) as well as accomplished using a continuous unitary transformation; this lets us make a more direct connection to ideas about holographic bulk/boundary correspondence where the radial direction into the bulk is most naturally related to the flow parameter. When the Hamiltonian is fully MBL, our representation will be compact and generated efficiently.

To benchmark our algorithm, we study the standard model of MBL, the Heisenberg chain with random magnetic fields with open boundary conditions as defined in Eq. (1.13).
B.2 Building unitary tensor networks using Wegner flow

Wegner flow, which can be interpreted as a renormalization group (RG) flow that diagonalizes successive energy scales, provides a continuous unitary transformation from the physical spin degrees of freedom (p-bits) to the l-bits. The difficulty of applying Wegner flow numerically lies in the exponentially growing Hilbert space size. At small system sizes, one can afford numerically integrating the flow equations using a sparse matrix format. For arbitrary disorder strength, we can use the Runge-Kutta method with dynamical time step to perform Wegner flow until the average variance of the Hamiltonian drops close to machine precision. At larger system sizes, the sparse matrix representation is generally impractical. Below we describe a method to perform Wegner flow using matrix product operators (MPO) for FMBL systems. Because FMBL systems’ eigenstates have area-law entanglement entropy, arguably it is efficient to store the Hamiltonians and the unitary transformations using MPO representation.

The steps are explained below.

1. The generator $\eta(\beta)$ can be rewritten as

$$\eta(\beta) = [H_0(\beta), H(\beta)], \quad (B.1)$$

where the diagonal MPO $H_0(\beta)$ can be constructed easily by setting the off-diagonal matrices $A^{\uparrow \downarrow}$ and $A^{\downarrow \uparrow}$ to zero on each site of $H(\beta)$’s MPO.

2. To time evolve the flow equations (4.3) using the explicit method, we find it necessary to perform higher order expansions. During a small, finite time step $\Delta \beta$, the unitary operator becomes

$$U(\beta + \Delta \beta) = e^{\eta(\beta)\Delta \beta} U(\beta). \quad (B.2)$$

The small multiplicative change $e^{\eta(\beta)\Delta \beta}$ to the unitary operator from here on will be called ‘$dU$’ whenever it is not confusing. To obtain $dU$, it is straightforward to use the Taylor series approach to approximate the exponentiation[243]. After obtaining $dU$, one may use it directly to evolve the Hamiltonian $H(\beta)$ according to

$$H(\beta + \Delta \beta) = e^{\eta(\beta)\Delta \beta} H(\beta) e^{-\eta(\beta)\Delta \beta}. \quad (B.3)$$

But in practice we find it more stable and accurate to expand and approximate $H(\beta + \Delta \beta)$ directly
using the Baker-Campbell-Hausdorff (BCH) formula.

\[
H(\beta + \Delta \beta) = H + \Delta \beta [\eta, H] + \frac{\Delta \beta^2}{2!} [\eta, [\eta, H]] + \frac{\Delta \beta^3}{3!} [\eta, [\eta, [\eta, H]]] + \cdots
\]  

(B.4)

The slight change of form in the last line allows us to repeatedly evaluate terms like \( H + \Delta \beta n [\eta, H'] \), whose bond dimensions are much better controlled compared to the exponentially growing bond dimensions (with respect to the number of \( \eta \)) of \([\eta, [\eta, [\eta, H]]]...\).

During the above procedure, we usually use a fixed SVD cutoff. It is important to notice that time evolutions of \( H(\beta) \) and \( U(\beta) \) can be carried out independently, and the former is possible without even building the \( U(\beta) \).

In Fig. B.1, we show the decrease of ensemble average of \( \log_{10}(V/L) \) as a function of \( \beta \), as well as the ensemble average of bond-dimension \( M \) for disordered Heisenberg chain of \( L = 16, 32 \). This set of computation is done with fixed amount of wall clock time. Because the small disorder strength samples are more entangled, they are harder to evolve, which is reflected in the lengths of the curve in Fig. B.1. In general, we find that deep in the MBL phase, the MPO version of the Wegner flow is easier, as reflected in their smaller bond dimensions through the process. To verify that the SVD cutoff we used is appropriate, we also compared the Wegner flow results for \( L = 32 \) using two different SVD cutoffs, as shown in Fig. B.2. One can see that at these two cutoffs, there is no significant deviation.

The computational complexity at each step scales roughly as \( O(M^5) \). We primarily run at a fixed \( \delta \beta \) (for very small \( \beta \) we use slightly finer steps) but if one switched over to an implicit time stepping method one could ramp up the time step exponentially faster.

### B.2.1 Geometry of unitary tensor networks

By stacking together the unitary operators in the Wegner flow process, we generate a unitary tensor networks, which look like a projected entangled pair state (PEPS). Although the PEPS naively appears like a grid, this fixed geometry is deceptive as the PEPS bond-dimension is dynamically adjusted which affects the geometry. We define both a radial as well as a circumferential distance metric on our geometry.

Our radial distance, the unitary distance, is adapted from the Bures distance in quantum information. Given two states described by density matrices \( \rho_1 \) and \( \rho_2 \), the Bures distance \( D_B \) between them is defined.
where

\[ L = 16 \]

\[ W = 4 \]

\[ W = 8 \]

\[ W = 12 \]

\[ W = 16 \]

\[ L = 32 \]

\[ 0.00 \]

\[ 0.05 \]

\[ 0.10 \]

\[ D_c \]

\[ 0.0 \]

\[ 0.5 \]

\[ 1.0 \]

\[ \beta \]

\[ M \]

\[ 5 \]

\[ 10 \]

\[ 15 \]

\[ 0.0 \]

\[ 0.5 \]

\[ 1.0 \]

\[ \beta \]

\[ -2 \]

\[ -4 \]

\[ -6 \]

\[ 0.0 \]

\[ 0.5 \]

\[ 1.0 \]

\[ 1.5 \]

\[ \ln(V/L) = 16 \]

\[ W = 4 \]

\[ W = 8 \]

\[ W = 12 \]

\[ W = 16 \]

\[ L = 32 \]

\[ 0.00 \]

\[ 0.05 \]

\[ 0.10 \]

\[ DU \]

\[ 0.0 \]

\[ 0.5 \]

\[ 1.0 \]

\[ 1.5 \]

\[ \beta \]

\[ 5 \]

\[ 10 \]

\[ 15 \]

\[ M \]

\[ 0.0 \]

\[ 0.5 \]

\[ 1.0 \]

\[ \beta \]

Figure B.1: (Colored online) MPO Wegner flow data for \( L = 16, 32 \). Different colors represent different disorder strength – blue for \( W = 4 \), orange for \( W = 8 \), red for \( W = 12 \), and green for \( W = 16 \). The SVD cutoffs used for \( L = 16, 32 \) are \( 4 \times 10^{-12} \) and \( 2 \times 10^{-12} \), respectively. The simulations are not converged at this \( \beta \) but run for a finite wall-clock time. **Left:** Ensemble average of \( \ln(V/L) \) and ensemble average of bond dimension \( M \) for \( H \) (solid) and \( dU \) (dashed) as a function of \( \beta \), with 160 samples and \( L = 16 \). **Right:** Ensemble average of \( \ln(V/L) \) and ensemble average of bond dimension \( M \) for \( H \) (solid) and \( dU \) (dashed) as a function of \( \beta \), with 160 samples and \( L = 32 \). through

\[ D_B^2 = 2(1 - Tr(\sqrt{\rho_1^{1/2} \rho_2 \rho_1^{1/2}})). \]  

(B.5)

For pure states \( \rho_1 = |\psi_1\rangle\langle\psi_1| \) and \( \rho_2 = |\psi_2\rangle\langle\psi_2| \), one gets

\[ D_B^2 = 2(1 - \langle\psi_1|\psi_2\rangle)). \]  

(B.6)

It is easy to see that the \( D_B^2 \) defined here depends on the system size \( L \). Especially, when that \( |\psi_1\rangle \) is translational invariant and \( |\psi_2\rangle \) is the result of a local basis rotation applied to every site of \( |\psi_1\rangle \), this dependence is obviously linear in \( L \).

Inspired by Ref. [230, 233], we defined the radial metric of the unitary tensor network as

\[ g_{rr}d\tau^2 = \frac{2}{\text{Dim}(H)L} Tr(\| - e^{\eta d\tau}) = \frac{Tr(\eta^4 \eta)}{\text{Dim}(H)L} d\tau^2, \]  

(B.7)
Figure B.2: (Colored online) Comparison of ensemble averages of $\ln(V/L)$ between SVD cutoffs of $2 \times 10^{-10}$ (dots) and $2 \times 10^{-12}$ (lines), at $L = 32$ and with the same 160 disorder realizations. Different colors represent different disorder strength – blue for $W = 4$, orange for $W = 8$, red for $W = 12$, and green for $W = 16$. It can be seen that there is no significant difference between the two sets of curves.

where $\eta$ is the anti-Hermitian generator and $L$ is the system size. The metric defined above is essentially the infinitesimal per unit length Bures distance brought by the unitary transformation of $e^{-\eta d\tau}$, averaged over a complete set of pure states. We include a factor of $1/L$ to remove some system size dependence from the radial distance of the RG flow.

The radial distance from the boundary (p-bits) to flow parameter of $\beta$ in the bulk of the unitary tensor network is given by

$$D_U(\beta) = \int_0^\beta \sqrt{g_{\tau\tau}} d\tau = \int_0^\beta \sqrt{\text{Tr}(\eta^\dagger \eta) \text{Dim}(H)L} d\tau.$$  \hspace{1cm} (B.8)

This distance is a generalization of a metric used in cMERA [230, 233] from states to UTN. This notion of distance is based on the rate of change of a quantum state throughout the RG flow, which is an extremely natural metric in the context of the Wigner flow as it follows from Eq. 4.6 that

$$D_U(\beta) = \int_0^\beta \sqrt{-\frac{1}{2L} \frac{dV(\tau)}{d\tau}} d\tau.$$  \hspace{1cm} (B.9)

Having defined a metric, we now explore the induced geometry. We first explore the relationship of $U_D(\infty)$ with the averaged entanglement entropy. We find a universal quadratic relationship between these two quantities, as in Fig. B.3.

Our circumferential metric will be defined as the number of tensors in our PEPS whose bond-dimension is greater than one. The intuition beyond this is that if the bond-dimension of the unitary is one around a given site, this roughly corresponds to an emerged l-bit, then the system becomes block-diagonal with
Figure B.3: Disorder averaged entanglement entropy vs final disorder averaged unitary distance $D_U$ for Heisenberg chain with $L = 6, 8, 10$ and $W = 0.5, 1, 2, 3, 4, 6, 8, 10, 12, 14, 16, 24, 32$. Each point represent one disorder strength of a specified system size. Curve fitting shows that these data points sit on a quadratic curve, irrespective of the system size $L$, which suggests a universal behavior.

respect to this l-bit. To remove some of the finite size effect, we define the normalized circumference across the system as

$$C = \frac{L - n_b}{L}, \quad (B.10)$$

where $n_b$ denotes the number of bonds of the small unitary MPO $dU$ that has bond dimension 1. To see how the circumference of the system change as the one goes into the bulk of the UTN, we looked at the relation between the circumference of the system and the unitary distance during the RG flow, as shown in Fig. B.4.

### B.3 Wegner flow and energy scale separation in the MBL phase

Typical numerical renormalization group (RG) approaches to MBL Hamiltonian systems, like RSRG-X [92] and SBRG [93], make use of the hierarchy of leading coupling strengths or energy scales to formulate the coarse graining and disentangling operations. During the RG process, l-bits emerge one after another with decreasing coupling strengths or energy scales.

Wegner flow is in general an energy scale separation renormalization flow. Empirically, for Wegner flow as in Eq. (4.3), Eq. (4.4) and Eq. (4.5), it separate out the energy scale of

$$E = \frac{1}{\sqrt{\beta}} \quad (B.11)$$
Figure B.4: Disorder averaged logarithmic circumference (\(\ln C\)) of the system vs the disorder averaged unitary distance \(D_U\) into the UTN. **Left:** Disordered Heisenberg chain of length \(L = 32\) at disorder strength of \(W = 4, 8, 12, 16\). **Right:** Disordered Heisenberg chain of length \(L = 16\) at disorder strength of \(W = 4, 8, 12, 16\). For both system sizes, we can see that \(\ln C\) decays linearly with \(D_U\) after an initial stage. If one plot the slopes of the linear fit curves vs the disorder strengths (see the two insets), one noticed that the extrapolated slope will reach zero around the disorder strength of \(W = 5\).

At RG time \(\beta\), which follows conceptually from dimension analysis. More rigorously, one can look at the flow equations for the off-diagonal Hamiltonian \(H_1\). Expanding Eq. (4.3), one has the following equation for an off-diagonal element \((H_1)_{ij}\),

\[
d(H_1)_{ij} = -(E_i - E_j)^2(H_1)_{ij} d\beta + O((H_1)^2),
\]

(B.12)

where \(E_i\) and \(E_j\) are the \(i\)-th and \(j\)-th diagonal elements of \(H_0\). Clearly the off-diagonal elements connecting larger energy differences are driven to zero faster than the others, effectively diagonalizing blocks successively depending on their energy hierarchy.

Assume \(H\) is only made up of Pauli operators. At time \(\beta_0\), Wegner flow with canonical generator divides up the Hamiltonian into the diagonal part and the off-diagonal part.

\[
H = \sum_i \hat{\alpha}_i P^z_i + H_1,
\]

(B.13)

where the diagonal part is further written as a summation over all Pauli strings \(P^z_i\) made up of identity operator \(I\) and \(\sigma_z\). There are two immediate consequences. Firstly, in the MBL phase, usually a shorter-ranged \(P^z_i\) with fewer \(\sigma_z\) will have a larger \(\alpha_i\). Secondly, for any Pauli string \(P^z_i\), the off-diagonal part \(H_1\) can be separated into \(H^A_i\) and \(H^C_i\), where the former anti-commute with \(P^z_i\) and the latter commute with \(P^z_i\).
The generator of the Wegner flow is

\[
\eta = \left[ \sum_i \tilde{\alpha}_i P_i^z, H_1 \right] = 2 \sum_i \tilde{\alpha}_i P_i^z H_i^A.
\]  

(B.14)

So

\[
\frac{dH}{d\beta} = [\eta, H] = [\eta, \sum_i \tilde{\alpha}_i P_i^z] + [\eta, H_1].
\]  

(B.15)

One can show that, all the change to the diagonal part of \( H \) solely comes from \([\eta, H_1]\)

\[
\frac{d}{d\beta} \sum_i \tilde{\alpha}_i P_i^z = 4 \sum_i \tilde{\alpha}_i P_i^z ||H_i^A||^2 + \text{cross terms},
\]  

(B.16)

and the leading order change of the off-diagonal part comes from \([\eta, \sum_i \tilde{\alpha}_i P_i^z]\)

\[
\frac{d}{d\beta} H_1 = -4 \sum_i |\tilde{\alpha}_i|^2 H_i^A + \text{cross terms} + O(||H_1||^2).
\]  

(B.17)

From the two equations above, it is clear that when there is a leading energy scale \( \alpha_i \) with a large anti-commuting \( H_i^A \), then they will dominate the flow at that stage, resulting in (note \( H_1 \neq \sum_i H_i^A \))

\[
\frac{d}{d\beta} \tilde{\alpha}_i = 4 \tilde{\alpha}_i ||H_i^A||^2,
\]  

(B.18)

and

\[
\frac{d}{d\beta} ||H_i^A||^2 = -8 \tilde{\alpha}_i^2 ||H_i^A||^2.
\]  

(B.19)

From the two equations above, we have

\[
\frac{d}{d\beta} ||H_i^A||^2 + \frac{d}{d\beta} \tilde{\alpha}_i^2 = 0,
\]  

(B.20)

which roughly comes from the fact that the L2 norm of \( H \) should be conserved during Wegner flow.

This means at this energy scale, we have

\[
H_i^A(\beta) = e^{-4\tilde{\alpha}_i^2(\beta - \beta_0)} H_i^A(\beta_0),
\]  

(B.21)

which resembles Eq. (B.12), and means that the variance at this stage decays exponentially according to \( \exp[-8\tilde{\alpha}_i^2(\beta - \beta_0)] \).

Define the slope of the linear segments of \( \ln V \) versus \( \beta \) as \( \alpha \), then we have the following relation between
the slope \( \alpha \) and the leading energy scale \( \tilde{\alpha} \),

\[
\alpha = 8\tilde{\alpha}^2. \tag{B.22}
\]

Qualitatively speaking, the off-diagonal part relevant at this regimes of the RG flow parameter (or energy scale) decreases exponentially with an exponent proportional to the square of the leading coefficient of the emerging l-bit. At the same time, new off-diagonal elements are generated at an higher order. The unitary distance accumulated through this stage can be estimated as

\[
\Delta D_U = \int_{\beta_0}^{\beta_0+\Delta \beta} \sqrt{\frac{\text{Tr}(\eta^1 \eta)}{\text{Dim}(H)L}} d\tau = \frac{\gamma}{2|\tilde{\alpha}|\sqrt{L}} (1 - e^{-4\tilde{\alpha}^2 \Delta \beta}),
\]  

(Eq. B.23)

where \( \gamma = \sqrt{\frac{\text{Tr}(H_A^2(\beta_0))}{\text{Dim}(H)}} \), and \( \gamma^2 \) is essentially the sum of square of all the coefficients of the Pauli strings in \( H_A \). Similarly, one can show that the change of average variance is

\[
\Delta V = -2 \int_{\beta_0}^{\beta_0+\Delta \beta} \frac{\text{Tr}(\eta^1 \eta)}{\text{Dim}(H)} d\tau = -\gamma^2 (1 - e^{-8\tilde{\alpha}^2 \Delta \beta}). \tag{B.24}
\]

The validity of these equations can be shown in Fig. B.5.

![Figure B.5: Comparison between actual change of \( D_U \) with the estimated change of \( D_U \) for \( L = 8 \) over the obtained linear segments, based on Eq. (B.23) and Eq. (B.24). Specifically, we used the linear segments’ change of average variance \( \Delta V \), slope \( \alpha \), RG time \( \Delta \beta \) to infer \( \gamma \), and used them to estimate \( \Delta D_U \) based on Eq. (B.23). The linear segments are obtained using our top-down linear segmentation method adapted from the Ramer-Douglas-Peucker (RDP) algorithm. For a given curve, the collection of all linear segments returned by this method do not cover the entire range, and is controlled by a tolerance parameter describing the maximum deviation from the linear segments of the points on the curve. The black straight line is \( y = x \).](image)

Further more, we performed Wegner flow at small system sizes at \( L = 4, 6, 8 \) with ED method, where we can afford to run the flow equations until all l-bits emerge from the systems and the Hamiltonians become
diagonalized. This can give us the complete log average variance $\ln V$ vs $\beta$ curve at any disorder strength $W$. Using these curves and the Ramer-Douglas-Peucker (RDP) algorithm, we can extract all the linear segments from a given $\ln V$ vs $\beta$ curve, where different linear segments represent regimes of different energy scales. After collecting all the slopes $\alpha$ from the linear segments, we found interesting behaviors of the largest slopes $\alpha_{\text{max}}$ (largest among all segments for a every curve) and the smallest slopes $\alpha_{\text{min}}$ (smallest among all segments for a every curve) as shown in Fig. B.6.

![Figure B.6: Left: Disorder averaged $\alpha_{\text{max}}$ vs $W$, on a log-log scale, for $L = 4, 6, 8$, using 200 disorder realizations. $\alpha_{\text{max}}$ is the largest slope (in magnitude) among the slopes of all the linear segments of a $\ln V$ vs $\beta$ curve. Usually $\alpha_{\text{max}}$ comes from the first segment which has the largest energy scale. As can be seen, we recover the $W^2$ behavior (because of $(E_i - E_j)^2$) in the MBL region. Left: Disorder averaged $\alpha_{\text{min}}$ vs $W$, on a log-log scale, for $L = 4, 6, 8$, using 200 disorder realizations. $\alpha_{\text{min}}$ is the smallest slope among the slopes of all the linear segments of a $\ln V$ vs $\beta$ curve. Usually $\alpha_{\text{min}}$ comes from the last segment which has the smallest energy scale. Interestingly, we find a system-size dependent power-law behavior in the MBL region, which is likely related to the renormalization of the energy scales during the Wegner flow. Notice that there seems to be a transitioning behavior at $W = 3$ (the black vertical line), which is close to the MBL transition point for the disordered Heisenberg chain.](image)