Quantum Many-Body Scars: Measures of Entanglement in the Spin $\frac{1}{2}$ Heisenberg XY model

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Abstract

Quantum-many-body scarring is a phenomena where there exists a small set of non-thermalizing eigenstates in an otherwise thermalizing system. These thermal eigenstates lead to interesting dynamics. In this report we explore the different phenomena that reveal the quantum scars in the spin $\frac{1}{2}$ XY model.

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Abbreviations

ETH	Eigenstate Thermalization Hypothesis	QMBS	Quantum Many-Body Scars
SSH	Su-Schrieffer-Heeger		

Chapter 1 : Introduction

With the recent experimental advancements allowing for the study of the quantum mechanics of individual atoms in isolated many-body systems there has been an increasing interest in describing the fundamental actions of these small systems. In particular we are interested in a phenomena called Quantum Many-Body Scarring, wherein certain non-equilibrium eigenstates show unexpected periodic revivals. These revivals provide an intriguing avenue of research with potential applications such as increasing the availability of long lasting quantum states in order to preserve quantum information within fields such as quantum algorithms or quantum metrology.

Chapter 2 : Background Physics

2.1 Classical Chaos

The concept of time evolution is one of the fundamental challenges in physics, how does a non-equilibrium state evolve over time? Even classically this problem can be challenging to approach. Chaos is typically defined such that a system is chaotic if its trajectory shows a significant dependence on its initial state. This causes its projection to be extremely weak to even small perturbations especially at longer times.
There exists however a set of systems which show non chaotic dynamics, these are known as integrable systems. [1]

2.2 The Ergodic Hypothesis

The first concept relevant to QMBS is the idea of ergodicity, the idea that underpins the idea of thermalization in microscopic systems. Ergodicity introduces the concept that a large enough sample of individual measurements can represent the bulk average of the entire system. The ergodic hypothesis, originally conjectured by Boltzmann as a method to link the microscopic dynamics with the ensemble average, implies that given long enough time, any non-equilibrium initial state will fully explore the entire phase space available from that initial state with the amount of time spent there being proportional to its volume.

2.3 Thermalization

Thermalization or Quantum Ergodicity is a quantum analogue to the classical ergodicity described above, wherein a many body system is separated into two subsystems one of which acts as a thermal sink which either disperses or absorbs energy to or from the other subsection such that it is possible to tend towards the thermal value as predicted by the statistical mechanics of the microcanonical ensemble. There are however examples of systems which are non ergodic, these systems have interesting non thermal dynamics even at long times. Understanding how these non-ergodic systems are produced and their dynamics is a growingly large field of research, there are a number of

methods known as ergodicity breaking which describe different potential causes for the lack of ergodicity in a given quantum system are described below. These systems are of particular interest as these systems which avoid thermalization allow for quantum information encoded into the initial parameters to exist at long times.

2.3.1 Eigenstate Thermalization Hypothesis

One of the key ideas within quantum many-body scaring is the idea that certain initial states can delay the process known as thermalization as is predicted by the Eigenstate Thermalization Hypothesis (ETH)[2]. This phenomena is what allows for the periodic revivals as have been both experimentally and theoretically. The eigenstate thermalization hypothesis states that individual eigenstates of quantum ergodic systems act as thermal ensembles, therefore the systems long term dynamics are not defined by the initial conditions of the system. if we take a generic state $|\Psi(0)\rangle = \Sigma_a A_a |a\rangle$ where $|a\rangle$ is a many-body eigenstate of the system the time evolution of the state is described purely by the initial probabilities of finding the system in a given eigenstate, $P_a = |A_a|^2$.

$$|\Psi(t)\rangle = e^{-i\hat{H}t} |\Psi(0)\rangle = \Sigma_a A_a e^{-iE_n t} |a\rangle \tag{2.1}$$

The expectation value of an operator for a specific time T is given by $\langle \hat{O} \rangle = \langle \Psi(T)|\hat{O}|\Psi(T)\rangle$ and we would expect the infinite time limit of this to approach the values predicted by the microcanonical ensemble

$$\langle \hat{O} \rangle_\infty = \lim_{T\to\infty} \frac{1}{T} \int_0^\infty \langle \Psi(T)|\hat{O}|\Psi(T)\rangle \, \mathrm{d}t = \Sigma_a |A_a|^2 \langle a|\hat{O}|a\rangle \tag{2.2}$$

Since the infinite time value should be independent of the initial conditions it is reasonable to enforce that $\langle a|\hat{O}|a\rangle$ agrees with the canonical average since $|A_a|^2$ is dependent on $|\Psi(0)\rangle$. [3]
The ETH also has significant implications on the entanglement of a many body system,

2.4 Ergodicity Breaking

2.4.1 Strong Ergodicity Breaking

There are two different forms of ergodicity breaking, these are split into strong and weak ergodicity breaking. We define strong ergodicity breaking with the requirements that all eigenstates are non-ergodic, that is that the system never thermalizes.

2.4.2 Weak Ergodicity Breaking

The weak ergodicity breaking on the other hand requires for the system to almost always thermalize, that is there exists a small subset of eigenstates which fail to thermalize.

2.5 Quantum Many Body Scars

2.5.1 PXP Model

The PXP model which is commonly used in QMBS experiments is based upon the idea of the Rydberg blockade and has experimentally shown non thermalizing dynamics [4]. The experiment consists of a system of two level atoms described by the states $|\circ\rangle$ and $|\bullet\rangle$ representing the ground and excited states. These states are allowed to flip freely when acted on by a microwave field via Rabi Oscillation. $|\circ\rangle \leftrightarrow |\bullet\rangle$. However when these Rydberg atoms are positioned close enough together the van der Walls forces repel. This distance can be tuned such that the interaction is strong enough to ensure that there are no two adjacent sites excited at the same time, $|...\bullet\bullet...\rangle$. This is known as a Rydberg Blockade, a kinetic constraint on the system.

This model is effectively represented by the Hamiltonian

$$\hat{H} = \sum_i P_{i-1} X_i P_{i+1} \tag{2.3}$$

Where X_i is the Pauli X gate $\sigma_i^x = |\circ\rangle_i \langle\bullet|_i + |\bullet\rangle_i \langle\circ|_i$, and P_i acts as a projector onto the groundstate $P_i = |\circ\rangle_i \langle\circ|_i$. Hence the name PXP. These projectors enforce the rydberg blockade constraint on the system.

This constrained model has an interesting Hilbert Space. if we consider the simplest case with only two sites only the following sites are allowed $|\circ\circ\rangle$, $|\circ\bullet\rangle$, $|\bullet\circ\rangle$ since the $|\bullet\bullet\rangle$ is in violation of the Rydberg Blockade. From this it is apparent that the Hilbert Space cannot be represented as a tensor product state of the two separate Hilbert Spaces. The majority of states in the PXP model thermalize rapidly, however there are a handful of states that fail to thermalize, one of such states is the Néel state or $\mathbb{Z}_2 = |1010101...\rangle$. [5, 6]

2.5.2 XY Heisenberg model

Recently QMBS were discovered experimentally in a 2D array of superconducting qubits [7], wherein an approximate Su-Schreiffver-Heeger (SSH) model [8] constructed by al-

ternating the coupling strengths between pairs of qubits. Experimentally a chain of pairs of qubits was produced within a 6x6 lattice of superconducting qubits. These pairs of qubits form 'dimers' where the intra-dimer coupling J_a is larger than the inter-dimer J_e coupling between them. If the system is constructed such that J_a is significantly larger than J_e and the system is half filled, that is when there are $L/2$ photons, where L is the length of the chain, then each dimer acts as an independent two level system with one photon per dimer. The control of the photons in this model shows similarities to how electrons transfer through the polyacetylene in the SSH model.

Experimentally this model also has to consider the cross couplings between the qubits, the chosen physical layout of the dimers introduces a cross coupling term J_x, this cross coupling breaks the inegrability of the system and should allow the system to thermalize.

This system uses an XY model where finely tuned microwave pulses force rotations in the X and Y directions. This system shows different scarred states to the PXP model, in this model the states $|\Pi\rangle = |D_+D_-D_+D_-...\rangle$, $|\Pi'\rangle = |D_-D_+D_-D_+...\rangle$, where $|D_-\rangle = |01\rangle$ and $|D_+\rangle = |10\rangle$ are found to have the non thermalizing dynamics expected of a QMBS.

This system is an effective spin 1/2 XY model with the following effective hamiltonian.

$$\mathcal{H}_{eff}/\hbar \approx \sum_{<i,j>} J_{ij}(S_i^+ S_j^- + S_i^- S_j^+) + \sum_i \Omega_i S_i^+ S_i^- \tag{2.4}$$

where J_{ij} is the effective coupling strength and Ω_i is the transition frequency which are both defined by the system design and coupling ratios.

SSH model

The Su-Schriefer-Heeger model is based on the electron transfer in a polyacetaylene molecule [8]. The SSH model is one of the simplest examples of non trivial 1D topological chains. The SSH model shown in figure 2.1 was the influence of the alternating couplings in an attempt to partially decouple the subspaces within the superconducting XY model [7], where they found QMBS phenomena within the subspace.

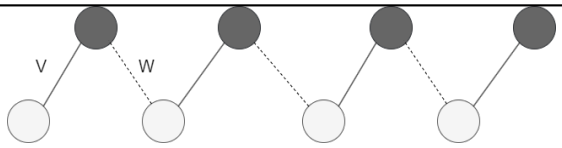

Figure 2.1: Simple graphical representation of the SSH model, with alternating bond strengths. This is a representation of the repeating chain of double and single carbon-carbon bonds found in a molecule of polyacetylene.

2.6 Entanglement

2.6.1 Quantum Fisher Information

Chapter 3 : Methodology

3.1 Simulating the Spin $\frac{1}{2}$ XY Model

Within this project the spin $\frac{1}{2}$ model is simulated using Python 2.7. This choice was made primarily due to personal familiarity with the language, as well as the large range of libraries suited to this kind of programming. When I initially started this project the first couple of iterations of code used only the standard Python libraries and Numpy. Due to the exponential scaling of the Hilbert space dimensions of the system and poorly constructed quantitative methods for calculating certain values this scaled extremely poorly with system size. This challenge had numerous solutions which I explored throughout the extent of this project.

3.1.1 Conserved Magnetization Subspace and Reducing Hilbert Space Dimension

The first problem I reached was the size of the Hamiltonian as a numpy array. originally attempting to store the full Hamiltonian in a numpy array reaches memory limits relatively quickly, with the Hilbert space scaling $Dim(\mathcal{H}) = 2^N$ where N is the chain length, the array will be of size $2^N, 2^N$, if we assume numpy stores a complex number as 2 floats which in python are each 8 bytes, the hamiltonian alone for a system of length $N = 16$ would require $\approx$ 67 GB of RAM to store. This is clearly a problem that requires solving such that the system is runnable. The first approach to this is to reduce the Hilbert space by creating a conserved magnetization basis, throughout this project we deal almost exclusively with the half filled basis of the Hamiltonian. This alone reduces the system size significantly as seen in figure 3.1. This alone allows for system sizes of upwards of 16 qubits to be simulated.

Another simple implementation that can significantly reduce the memory requirements for constructing a Hamiltonian is the concept of a sparse matrix, as opposed to initiating a matrix with empty values in all of the possible matrix elements, each matrix element is stored in 3 parts; the value in the element, and the corresponding position in the rows and columns. These sparse matrices require significantly less memory to store, however they require slightly special handling in terms of using them in calculations. Two of the main Python modules for scientific computing are Numpy[9], and SciPy[10]

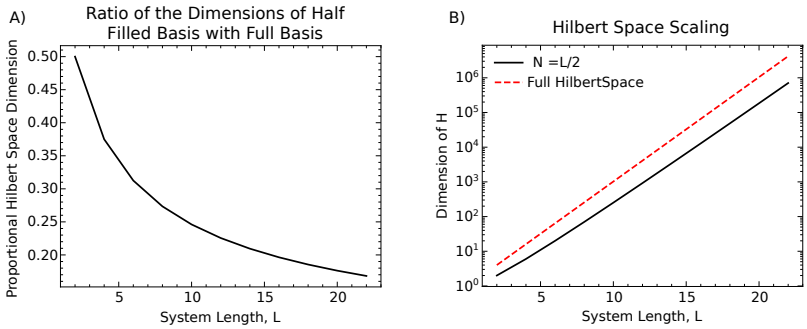

Figure 3.1: Scaling of Hilbert space dimensions. **A,** The ratio of Hilbert space dimension between the half filled basis and the full hilbert space of a qubit chain of length L. **B,** showing the exponential increase of the Hilbert space dimension with system size.

these both have sparse functionality, throughout my work scipy was mainly used for its wider range of functions. Although the memory saving is useful sparse matrices encounter problems with certain functions which require rebuilding the full matrix from the sparsely stored version before it can be calculated. Therefore you could store significantly larger matrices however calculating with them still proves challenging. For example the exponentiation of the Hamiltonian to produce the time evolution operator requires the full array, and the sparse variations in Numpy and Scipy simply produce the full array and then act with their exponentiation algorithm.

3.1.2 Quantum Python Libraries

Although this approach was possible and I produced functioning code it wasn't very efficient. This made producing and verifying results extremely time expensive, having spent a large amount of time attempting to improve this myself I turned my attention to pre-existing python libraries which should simplify some portions of the programming. In the end I used a mixture of two different libraries: Qutip - Quantum Toolkit for python[11], and Quspin a library designed for the simulation of quantum many body systems and their exact diagonalization[12]. Both of these libraries include significant speed ups over the code that I produced. Part of this is through the implementation of Cython to run certain common equations using C, as well as multi threading where possible. Each of these programs have their advantages, Qutip is a more commonly used library however the wide range of potential applications makes certain implementations

that were required for this project slightly more intricate to implement. Therefore after a while I explored the QuSpin library which was more explicitly created with the idea of quantum many body dynamics, allowing for easier implementation of many body problems.

3.1.3 Constructing the Hamiltonian

In order to construct the Hamiltonian we first need to consider the half filled basis. We consider each basis state as a string of zeroes and ones representing the spin up and spin down states, therefore the full basis is trivial to construct. The half filled basis however requires slightly more care. There is no trivial method to calculating the integer values of the binary numbers that have exactly L/2 zeroes within the string, Therefore we simply iterate through the full basis and check each individual string counting the occurrence of zero matches L/2. Using this it is possible to construct a mapping operator that moves between the half filled and full basis. This process is simplified within Quspin, which has its own basis generating functions which allow for simply defining the magnetization subspace symmetry that you want to generate.

To construct the matrix representation for the Hamiltonian for the XY model 2.4 we simply act the Hamiltonian on each of the basis states and find the respective output. That is the matrix element $\hat{\mathcal{H}}_{ij} = \langle i|\hat{\mathcal{H}}|j\rangle$ allows us to find the matrix elements for the Hamiltonian.

Using Quspin to construct Hamiltonian

The effective Hamiltonian of the spin $\frac{1}{2}$ XY model 2.4 is in that form an integrable model. Therefore in order to observe quantum many body scar effects we must break that integrability. In the paper by Zhang et al.[7] the integrability is broken by the cross coupling terms which come from the physical layout of the device. Therefore it is critical that we add a perturbation to the Hamiltonian such that the integrability is broken. Zhang et al[7] use a next-next-nearest neighbour coupling in order to break the integrability of the system for their numerics, we will later explore the impact of changing this, as well as a stepping function in order to speed up thermalization from random states whilst maintaining the dynamics of the pure dimerized states.
Using Quspin we initialize a 1D spin $\frac{1}{2}$ basis, with the $\sum_i^l \hat{S}_i^z = 0$ where $\hat{S}i^z$ is the Pauli Z spin operator acting on site i.

we then construct a Hamiltonian of the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 + \hat{\mathcal{H}}_3 \tag{3.1}$$

where $\hat{\mathcal{H}}_1$ is the nearest neighbour interaction 3.2, $\hat{\mathcal{H}}_2$ is the next-next nearest interaction 3.3, and $\hat{\mathcal{H}}_2$ is the step function described above 3.4.

$$\hat{\mathcal{H}}_1 = J_a \sum_{i \in Even}^{L-1} (\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+) + J_e \sum_{i \in Odd}^{L-1} (\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+) \tag{3.2}$$

where J_a, J_e refer to the intra-dimer and inter-dimer couplings respectively, this alternating coupling strengths are what cause this model to be a representation of the SSH model describe in section 2.5.2.

$$\hat{\mathcal{H}}_2 = J_{nnn} \sum_{i}^{L-3} (\hat{S}_i^+ \hat{S}_{i+3}^- + \hat{S}_i^- \hat{S}_{i+3}^+) \tag{3.3}$$

J_{nnn} is a constant that describes the next-next-nearest neighbour coupling. This is required to break the integrability of the XY model.

$$\hat{\mathcal{H}}_3 = \sum_{i}^{L} \Omega \hat{S}^+ \hat{S}^- \tag{3.4}$$

The $\hat{\mathcal{H}}_3$ term relates to a transition frequency acting on all sites. As previously described this matrix is stored as a sparse matrix in order to save on memory. This is the default for Hamiltonians in Quspin so requires no additional programming.

3.1.4 Time Evolution

In order to analyse the dynamics of the system we must calculate the time evolution of this Hamiltonian from varying initial states. One of the states that we will use is the $|\Pi\rangle = |10011001...\rangle$ state. This state is chosen due to it being an experimentally preparable state showing scarred dynamics.

We will use the Schrodinger equation in order to probe the time evolution of the Hamiltonian.

$$|\psi(t)\rangle = e^{\frac{-i}{\hbar}\hat{H}t} |\psi(0)\rangle \tag{3.5}$$

3.2 Quantum Scarring Phenomena

After constructing the dynamics of the system we will start by looking at some of the common metrics of QMBS, the first of which is the fidelity or overlap. This is measured between $|\psi(0)\rangle$ and $|\psi(t)\rangle$. This is the one of the observables that shows the periodic revival for the QMBS states. The fidelity is calculated as

$$\mathcal{F} = |\langle\psi(0)|\psi(t)\rangle|^2 \tag{3.6}$$

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