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IIT (BHU) Varanasi

On

Entanglement and Mutual Information in Many-Body Localized Quantum Systems.

Presented by

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1st Year, 16MS156

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Certificate

This is to certify that ***Mr. Amlan Datta (1st year, 16 MS Batch, Indian Institute of Science Education & Research, Kolkata)*** has done his Summer Research Project titled ***"Entanglement and Mutual Information in Many-Body Localized Quantum Systems"*** at **Department of Physics, IIT (BHU), Varanasi** during the period from **22nd May 2017 to 14th July 2017**. He has completed his project within the stipulated time. Moreover, his conduct and behavior was quite satisfactory throughout the project.

[Dr. Debaprasad Giri]	**[Dr. Rajeev Singh]**
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1st Year, 16MS156

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Date: 14th July 2017

Abstract

In this project we have two models for both interacting and non interacting particles (Many-body localization and Anderson localization respectively). We study entanglement entropies and mutual information for the two models and understand the structure of the many-body localization by analyzing structures of single site entanglement entropy, two site entanglement entropy, mutual information and half chain entanglement entropy for both time independent and time dependent Schrodinger equation. We find that the entanglement entropies decrease almost monotonically with increase in disorder strength, whereas mutual information is not monotonic. We also see some interesting properties which depend on the periodic boundary condition.

Contents:

- ***Introduction:***

In this project work, single site entanglement entropy, two site entanglement entropy and mutual information are calculated for disordered quantum systems. All these quantities are reproduced from the research paper "Multipoint entanglement in disordered system" by Javier M. Magan, Simone Paganelli and Vadim Oganesyan [Ref. 1]. Also some other quantities like half chain entanglement entropy, single site and two site entanglement entropies for time evolved states, mutual information between two subsystems different from the given one and some other quantities discussed later are calculated and analyzed to properly understand the many-body localization.

- ***Models***:

For this project we have two models with spin chains for our discussions. These models represent quantum magnetism spin chains with spin half particles. Disorder is applied to the spin chain system in the external field.

✓ Model 1 (XX model):

The Hamiltonian we have for the discussion of some quantities like single site, two site entanglement entropies etc. is:

$$H = \sum_{j=1}^{L-1} \sigma_j^{\pm}\sigma_{j+1}^{\mp} + h_j \cdot \sigma_j^z$$

where $\sigma_j's$ are Pauli matrices and h_j only has x and z components and L is the system size.

$$\sigma^+ = \frac{\sigma_x + i\sigma_y}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad , \quad \sigma^- = \frac{\sigma_x - i\sigma_y}{2} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Pauli Matrices: $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

The above Hamiltonian can be explicitly rewritten as:

$$H = \sum_{j=1}^{L-1} (\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+) + \sum_{j=1}^{L} (h_j \sigma_j^x + h_j \sigma_j^z)$$

In addition to the first part of the Hamiltonian, periodic boundary condition is also applied. So we have the Hamiltonian as:

$$H = \sum_{j=1}^{L-1} (\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+) + (\sigma_1^+ \sigma_L^- + \sigma_1^- \sigma_L^+) + \sum_{j=1}^{L} (h_j \sigma_j^x + h_j \sigma_j^z)$$

- ✓ Model 2 (XXZ model):
  We again have another Hamiltonian which is defined as:

$$H = \sum_{i=1}^{n-1} J_{\perp}(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + J_z(\sigma_i^z \sigma_{i+1}^z) + \sum_{i=1}^{n} h_i \sigma_i^z$$

This Hamiltonian is different from the previous one as there is one extra term J_z which is for interaction. Model 1 is for non-interacting particles and the phenomenon is known as "Anderson Localization". And the second one is for interacting particles and the phenomenon is called "Many-Body Localization". [Ref. 2, 3]

If the $J_{\perp}$ and J_z are same then it is known as the Heisenberg model. For our discussion it is XXZ model as here $J_z/J_{\perp} = 0.2$.

• *Entanglement:*

In quantum mechanics when a state of composite system cannot be written as a product of its component systems, then it is an entangled state.

Example: Let us consider a two qubit state $|\Psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. Let us assume that this state is a product of $|a\rangle$ and $|b\rangle$.

Let $|a\rangle = c|0\rangle + d|1\rangle$ and $|b\rangle = e|0\rangle + f|1\rangle$. So, $|a\rangle|b\rangle = ce|00\rangle + cf|01\rangle + de|10\rangle + df|11\rangle$

And we already have, $|\Psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, comparing the equations we get $cf = 0\ i.e.$ either $c = 0$ or $f = 0$, but if $c = 0$ then $ce = 0$

In that case $ce \neq 1/\sqrt{2}$ so we cannot get the first part of $|\Psi\rangle$ and if we also do same calculation for d and f we get $df = 0$ and we cannot get the second part of $|\Psi\rangle$.

Hence it follows that the composite quantum state $|\Psi\rangle$ cannot be written as a product of its component systems $|a\rangle$ and $|b\rangle$. So $|\Psi\rangle$ is said to be entangled.

But from this we can only come about whether it is entangled or not. To know how much entanglement is there, we need to calculate entanglement entropy which is discussed in the next section.

• *Entanglement Entropy:*

Entanglement entropy is an entanglement measure for a quantum system. For classical information theory we work with Shannon entropy and for quantum information theory we have von Neumann entropy.

- ✓ Shannon Entropy: As mentioned above the key concept of classical

information theory is the Shannon entropy. Suppose we have a random variable X and the Shannon entropy of X quantifies the amount of information we gain when we study X. In other way the entropy of X tells us the amount of uncertainty about X before we learn its value. We often write the entropy as a function of a probability distribution $p_1, \ldots, p_n$. The Shannon entropy associated with this probability distribution is defined by

$$H(X) = H(p_1, \ldots, p_n) = -\sum_x p_x \log_2 p_x$$

- ✓ *von Neumann Entropy* : In contradiction to classical states, quantum states

are described in density operators replacing probability distributions. von Neumann entropy of a quantum state ρ is defined by the formula, $\boldsymbol{S(\rho) = -tr(\rho \log_2 \rho)}$

This formula can be re-expressed with the eigenvalues of ρ i.e.

$$S(\rho) = -\sum_x \lambda_x log \lambda_x$$

where λ_x are the eigenvalues of ρ.

And the latter formula is used for calculating single site entanglement entropy, two site entanglement entropy, mutual information and half chain entanglement entropy discussed later.

- ***Entanglement entropy and disorder strength:***

For higher disorder strength the state corresponds to many-body localized (MBL) phase. For lower disorder strength we have thermal/random state or ergodic phase.

With the increase in disorder strength (η), the ergodicity decreases and also the entanglement entropy decreases. This is the signature of localization in spin chain system.

- ***Single site and two site entanglement entropy:***

A quantum state Ψ is chosen and the density matrix (ρ) is obtained to calculate the single site and two site entanglement entropy. We are dealing with eigenstates of Hamiltonian with intermediate energy. The plots (Fig 1) obtained show different maximum values for single site and two site entanglement entropy for different system sizes (n).

Higher the system size (n) higher is the maximum value for both single site and two site entanglement entropy.

For $n = 10$ the single site entanglement entropy value approaches 1.0 and two site entanglement entropy value approaches 2.0.

In the plots the W is the disordered strength i.e η. So $\eta = W = 2^x$, where x is the value in the X-axis.

The $S1$ and $S2$ is the (normalized by log2) average value of single site and two site entanglement entropy respectively averaged over 1000 realizations for $n = 6$ and 8 and over 100 realizations for $n = 10$.

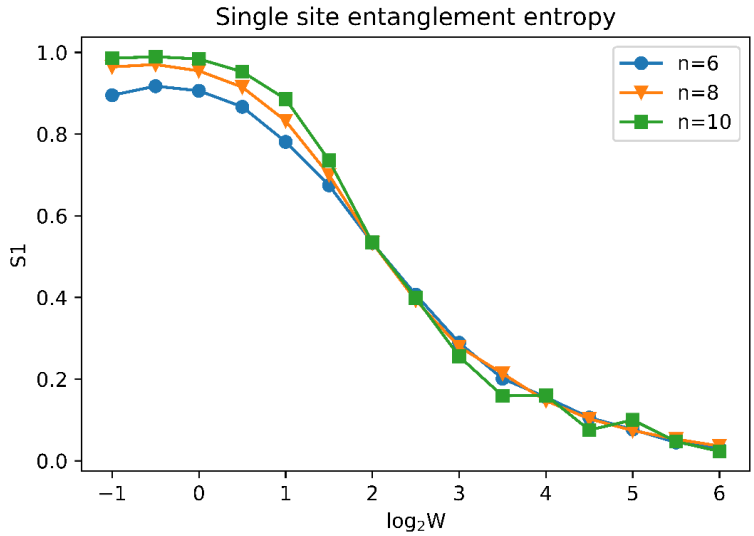

Fig 1(a): Single site entanglement entropy (normalized by log2)

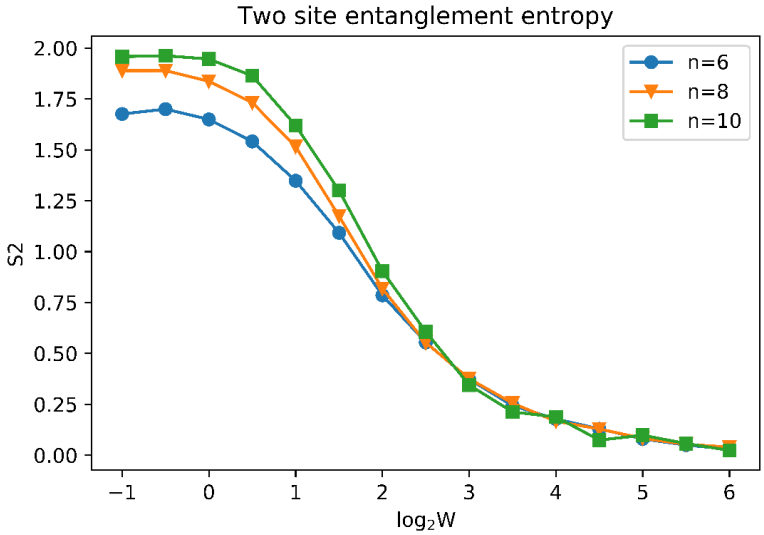

Fig 1(b): Two site Entanglement entropy (normalized by log2)

As we can see for higher disorder strength both the single site and two entanglement entropy for any system sizes approach zero value. So the state then is in localized phase. In case of ergodic phase the quantum information is very much delocalized over the system.

This $(-logS1\ vs.\log_2 W)$ illustrates the simple scaling of entanglement in localized phase.

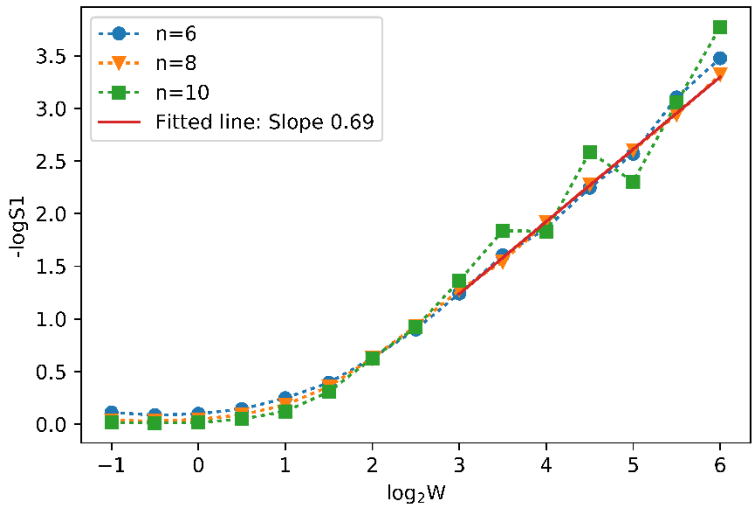

Fig 2: $-logS1\ vs\log_2 W$; The slope of the fitted line is 0.69

- ***Classical Mutual Information:***

In probability theory and information theory, the **mutual information** (**MI**) of two random variables is a measure of the mutual dependence between the two random variables. More specifically, it quantifies the amount of information obtained about one random variable, through the other random variable.

Mutual information measures how much information two states have in common. Suppose we have two random variables A and B. Now mutual information tells us about the correlations between the information of those two variables A and B. The conditional entropy is defined as,

$$\boldsymbol{H(A|B) = H(A,B) - H(B)}$$

And the classical mutual information of A and B is given by:

$$\boldsymbol{H(A:B) = H(A) - H(A|B)}$$

$$\boldsymbol{= H(A) + H(B) - H(A,B)}$$

This is also known as Shannon mutual information.

- ***Quantum Mutual Information:***

In quantum information theory, **quantum mutual information**, or **von Neumann mutual information** is a measure of correlation between subsystems of quantum state. It is the quantum mechanical analog of Shannon mutual information.

As mentioned above, by analogy with Shannon entropy it is possible to express quantum mutual information, for composite quantum systems using density operators or density matrices.

The joint entropy $S(A,B)$ for a composite system with two components A and B is defined as, $S(A,B) \equiv -tr(\rho^{AB} \log(\rho^{AB}))$, where ρ^{AB} is the density matrix of the system AB.

We define the conditional entropy and mutual information by:

$$S(A|B) = S(A,B) - S(B)$$

$$S(A:B) = S(A) + S(B) - S(A,B)$$

$$= S(A) - S(A|B) = S(B) - S(B|A)$$

Now we have the plot of mutual information calculated using the Model 1 mentioned earlier in Fig 3. The mutual information is calculated between a point at the end of the chain and adjacent site (neighbor site).

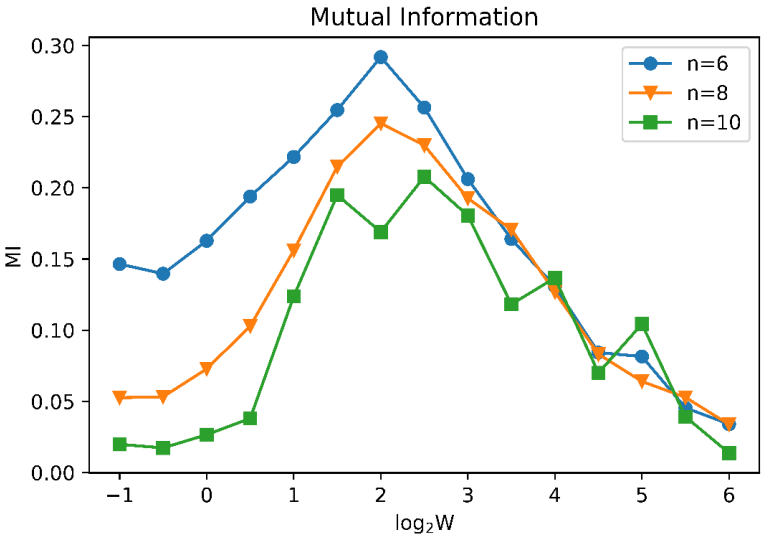

Fig 3: Mutual information (normalized by log2)

Here also MI is averaged over 1000 realizations for $n = 6, 8$ and over 100 realizations for $n = 10$.

We can see a different behavior in the plot of mutual information. In both the cases for low disorder strength and high disorder strength mutual information is low, but for intermediate disorder strength mutual information attains its maximum value. But if we look at the single site entanglement entropy and two site entanglement entropy plots, both quantities are almost monotonic whereas the mutual information is not monotonic in nature. It first increase and then decreases.

- *Peak to Volume Mutual Information:*

Now we are interested to calculate the mutual information between a point at the end of the chain and the adjacent group of sites B. This is known as "peak-to-volume" mutual information

(PVMI) which is denoted by $I(1, B)$. The value of B need not be the same as the size of the chain, it can be smaller than the size of the spin chain. We have considered two disordered strength $\eta = 2$ and $\eta = 12$ and in the discussion the system size is 8. Also for comparison PVMI up to tail of the chain of a random state in the Hilbert space is also calculated. For this calculation we have the random field XXZ chain (Model 2). In the Model 2 the h_i which has only the z component is the random variable with uniform probability distribution in the range $[-\eta, \eta]$ where η is the disorder strength.

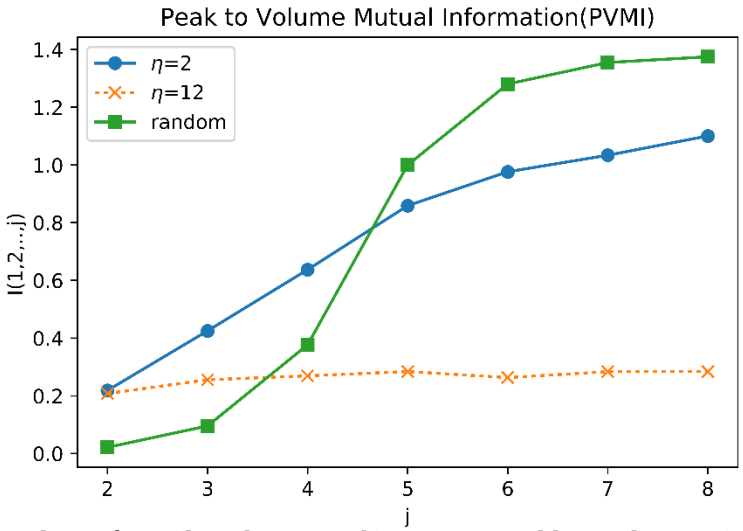

Fig 4:(a) For two values of eta (disorder strength) two curves (blue and orange); (b) A random state in Hilbert space (or, ergodic phase) (green) .

We observe that for $\eta = 12$ the PVMI line increases slightly with increase in size of B and then it is more or less constant throughout. This phenomenon is deep inside many-body localization (MBL). This shows that adding more spins does not increase the mutual information significantly. The PVMI for low disorder strength ($\eta = 2$) behaves like ergodic phase.

From the plot we can see that the average structure of **many-body localized** phase significantly differs from that of the structure of random state. But when the disordered strength is very high, just like the case of $\eta = 12$, none of the curve (the random state and the low disorder one) has any similarity with this high disorder one.

- *Time evolution:*

All the quantities we have calculated so far are all for non-equilibrium unitary processes i.e. we can say for time independent Schrodinger equation. But we are now interested in the time dependent Schrodinger equation and will calculate all those above values at stationarity. We now need to consider the product states selected from the group of initial conditions.

For $|\psi\rangle_\theta = cos\left(\frac{\theta}{2}\right)|\downarrow\rangle + isin\left(\frac{\theta}{2}\right)|\uparrow\rangle$, we have the family of initial states parameterized by θ as,

$$|\Psi\rangle_\theta = |\psi\rangle_\theta \otimes |\psi\rangle_{\pi-\theta} \otimes |\psi\rangle_\theta| \otimes \psi\rangle_{\pi-\theta} \otimes |\psi\rangle_\theta \otimes |\psi\rangle_{\pi-\theta} \otimes |\psi\rangle_\theta \otimes |\psi\rangle_{\pi-\theta}$$

with $0 \leq \theta \leq \pi/2$.

This is for system size of 8 spins and it will change for corresponding system sizes $i.e.$ for 6 spins system there will be 3 pairs and for 10 spins system there will be 5 pairs and this will increase with further increase in system size.

As we are now concerned about time evolution, let us first consider the Model 1 and again single site and two site entanglement entropy and mutual information of first two sites are calculated . But this time we have fixed disorder strength ($\eta = 1$) and everything is calculated as function of time so that we can see clearly how those quantities vary within a short range of time.

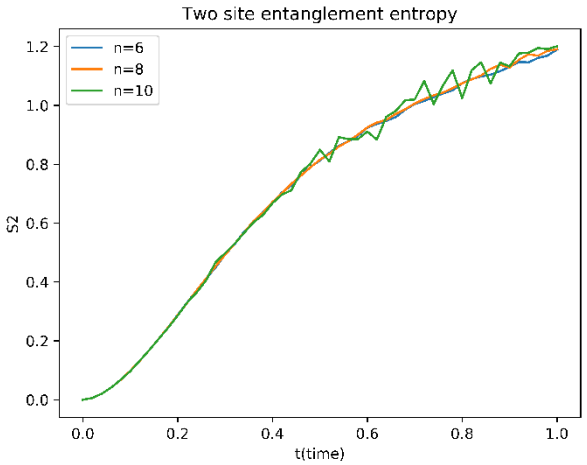

Fig 5(a):

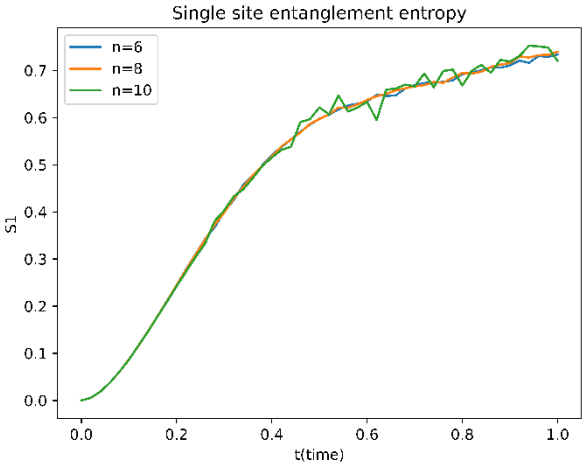

Fig 5(b):

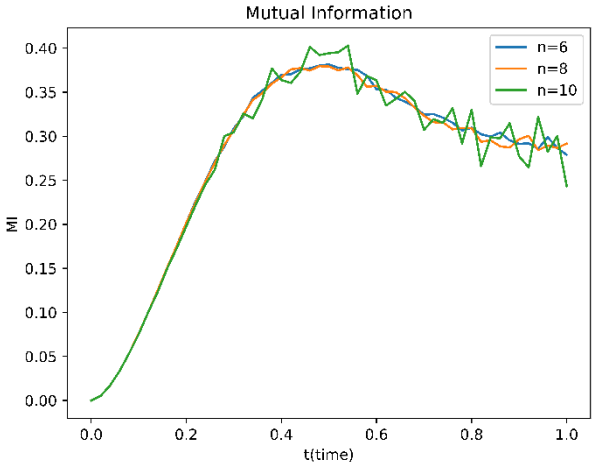

Fig 5(c):

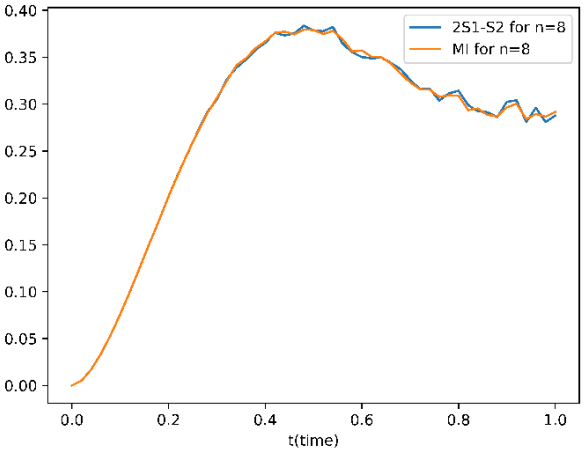

Fig 5(d):

Roughly for mutual information we can say that it is the value we get by subtracting two site entanglement entropy value from two times the single site entanglement entropy $i.e.$ $(2 * S1 - S2)$. For comparison $(2 * S1 - S2)$ is also plotted with MI against time in Fig 5(d). And it almost same as that of the mutual information we have plotted. We can see that both the single site and two site entanglement entropy are monotonic but as per calculation mutual information is not monotonic. It first increases then decreases and abnormally has a peak in it which is quite strange.

Now if we calculate "peak-to-volume" mutual information $I(1, B)$ between a point at the end of the chain and the adjacent group of sites B with Model 2 for time evolved state we get the plot shown in Fig 6 for disorder strength $\eta = 6$.

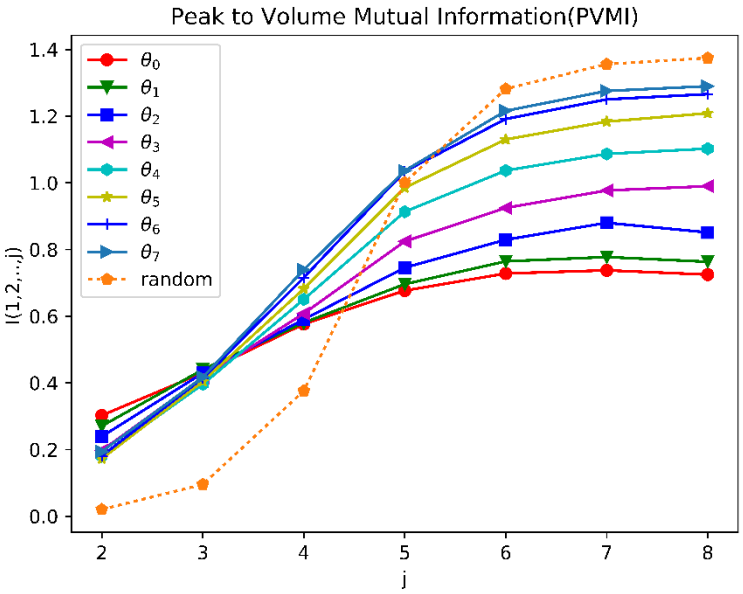

Fig 6: Peak-to-volume mutual information at stationarity.

Each curve corresponds to one of the initial states parameterized with $\theta_k = \frac{k\pi}{14}$, $k = 0,1,\ldots,7$. A random state (low disorder strength) is also plotted for comparison. We see that even for high disorder the long term mutual information at $\theta = \pi/2$ behaves like ergodic phase. For $\theta = \pi/2$ the PVMI approaches the random state.

- *Magnetization Imbalance:* Now we have the quantity called magnetization imbalance for odd and even sites, defined as $\Delta m = \sum_j \langle \sigma_{2j}^z - \sigma_{2j+1}^z \rangle$, for our spin chain system.

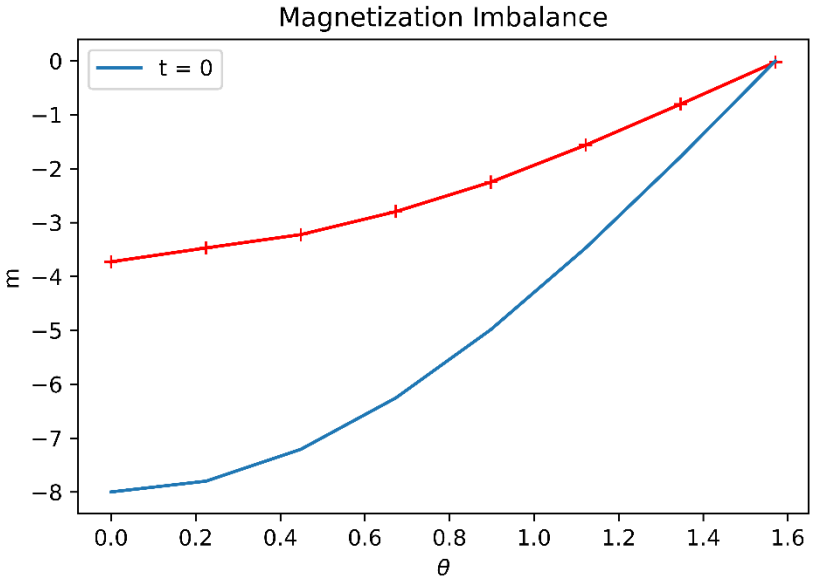

Fig 7: Magnetization imbalance as a function of θ at stationarity.

From Fig 7 it is clear that as the initial state approaches $\theta = \pi/2$, the magnetization imbalance value approaches to zero. The blue curve corresponds to magnetization imbalance of initial state.

- *Half Chain Entanglement Entropy:* Now we are interested to calculate the **half chain entanglement entropy** for Model 2 with time evolved states.

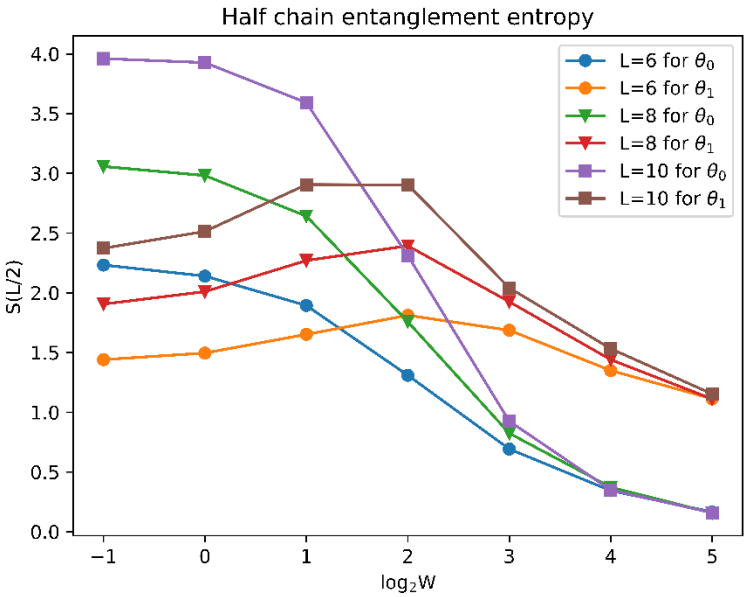

Fig 8: Half chain entanglement entropy (normalized by log2)

For different system sizes (L=6, 8 & 10) the half chain entanglement entropy is plotted for different initial states. In the plot above L is the system size and $\theta_0 = 0$ and $\theta_1 = \pi/2$.

Now instead of taking the initial state as discussed earlier for $\theta = \pi/2$ if we take the initial state as $|\Psi\rangle = |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle \otimes |\psi\rangle$ for $|\psi\rangle = (|\downarrow\rangle + |\uparrow\rangle)/\sqrt{2}$ and we get same result as we have for $\theta = \pi/2$.

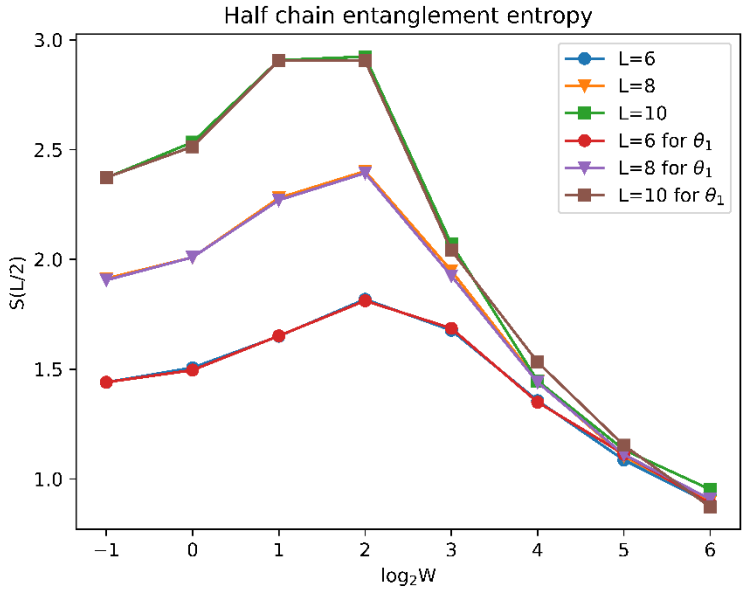

Fig 9: Comparison of half chain entanglement entropy for two initial conditions.

If we look at the Hamiltonian of Model 2 we see that there is no difference for x and y. Even if we interchange x and y the Hamiltonian remains same. As $\theta = \pi/2$ is eigenstate for σ^y and we can choose the ψ which is eigenstate for σ^x and both are interchangeable. And we get the same values of half chain entanglement entropies and almost same as plotted on Fig 9.

Now as we have the Hamiltonian (Model 2) and we also know how the mutual information is to be calculated, so we now calculate a new type of mutual information. Previously we calculated mutual information between first site and subsystem composed of several sites up to tail of the chain. But this time we are taking first two sites of the chain instead of only one site and calculating mutual information with other sites $i.e. I(2,\ldots,j)$ where j is the maximum numbers of sites. So Fig 10 is the plot of that newly calculated mutual information.

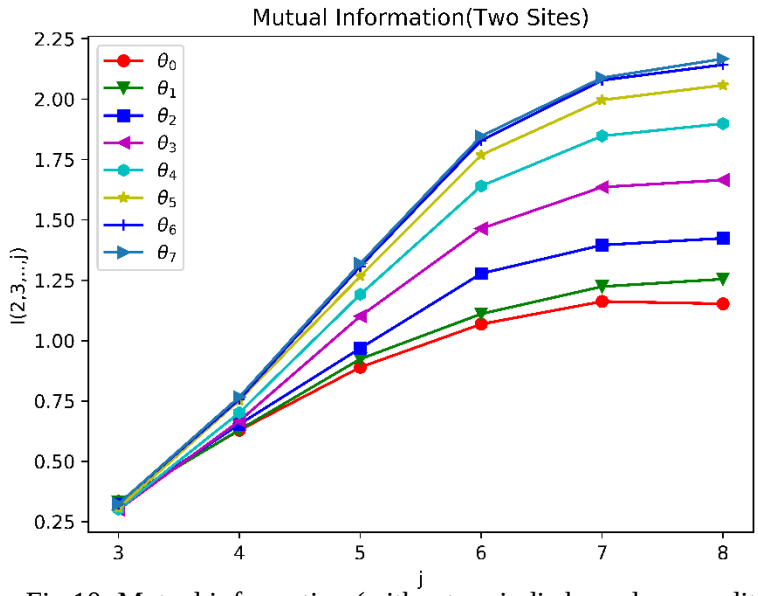

Fig 10: Mutual information (without periodic boundary condition)

This is calculated for Model 2 Hamiltonian without periodic boundary condition. Now if we apply periodic boundary condition to both $I(1,\ldots,j)$ and $I(2,\ldots,j)$ we can see that for $j = 3$ both the plots have same value.

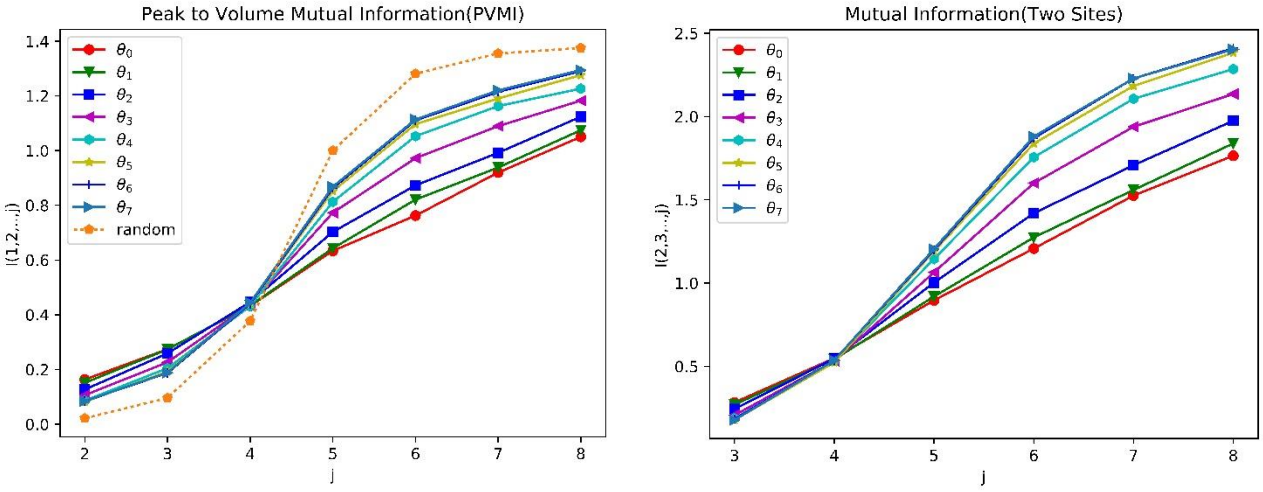

Fig 11: Comparison of different MI plots (with periodic boundary condition).

We get close values for $I(1,3)$ and $I(2,3)$ $i.e.$ for $j = 3$, only if the periodic boundary condition is applied.

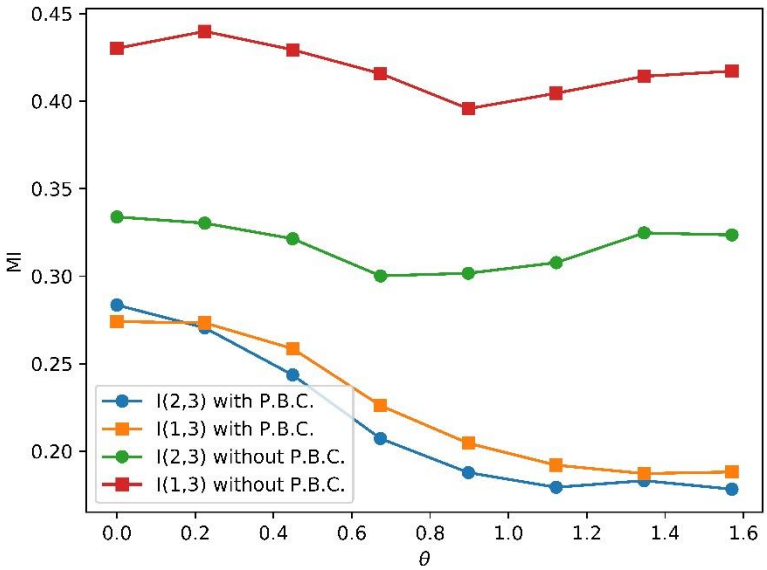

Fig 12: Similarity between $I(1,3)$ & $I(2,3)$

(P.B.C = Periodic boundary condition)

In case of periodic boundary when we are calculating mutual information between two subsystem e.g. 1 site vs. 2 sites ($I(1,3)$) and 2 sites vs. 1 site ($I(2,3)$) become same thing as both are actually mirror image of each other because the tail of the spin chain is connected to the beginning of the spin chain i.e. the chain has no open end due to periodic boundary condition. But when the periodic boundary condition is not there then there are open ends in the spin chain. So 1 site vs. 2 sites ($I(1,3)$) and 2 sites vs. 1 site ($I(2,3)$) will not be same as before and it will have significant difference in the value of mutual information shown in the Fig 12.

Now there is a very interesting behavior in the calculation of entanglement entropy of the density matrices which form the composite quantum system. As we have the composite quantum system as ρ^{AB} in pure state i.e. $\rho^{AB} = |\psi\rangle\langle\psi|$ and the reduced density matrices ρ^{A} and ρ^{B}, if we calculate the entanglement entropy for ρ^{B} we get very interesting information which is shown in the Fig 13. The values of entanglement entropies are in pairs and they are almost similar for different subsystem size. If we a have a big quantum system in pure state and we break it into two subsystem A and B, the von Neumann entropy for both the subsystem will be same irrespective of the size of the subsystem. So here for $j = 2$ and $j = 8$ we are having the same von Neumann entropy value. For $j = 2$, B has 1spin and for $j = 8$, B has 7 spins. But as mentioned earlier that the entropy will be same for both subsystems irrespective of the size of the subsystem and here for the case of 1 spin and 7 spins, they have same value of von Neumann entropy value as shown in Fig 13. It is also followed by other $j's$.

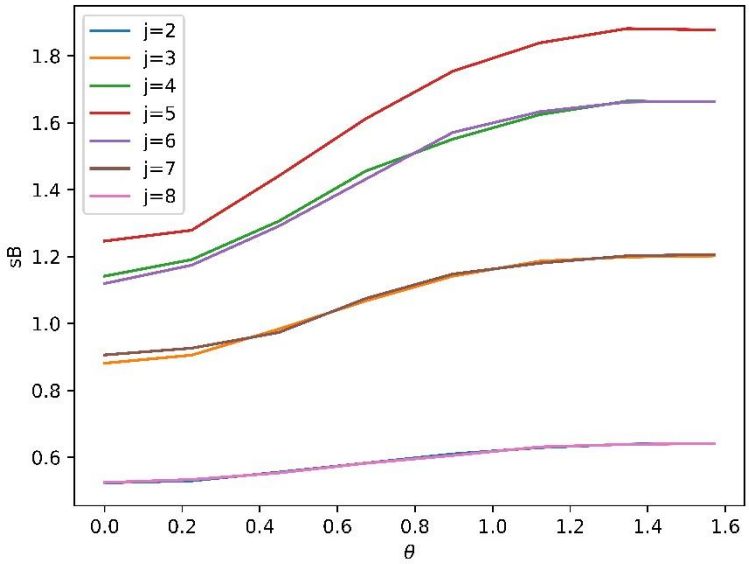

Fig 13: von Neumann entanglement entropy for ρ^B

Now if we look at the plot of half chain entanglement entropy (Fig 8), for system size 8 we have the value of entanglement entropy for θ_0 around 2 (without normalization). And in the Fig 13 the value of sB for $j = 5$ at $\theta = \pi/2$ is also around 2 which is actually the half chain entanglement entropy.

- ***Summary:***

We have studied the two models with non-interacting and interacting particles i.e. Anderson localization (Model 1,XX) and many-body localization (Model 2,XXZ) respectively. Single site entanglement entropy, two site entanglement entropy, mutual information and half chain entanglement entropy have been calculated for both eigenstates of the Hamiltonian with intermediate energy and time evolved product states. We have seen that we can get an initial state in many-body localization which thermalizes. We have also analyzed how peak-to-volume mutual information depends on the size of subsystems in a spin chain for both with and without periodic boundary condition.

- ***References:***

1. Multipoint entanglement in disordered systems; Javier M. Magan, Simone Paganelli and Vadim Oganesyan, Phys. Lett. A **381**, 535 (2017)
2. Signature of the many-body localization transition in the dynamic of entanglement and bipartite fluctuations; Rajeev Singh, Jens H Bardarson and Frank Pollmann, New J. Phys. **18**, 023046 (2016).
3. Many-body localization phase transition; Arijeet Pal and David A. Huse, Phys. Rev. B **82**, 174411 (2010).