Single-particle Entanglement of the Entanglement Hamiltonian Eigen-modes

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Single-particle entanglement entropy (SPEE) is calculated for entanglement Hamiltonian eigen-mode in a one-dimensional free fermion model that undergoes a delocalized-localized phase transition. In this numerical study, we show that SPEE of entanglement Hamiltonian eigen-mode has the same behavior as EPEE of Hamiltonian eigen-mode at the Fermi level: as we go from delocalized phase toward localized phase, SPEE of both modes decreases in the same manner. Furthermore, fluctuations of SPEE of entanglement Hamiltonian eigen-mode – which can be obtained through the calculation of moments of SPEE – signature very sharply the phase transition point. These two modes are also compared by calculation of single particle Réyni entropy (SPRE). We show that SPEE and SPRE of entanglement Hamiltonian eigen-mode can be used as a phase detection parameter.

I. INTRODUCTION

Entanglement as a pure quantum concept with no classical counterpart, has been used as a phase detection parameter. It is borrowed from quantum information science, and people in condensed matter physics found it useful to distinguish different phases. I.e. its behavior depends on the phase of the system. Specially, for a delocalized-localized phase transition, the concept of entanglement entropy (EE) is useful. In the delocalized phase, where the system is extended over many sites, we expect large correlation in the system, and thus EE – which indirectly measures the correlation among the system – is larger than when the system is localized. Réyni entropy (RE) is another measure of entanglement in a system, by which people distinguish localized from delocalized phases. However, beside the entanglement, there are other source of information contained in the reduced density matrix. Eigen-values of the entanglement Hamiltonian are also another way to distinguish different phase. In addition, eigen-modes of the entanglement Hamiltonian also carry physical information.

Let’s review the concept of entanglement. For a free fermion Hamiltonian, we obtain single-particle eigen-modes of the Hamiltonian, and the ground state of the system $|\psi\rangle$ will be the Slater determinant of filled single-particle eigen-mode up to Fermi level. We know that all physical information contained in the state can also be understood using the density matrix which is defined as $\rho = |\psi\rangle\langle\psi|$. Now, we consider a system divided into two subsystems. For each subsystem, we can obtain a reduced density matrix, which is obtained by tracing over the other subsystem. In this paper we consider a lattice system with $N$ sites and divide the system into two equal parts: subsystem $A$ is from site number 1 to site number $N_A$ and the rest is subsystem $B$. Thus, the reduced density matrix of subsystem $A$ for example, is obtained by tracing over sites of subsystem $B$: $\rho_A = \text{tr}_B \rho$. Then, entanglement entropy is $EE = -\text{tr}[\rho_A \log \rho_A]$. Note that entanglement entropy is defined for a many-body state of the system. In a free fermion lattice system, which we focus on in this study, we can write the reduced density matrix as $e^{-H_{ent}}$ in which the $H_{ent}$ is a free fermion Hamiltonian and called entanglement Hamiltonian. This procedure can be done to calculate the reduced density matrix for subsystem $B$ as well.

In this paper, the single-particle eigen-modes of the entanglement Hamiltonian are considered. Note that for each entanglement Hamiltonian eigen-mode of subsystem $A$, there is a counterpart eigen-mode in subsystem $B$. To obtain a mode that characterizes the entire system, we attach these two eigen-modes. Ref. introduces a method for attaching these two modes together. For a system with size $N$ that is divided into two equal subsystems, we have $N/2$ of such single particle eigen-modes for each subsystem. But, one of them is particularly very important. Note that each eigen-mode of the entanglement Hamiltonian, correspond to an eigen-value, that is the corresponding entanglement energy. One of these eigen-values that is closest to zero has the largest contribution to the EE. The corresponding eigen-modes in two subsystems are attached together to make a mode that is called maximally entangled mode (MEM) for the whole system.

In recent studies, we showed that MEM has physical information very similar to those information we can obtain from eigen-mode of the Hamiltonian at the Fermi level, $|E_F\rangle$. It is shown that both MEM and $|E_F\rangle$ are extended in the delocalized phase and both are localized in localized phase and thus, by studying the MEM behavior we can distinguish different phases: MEM introduces another way of studying the behavior of the system.

For a single-particle eigen-mode, it is possible to define single-particle entanglement entropy (SPEE)(see below for definition). And since the MEM is a single-particle eigen-mode, we can obtain its SPEE, as we do for the single-particle eigen-mode of the Hamiltonian at the Fermi level. On the other hand, we have seen that the behavior of the MEM is similar to the behavior of Hamiltonian eigen-mode at the Fermi level. We conjecture that there is a physics in the MEM that can be captured by measuring its correlation, through the calculation of its entanglement. Although the MEM and $|E_F\rangle$ are not the same, but since the behavior of both are similar, we ex-
pect that the correlation in the MEM to have the same trend as the correlation of the \(|E_F|\). As a single-particle eigen-mode, we can calculate the single-particle entanglement entropy of MEM to obtain the correlation information in the MEM. In this paper, we show that SPEE of the MEM distinguishes different phases and it locates the phase transition point, and thus can be used as a phase detection parameter.

Summary of our results are the followings: SPEE of MEM has the same behavior as SPEE of \(|E_F|\). As we go from delocalized phase to localized phase, SPEE of both modes decreases. In addition, amount of fluctuations in SPEE of MEM can be used as a signature of the phase transition point: in the delocalized phase moments of the SPEE of MEM is very small, but its magnitude sharply increases at the phase transition point. Furthermore, we calculate the single-particle RE of both these modes and show that they have the same behavior, i.e. both modes have same entanglement information about the system.

Paper is structured as follows: first, in section II we explain the concept of single-particle EE along with the models we employ in this paper, and then we compare the SPEE of \(|E_F|\) and MEM. In section III we use the notation of RE as another comparison of these two modes. Paper is finished with a conclusion in section IV.

II. SINGLE-PARTICLE ENTANGLEMENT ENTROPY OF MEM

In this paper, single-particle eigen-modes of entanglement Hamiltonian are considered and they should not be confused with the many-body states of the system of the original Hamiltonian. In what follows, we explain the SPEE which will be applied to single-particle MEM as well as to single-particle \(|E_F|\). As explained in Ref. 22 and 23 to define the SPEE, we use occupation number basis. For a lattice system with size \(N\):

\[ |\psi\rangle = \sum_{i=1}^{N} \psi_i |1\rangle_i \bigotimes_{j \neq i} |0\rangle_j, \]

where \(|\psi\rangle\) can be the \(|E_F|\) or the MEM. We divide the system into two equal parts, \(A\) and \(B\). We can define:

\[ |1\rangle_A = \sum_{i=1}^{N_A} \psi_i |1\rangle_i \bigotimes_{j \neq i} |0\rangle_j, \]
\[ |0\rangle_A = \bigotimes_{i=1}^{N_A} |0\rangle_i. \]

To obtain the reduced density matrix for subsystem \(A\), we trace over sites in \(B\) and we obtain:

\[ \rho_A = |1\rangle_A \langle 1| + p_B |0\rangle_A \langle 0|, \]

where:

\[ p_A = \sum_{i=1}^{N_A} |\psi_i|^2, \]
\[ p_B = \sum_{i=N_A+1}^{N} |\psi_i|^2 = 1 - p_A, \]

and finally we obtain the SPEE:

\[ EE = -tr \rho_A \log \rho_A = -(p_A \log p_A + p_B \log p_B). \]

We note that the above mentioned procedure to calculate the single-particle entanglement entropy can be applied to any single-particle wave-function in lattice system; it can be applied to \(|E_F|\) as well as to MEM.

To verify our idea, we employ power-law random banded matrix model (PRBM) 22 that is a one-dimensional long range hopping model with the following Hamiltonian:

\[ H = \sum_{i,j=1}^{N} h_{ij} c_i^\dagger c_j \]

in which \(N\) is the system size and \(c_i^\dagger (c_j)\) is the creation (annihilation) operator for site \(j\) in the second quantization. Matrix elements \(h_{ij}\) are random numbers that are distributed by a Gaussian distribution. The mean value of the distribution is zero and it has the following variance:

\[ \langle |h_{ij}|^2 \rangle = \left[ 1 + \left( \frac{|i-j|}{b} \right)^{2a} \right]^{-1} \]

Where \(b\) is a parameter, by which we can tune hopping amplitudes. In the regime of \(b \lesssim 1\) we approach to the nearest-neighbor case; on the other hand, when \(b \gg 1\), all hopping amplitudes are non-zero. In this paper we set \(b = 1\) 22 To avoid the effect of finite size of system, we choose periodic boundary condition in the Hamiltonian of Eq. (9), where we replace \(i-j\) with the chord length and thus the Hamiltonian becomes:

\[ \langle |h_{ij}|^2 \rangle = \left[ 1 + \left( \frac{\sin \pi(i-j)/N}{b \pi/N} \right)^{2a} \right]^{-1}, \]
as it is proved numerically and analytically in Ref. 24, this system is localized for \(a > 1\) and it is extended in the regime of \(a < 1\). There is a phase transition at the point \(a = 1\) regardless the value of \(b\). This model is important since there is a parameter \(b\) in this model that can be tuned in a way that it resembles other typical models 25 and specially it can be tuned to have similar behavior like the three dimensional Anderson model. This model has attracted much attention and has been used in several recent studies (see for example Refs. 32–35). Because of such features, we choose this model to verify our ideas.
We calculate the SPEE of the MEM and $|E_F\rangle$ by Eq. (7). Results are presented in Fig. 1. Although the SPEE of both are not exactly the same, both have the same trend. In the delocalized phase, SPEE is almost constant and as we approach the the localized phase, SPEE decreases. This result makes sense, since as we approach to the localized phase, the amount of correlation and thus SPEE decreases.

On the other hand, we plot SPEE of both $|E_F\rangle$ and MEM as system size $N$ changes (see Fig. 2). SPEE for MEM and $|E_F\rangle$ are approximately constant as $N$ changes, thus we do not need a very large system size to verify the phase of the system.

PRBM model undergoes a disorder phase transition, i.e. by increasing disorder in system, it goes from delocalized phase to localized phase where quantum fluctuations are dominant. These fluctuations should be seen in observable quantities in system. To see how fluctuations are seen in the SPEE, we use moments of SPEE. Moments, $m_k$, of random numbers $\{x\}$ with mean value $<x>$ are defined as below:

$$m_k = \frac{1}{n_s} \sum_{i=1}^{n_s} (x_i - <x>)^k$$

where $n_s$ is the number of random numbers. Different moments of SPEE of MEM are plotted in Fig. 3 for $m = 2, 3, 4, 5$. As we can see, different moments that are a measure of fluctuations of SPEE in system, show very sharply the phase transition point: Moments are zero in the delocalized phase and they are non-zero in the localized phase. Thus, fluctuations of the SPEE of MEM can distinguish different phase.

### III. SINGLE PARTICLE RÉNYI ENTROPY OF MEM

Beside the single-particle entanglement entropy that contains information about correlation of the system and is a tool to distinguish different phases, we can also use the other related measure, namely the Rényi entropy. Similar to EE, RE can also be calculated for a many-body state as well as for a single-particle state. Here we apply single-particle Rényi entropy (SPRE) to the single-particle MEM and $|E_F\rangle$. The advantage of RE over EE is that, we can obtain more complete physical information by calculating different orders of Rényi entropy. Here,
FIG. 4. Single particle Rényi entropy of $|E_F\rangle$ and $|\text{MEM}\rangle$ as a function of $a$. We see that both have same trend. System size is fixed to $N = 500$ and for each point we have 1000 samples.

we calculate the RE of MEM and compare it with RE of $|E_F\rangle$ to show that, both have similar entanglement properties from the perspective of other measurement of entanglement, namely the RE.

because we have the freedom of choosing size of the subsystem, we choose subsystem $A$ to be a single site and the rest of the system as subsystem $B$. Since no site has privilege over other sites, we average over sites of the system. SPRE then will be

$$RE_q = \frac{1}{N} \frac{1}{1-q} \log tr\rho_A^q$$

$$= \frac{1}{N} \frac{1}{1-q} \log (p_A^q + p_B^q)$$

where $p_A$ and $p_B$ are defined in Eqs. (5) and (6). In Fig. 4 we plot SPRE of $|E_F\rangle$ and MEM for a fixed system size as we change $a$. As we can see from this figure, SPRE for both eigen-mode has similar behavior: SPRE is decreasing as we go from delocalized phase to localized phase. Thus, in the light of RE, both MEM and $|E_F\rangle$ have similar entanglement properties in the delocalized-localized phase transition.

IV. CONCLUSION

In this paper, we introduced a novel phase transition characterization, namely the single-particle entanglement and Rényi entropy of the MEM of Hamiltonian eigen-mode. By using a free fermion lattice model that undergoes delocalized-localized phase transition, we verified numerically that SPEE of MEM clearly distinguish different phases. In the delocalized phase, SPEE is very close to $\ln 2$ and it decrease in localized phase. Fluctuations of the SPEE of MEM was another phase detection characterization we introduced in this paper. In addition, to show that both MEM and $|E_F\rangle$ have similar entanglement properties, we used another measure of entanglement, namely the RE. We showed that SPRE for MEM and $|E_F\rangle$ have similar behavior in delocalized and localized phase.

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