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Bipartite entanglement and localization of one-particle states

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Abstract

We study bipartite entanglement in a general one-particle state, and find that the linear entropy, quantifying the bipartite entanglement, is directly connected to the participation ratio, characterizing the state localization. The more extended the state, the more entangled it is. We apply the general formalism to investigate ground-state and dynamical properties of entanglement in the one-dimensional Harper model.

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Entanglement is an interesting phenomenon of quantum systems which does not exist classically. It has attracted increasing interest due to its potential applications in quantum communication and information processing [1] such as quantum teleportation [2], superdense coding [3], quantum key distribution [4] and telecoloning [5]. On the other hand, entanglement has been proved to be playing an important role in condensed matter physics. There are many studies on entanglement in the Heisenberg spin models [6–8], Ising models in a transverse magnetic field [9, 10] and related fermionic systems [11]. In the context of quantum phase transition, entanglement is a convenient indicator of the transition [12, 13].

Recently, *pairwise entanglement* sharing in one-particle states was studied [14] using the concurrence [15] in the Harper model [16]. Here, we study another type of entanglement of one-particle states, the *bipartite entanglement*, which refers to entanglement between two subsystems when a whole system is divided into two parts. We reveal that the average bipartite entanglement directly connects to state localization.

The one-particle states permeate many physics systems. For example, for one electron moving on a substrate potential, the eigenfunctions are one-particle states. In quantum spin chain models with only one spin up (down) and all other spins down (up), the eigenfuntions of the model are one-magnon states.

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We consider a system containing N two-level systems (qubits) with $|0\rangle$ being the excited state and $|1\rangle$ the ground state. A general one-particle state is then written as [17]

$$|\Psi\rangle = \psi_1|1000\ldots0\rangle + \psi_2|0100\ldots0\rangle + \cdots + \psi_N|0000\ldots1\rangle. \tag{1}$$

Here, $\{|\psi_n|^2\}$ is a probability distribution, satisfying the normalization condition $\sum_{n=1}^{N}|\psi_n|^2 = 1$. When $|\psi_n| = 1/\sqrt{N}$, state $|\Psi\rangle$ reduces to the W-state [18, 8], one representative state in quantum information theory.

We now consider bipartite entanglement between a block of L qubits and the rest $N - L$ qubits. Bipartite entanglement of a pure state can be measured by the linear entropy of reduced density matrices

$$E(|\Psi\rangle) = 1 - \mathrm{Tr}\big(\rho_i^2\big), \qquad i \in \{1, 2\} \tag{2}$$

where ρ_i is the reduced density matrix for subsystem i. Of course, we can use other entropies such as the von Neumann entropy, and the *qualitative* results are not changed. The linear entropy adopted here is convenient to reveal the *quantitative* relation between bipartite entanglement and state localization.

To calculate bipartite entanglement, we first consider a simple situation, namely, the entanglement between the first qubit and the rest $N - 1$ qubits. The one-particle state can be written in the following form,

$$|\Psi\rangle = \psi_1|1\rangle \otimes |\alpha\rangle + \sqrt{\sum_{n=2}^{N}|\psi_n|^2}|0\rangle \otimes |\beta\rangle \tag{3}$$

where

$$\begin{aligned} |\alpha\rangle &= |00\ldots0\rangle, \\ |\beta\rangle &= \frac{1}{\sqrt{\sum_{n=2}^{N}|\psi_n|^2}}(\psi_2|100\ldots0\rangle + \psi_3|010\ldots0\rangle + \cdots + \psi_N|00\ldots1\rangle) \end{aligned} \tag{4}$$

are two orthonormal states of $N - 1$ qubits. Then the reduced density matrix for qubit 1 is easily found to be

$$\rho_1 = \begin{pmatrix} 1 - |\psi_1|^2 & 0 \\ 0 & |\psi_1|^2 \end{pmatrix} \tag{5}$$

in the basis $\{|0\rangle, |1\rangle\}$. Therefore, from equations (2) and (5), the linear entropy of qubit 1 is obtained as $E_{1,N-1}^{(1)} = 2(|\psi_1|^2 - |\psi_1|^4)$, where the superscript denotes the first qubit. In the same way, we may find the linear entropy for the nth qubit as

$$E_{1,N-1}^{(n)} = 2(|\psi_n|^2 - |\psi_n|^4), \tag{6}$$

quantifying the degree of bipartite entanglement between nth qubit and the rest.

Taking an average of entanglement over all qubits, we obtain

$$E_{1,N-1} = \big\langle E_{1,N-1}^{(n)}\big\rangle = \frac{2}{N}\sum_{n=1}^{N}(|\psi_n|^2 - |\psi_n|^4) = \frac{2}{N}\left(1 - \sum_{n=1}^{N}|\psi_n|^4\right) = \frac{2}{N}E_s, \tag{7}$$

where $E_s = \big(1 - \sum_{n=1}^{N}|\psi_n|^4\big)$ is the quantum state linear entropy [19] for state $|\Psi\rangle$.

We now consider more general situations, namely, the bipartite entanglement between a block of L qubits and the rest of the system. We pick up L qubits $\{1', 2', \ldots, L'\}$ from N qubits, and there are totally C_N^L options. In the same way as above, we can calculate the linear entropy of L qubits as

$$E_{L,N-L}^{\{1',\ldots,L'\}} = 2(|\psi_{1'}|^2 + \cdots + |\psi_{L'}|^2) - 2(|\psi_{1'}|^2 + \cdots + |\psi_{L'}|^2)^2. \tag{8}$$

Now, we make an average of the linear entropy $E_{L,N-L}^{\{1',\ldots,L'\}}$ over the C_N^L options. Formally, the average entropy is given by

$$E_{L,N-L} = \langle E_{L,N-L}^{\{1',\ldots,L'\}}\rangle = \left[\sum_{\{1',\ldots,L'\}} \frac{2}{C_N^L}(|\psi_{1'}|^2 + \cdots + |\psi_{L'}|^2) - \frac{2}{C_N^L}(|\psi_{1'}|^2 + \cdots + |\psi_{L'}|^2)^2\right]. \tag{9}$$

The first term in the summation of the above equation can be easily evaluated as

$$\frac{2}{C_N^L}\sum_{\{1',\ldots,L'\}}(|\psi_{1'}|^2 + |\psi_{2'}|^2 + \cdots + |\psi_{L'}|^2) = \frac{2L}{N}. \tag{10}$$

Next, we evaluate the second term of the summation in equation (9). The following relation

$$\sum_{n>m} 2|\psi_n|^2|\psi_m|^2 = 1 - \sum_{n=1}^{N} |\psi_n|^4. \tag{11}$$

is useful, resulting from the normalization condition of state $|\Psi\rangle$. Note that the summation on the left-hand side of the above equation contains C_N^2 terms. By applying the above relation, the second term of the summation in equation (9) is obtained as

$$-\frac{2L}{N}\sum_{n=1}^{N}|\psi_n|^4 - \frac{2C_L^2}{C_N^2}\left(1 - \sum_{n=1}^{N}|\psi_n|^4\right). \tag{12}$$

Substituting equations (10) and (12) into equation (9) leads to

$$E_{L,N-L} = 2\left(\frac{L}{N} - \frac{C_L^2}{C_N^2}\right)E_s = \frac{2L(N-L)}{N(N-1)}E_s. \tag{13}$$

As we expected, the average linear entropy is invariant under the transformation $L \to N - L$.

The above result (13) shows that the average bipartite entanglement between a block of L qubits and the rest $N - L$ qubits is proportional to the quantum state linear entropy E_s. For the W-state, the quantum state linear entropy $E_s = 1 - 1/N$, and thus the average linear entropy becomes

$$E_{L,N-L} = 2L(N-L)/N^2. \tag{14}$$

If N is an even number and $L = N/2$, the linear entropy $E_{L,N-L} = 1/2$ becomes maximal, equal to the amount of bipartite entanglement of a Bell state.

There exists a close relation between the average *pairwise entanglement* and *state localization* for one-particle states as discussed in [14]. We now study relations between *bipartite entanglement* and state localization. The degree of localization can be studied by a simple quantity, the participation ratio defined by [20]

$$p = \frac{1}{N\sum_{n=1}^{N}|\psi_n|^4}. \tag{15}$$

Then, from the above equation, the quantum state linear entropy can be written as

$$E_s = 1 - \frac{1}{Np}. \tag{16}$$

Substituting equation (16) into equation (13) leads to

$$E_{L,N-L} = \frac{2L(N-L)}{N(N-1)}\left(1 - \frac{1}{Np}\right), \tag{17}$$

which builds a direct connection between bipartite entanglement and state localization. It is evident that the more extended the one-particle state, the more entangled the state is.

In a recent work [21], we find that there is a relation between the average square of concurrence and the participation ratio given by

$$\langle C^2 \rangle = \frac{4}{N(N-1)}\left(1 - \frac{1}{Np}\right). \tag{18}$$

Then, from equations (17) and (18), we obtain a connection between bipartite entanglement and pairwise entanglement given by

$$E_{L,N-L} = \frac{L(N-L)}{2}\langle C^2 \rangle. \tag{19}$$

Therefore, for the one-particle state, the average linear entropy, the average square of concurrence and the participation ratio are interrelated by simple relations. Next, we consider an example of one-particle states, and study quantum entanglement and its relations to state localization induced by on-site potentials in the quasiperiodic one-dimensional Harper model [16].

The Hamiltonian describing electrons hopping in a one-dimensional lattice can be written as [16]

$$H = \sum_{n=1}^{N} \frac{1}{2}\left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n\right) + V_n c_n^\dagger c_n, \tag{20}$$

where $c_n^\dagger$ and c_n are the fermionic creation and annihilation operators, respectively, and V_n is the on-site potential. This Hamiltonian describes electrons moving on a substrate potential. The different forms of on-site potential V_n lead to different behaviours of electrons.

For the Harper model, the on-site potential is given by

$$V_n = \lambda \cos(2\pi n \sigma) \tag{21}$$

where σ determines the period of potential and λ is the amplitude of the potential. It is well known that the dynamics of the Harper model is characterized by parameter λ [22]. If $\lambda < 1$, the electron is in a quasiballistic extended state, but in a localized state when $\lambda > 1$. The critical Harper model corresponds to $\lambda = 1$, where the spectrum is a Cantor set.

We consider one-electron states in the Harper model. For studying entanglement in this fermionic system, we adopt the approach given in [11], namely, we first map electronic states to qubit states and study entanglement of fermions by calculating entanglement of qubits. After the mapping, the one-particle wavefunction of Harper model can be formally written in the form of a general state given by equation (1). Then, we may apply the general result (13) to calculate bipartite entanglement.

For convenience, we examine the average bipartite entanglement between one local fermionic mode (LFM) and the rest for the ground state of the system. The LFMs refer to sites which can be either empty or occupied by an electron [23]. Figure 1 gives results of the scaled linear entropy $NE_{1,N-1}$ for different lengths of system. We note that when the amplitude of the on-site potential increases but does not reach the value $\lambda = 1$, the average entanglement is almost keeping a constant value, varying a very small amount. The entanglement is not destroyed by the external potential in this region. However, when $\lambda = 1$, the entanglement exhibits a sudden jump down to a value close to zero. For larger λ, the ground state is almost

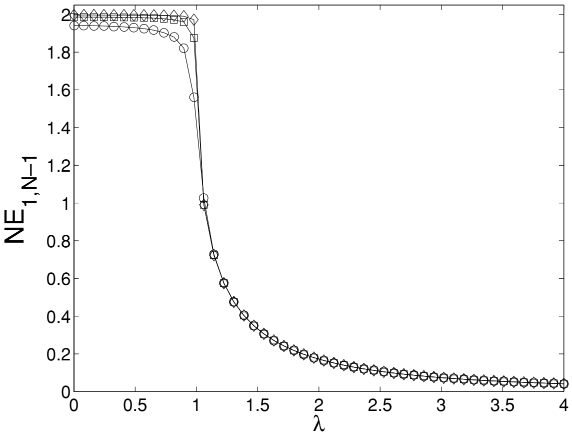

Figure 1. The scaled average linear entropy as a function of λ for different lengths of the chain, $N = 34$ (circle line), $N = 144$ (square line) and $N = 610$ (diamond line). The parameter σ is $F(n-1)/F(n)$ with $F(n) = N$, where $\{F(n)\}$ is the Fibonacci sequence.

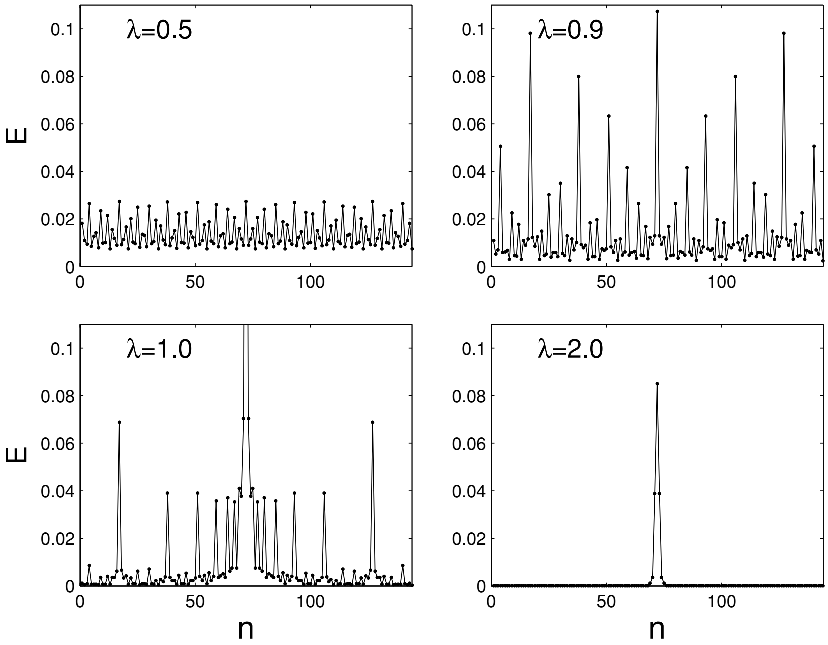

Figure 2. The distribution of the linear entropy for different λ with $N = 144$ and $\sigma = 89/144$.

not entangled. After the critical point, the three curves merge into one, implying that the scaled average entanglement is independent on N when $\lambda > \lambda_c$. From our analytical result (13), the scaled linear entropy is just the twice of the quantum state entropy E_s. In the limit of $N \to \infty$, the scaled linear entropy $NE_{L,N-L}$ (finite L) is equivalent to E_s up to a multiplicative factor $2L$.

To understand the underlying mechanism of the transition of entanglement induced by the change of on-site potential, we study the distribution of the linear entropy $E_{1,N-1}^{(n)}$. If the on-site potential is absent, the entanglement distributes evenly on the lattice sites. Figure 2

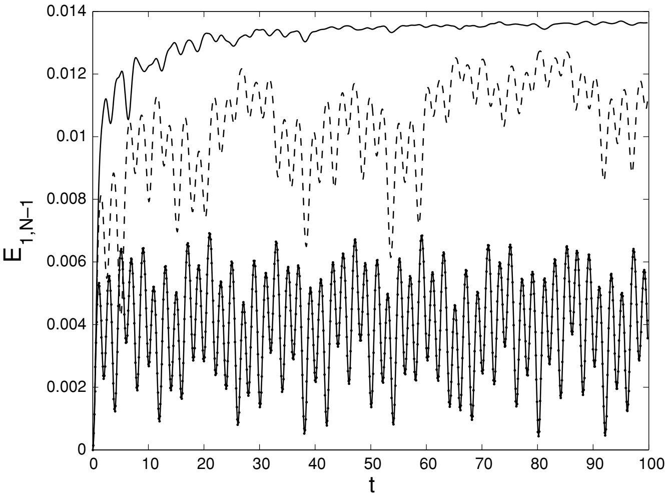

Figure 3. Dynamics of the linear entropy for $\lambda = 1/2$ (solid line), $\lambda = 1$ (dashed line) and $\lambda = 1.5$ (connected dotted line). The parameters $N = 144$ and $\sigma = 89/144$.

shows the distribution of the linear entropy for different λ. When $\lambda = 0.5$ smaller than λ_c, the entanglement shows small oscillations. When $\lambda = 0.9$ near to λ_c, the distinct uneven distribution is observed but the state is still not localized. When $\lambda = \lambda_c$, a significant change takes place, and a large peak of entanglement appears at the centre of the lattice and the entanglement at most of the other sites is suppressed. The entanglement between the LFM at the centre and the rest becomes dominant. The ground state is localized by the effects of on-site potential V_n in this case. When $\lambda = 2$ larger than λ_c, the entanglement at most sites is suppressed to zero except at a few sites near the centre of the lattice where it is still of finite value, although they are also suppressed. Thus, the localization is enhanced when the amplitude of the potential increases. Furthermore, the biparticle entanglement between a block of LFMs and the rest for such a one-particle state is also calculated and shows similar behaviours as the linear entropy $E_{1,N-1}$.

Having studied ground-state entanglement of the Harper model, we now examine dynamics of entanglement. The time evolution can be described by the following time-dependent equation:

$$\mathrm{i}\frac{\mathrm{d}\psi_n}{\mathrm{d}t} = \frac{1}{2}(\psi_{n+1} + \psi_{n-1}) + \lambda\cos(2\pi n\sigma). \tag{22}$$

The wave packet is localized initially at the centre of the chain and the above equation can be solved numerically by integration. In our calculations, we adopt the periodic boundary condition. The variance of the wave packet

$$\sigma^2(t) = \sum_{n=1}^{N}(n - \bar{n})^2|\psi_n(t)|^2 \tag{23}$$

is studied in [22] and different time evolution behaviours were shown.

When the state vectors at any time are obtained by integration, we can calculate bipartite entanglement between the block of LFMs and the rest of the chain. In figure 3, we plot the average entanglement $E_{1,N-1}$ for several values of λ. When $\lambda < \lambda_c$, $E_{1,N-1}$ exhibits a rapid initial increase, which corresponds to the variance $\sigma^2(t) \sim t^2$ [22]. This unbounded diffusion is caused by the existence of extended states. In the critical case $\lambda = \lambda_c$, $E_{1,N-1}$ increases slowly, which is in agreement with the clear-cut diffusion with the variance $\sigma^2(t) \sim t^1$. For $\lambda > \lambda_c$, $E_{1,N-1}$ exhibits rapid oscillations because of the localization.

To quantify the ability of entanglement generation, we use the average entanglement over a range of time. Mathematically, we define

$$\bar{E} = \frac{1}{T}\int_0^T E(t), \tag{24}$$

which may reflect the entanglement capability of the system. For our case, $\bar{E}(\lambda)$ is obtained from $E_{1,N-1}$ ($T = 100$) and λ-dependent. Then, we have $\bar{E}(1/2) = 0.0131$, $\bar{E}(1) = 0.0103$, and $\bar{E}(1/2) = 0.0040$. We see that the less the λ, the more the entanglement production.

In this paper, we have studied bipartite entanglement of one-particle states, and found a direct connection between the linear entropy, quantifying the bipartite entanglement and the participation ratio, characterizing state localization. The more localized the state is, the less the entanglement. Pairwise entanglement, bipartite entanglement and state localization are found closely connected together for one-particle states.

As an application of the general formalism, we have studied quantum entanglement of the ground state in the Harper model and found that the bipartite entanglement exhibits a jump at critical point $\lambda = \lambda_c$. The time evolution of entanglement was also investigated, which displays distinct behaviours for different amplitudes of the on-site potential, corresponding to extended, critical and localized states. It is interesting to consider the connections between entanglement and other measures of localization such as the Brody parameter [24], which are under consideration.

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