Two particle excited states entanglement entropy in a one-dimensional ring

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The properties of the entanglement entropy (EE) of two particle excited states in a one-dimensional ring are studied. For a clean system we show analytically that as long as the momenta of the two particles are not close, the EE is twice the value of the EE of any single particle state. For almost identical momenta the EE is lower than this value. The introduction of disorder is numerically shown to lead to a decrease in the median EE of a two particle excited state, while interactions (which have no effect for the clean case) mitigate the decrease. For a ring which is of the same size as the localization length, interaction increase the EE of a typical two particle excited state above the clean system EE value.

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INTRODUCTION

There has been a growing interest in the behavior of entanglement entropy (EE) in different physical fields. In condensed matter, much of the interest stems from the behavior of the ground state EE in the presence of quantum phase transitions (QPTs). The EE of a finite region A of a one-dimensional system grows logarithmically as long as the region’s size $L_A$ is smaller than the correlation length $\xi$ characterizing the system, while it saturates for $L_A > \xi$. This behavior may be used in order to extract $\xi$, for example the ground state localization length of the Anderson transition.

A natural question is what is the behavior of the EE for the excited states? Beyond the growing interest in EE coming from the quantum information circles, the question whether EE is a useful concept in studying the behavior of excited states, is relevant to the condensed matter community. Low lying excited states in the vicinity of a ground state quantum critical point (QCP) should be strongly influenced by the critical point, and one expects it to show in the behavior of the EE of these states. Moreover, the whole concept of the many-body localization transition is centered on the behavior of the excited states. The localization-delocalization transition occurring at a critical excitation energy should change the properties of excitations above it which should be manifested in the properties of the excited states. Although much effort went into trying to understand the transition using different properties of the excited states (such as level statistics, inverse participation ratio, conductance, and correlations), all these studies were performed for rather small systems, and many questions remain open. Recently, time evolution of the entanglement of an initial state was studied, and it showed signs of many-particle delocalization. Thus, EE seems as a useful tool to study the many-body localization transition.

Unlike the ground state EE for which universal results exist, the understanding of EE for the excited states is still a work in progress. Therefore, it would be useful to consider a system for which the EE of the excited states is simple enough to describe analytically, although it exhibits interesting behavior such as interaction induced delocalization of the excited states. In this paper we study the EE for such a system, namely two particles on a ring. The study of two interacting particle (TIP) in a disordered one dimensional system has a long history in the context of many particle delocalization problem. All single-electron states for any amount of disorder are localized. This continues to be true for two-electron states, however, the localization length becomes longer as the repulsive interaction becomes stronger. This interaction induced delocalization was confirmed numerically. It is important to emphasize that there is no enhancement of the localization length in the ground state. The delocalization becomes significant only for higher excitations.

CLEAN RING

For a clean ring composed of $N$ sites, the tight-binding Hamiltonian is given by:

$$ H = \sum_{j=1}^{N} \epsilon_j \hat{a}_j^\dagger \hat{a}_j - t \sum_{j=1}^{N} (\epsilon^\alpha \hat{a}_j^\dagger \hat{a}_{j+1} + h.c.), $$

where for the clean case $\epsilon_j = 0$, $t = 1$ is the hopping matrix element between neighboring sites, and $\hat{a}_j^\dagger$ is the creation operator of a spinless electron at site $j$ on the ring. In order to break symmetry (we shall see why this is important further on) a magnetic flux $\phi$ threading the ring is introduced, where $\alpha = 2\pi \phi/\phi_0 N$, and $\phi_0 = hc/e$ is the quantum flux unit. The single-electron eigenvalues are $\varepsilon(k) = -2t \cos(p - \alpha)$ where $p = 2\pi k/N$, and $k = 0, \pm 1, \pm 2, \ldots \pm N/2$. The eigenvectors are given by

$$ |k\rangle = (1/\sqrt{N}) \sum_{j=1}^{N} \exp(iyj) \hat{a}_j^\dagger |\emptyset\rangle, $$

where $|\emptyset\rangle$ is the vacuum state.
The two particle eigenvalues are $\varepsilon(k_1, k_2) = -2t (\cos(p_1 - \alpha) + \cos(p_2 - \alpha))$. The eigenvector
\[ |k_1, k_2\rangle = (1/N) \sum_{j_1, j_2 = 1}^{N} A(k_1, j_1, k_2, j_2) a_{j_1}^\dagger a_{j_2}^\dagger |\emptyset\rangle, \]
where
\[ A(k_1, j_1, k_2, j_2) = \left( \exp(i(p_1 j_1 + p_2 j_2)) - \exp(i(p_1 j_2 + p_2 j_1)) \right). \]

Once the eigenvectors of the system are available one can (in principal) calculate the EE. The entanglement between a region A (of length $N_A$) in the system and the rest of the system (denoted by B) for a given eigenstate $|\psi\rangle$ is measured by the EE $S_{A/B}$. This EE is related to the eigenvalues of the matrix $\rho_{A/B}$, defined in the following way:
\[ \hat{\rho}_{A/B} = \text{Tr}_{B/A}|\psi\rangle\langle\psi|, \]
where the trace is over region’s B or A degrees of freedom.

The two-particle eigenvalues are $\varepsilon(k_1, k_2) = -2t (\cos(p_1 - \alpha) + \cos(p_2 - \alpha))$. The eigenvector
\[ |k_1, k_2\rangle = (1/N) \sum_{j_1, j_2 = 1}^{N} A(k_1, j_1, k_2, j_2) a_{j_1}^\dagger a_{j_2}^\dagger |\emptyset\rangle, \]
where
\[ A(k_1, j_1, k_2, j_2) = \left( \exp(i(p_1 j_1 + p_2 j_2)) - \exp(i(p_1 j_2 + p_2 j_1)) \right). \]

One important result of this definition is the symmetry between the EE of the two regions $S_A = S_B$. Following Cheong and Henley [32], one can write the pure state $|\Psi\rangle = \sum_i |i_A\rangle |\phi_{B,i}\rangle$, where $|i_A\rangle$ is a complete orthonormal many-body basis of region A, while $|\phi_{B,i}\rangle$ is the state in region B associated with $|i_A\rangle$. Please note that $|\phi_{B,i}\rangle$ is not normalized. Using that notation, the reduced density matrix
\[ \hat{\rho}_{A} = \sum_{i, j = 1}^{N} |i_A\rangle \langle j_A|, \]
or in matrix form:
\[ \rho_{A}(i, j) = \langle \phi_{B,i}|\phi_{B,j}\rangle. \]

Utilizing the occupation basis in the A region, i.e., $|i_A\rangle = |n_1^i, n_2^i, n_3^i, \ldots, n_{N_A}^i\rangle$ (where $n_j^i = 0, 1$), one can define an operator, $K_i = \prod_{s=1}^{N_A} (n_s^i \hat{a}_s^\dagger + (1 - n_s^i) \hat{a}_s^\dagger \hat{a}_s^\dagger)$, resulting in:
\[ \rho_{A}(i, j) = \langle \Psi|K_i^\dagger K_j|\Psi\rangle. \]

It is important to note that $\rho_{A}(i, j) \neq 0$ only for states which have the same number of particles $n_s^i$ in region A, where $n_A^i = \sum_{s=1}^{N} n_s^i$. Thus, in this basis, the reduced density matrix is composed of blocks which increases in size with $n_A^i$. Thus for $n_A^i = 0$, the block size is one, for $n_A^i = 1$ it is $N_A$, for $n_A^i = 2$ it is $N_A(N_A - 1)/2$, etc.

Thus, the task of calculating the EE of a region A at a given excitation $|\Psi\rangle$ is equivalent to calculating the eigenvalues of the matrix $\rho_{A}(i, j)$. Since the blocks are uncoupled, it is possible to diagonalize each block with a given number of particles, $\rho_{A}(i, j)$, independently (where $\ell$ denotes the number of particles in region A). For a state $|\Psi\rangle$, which is the ground state of a half-filled ring at $N \rightarrow \infty$, it is possible (in several different ways) to show that $S_A = -(1/3) \ln(x) + \text{Const}$, where $x = N_A/N$. For the excited states the task becomes more difficult, and no simple and general result for $S_A$ exists [34]. Here we will calculate the $S_A$ for two-particle excitations.

For the sake of completeness lets first consider single particle state entanglement. In this simple case $\rho_{A}(i, j)$ is composed of two blocks: $\rho_A(0)(1, 1)$ and $\rho_A(1)(i, j)$ (where $i, j = 1 \ldots N_A$). Direct evaluation of Eq. (9) for any single-particle state $|\Psi\rangle = |k\rangle$ results in $\rho_A(0)(1, 1) = 1 - x$, while $\rho_A(1)(i, j) = (1/N) \exp(-i\phi(i - j))$. The latter is a Toeplitz matrix, with one eigenvalue equal to $x$ and $N_A - 1$ zero eigenvalues. As expected, the EE for any single particle eigenstate $|k\rangle$ is equal to
\[ S_A = -x \ln(x) - (1 - x) \ln(1 - x) \]
and does not depend on $|k\rangle$.

A note of caution is in place. Since the eigenvalues for $k$ and $-k$ are degenerate, any linear combination of $|k\rangle$ and $|-k\rangle$ are an excited state of Eq. (10). These linear combinations have different values of the EE, and therefore, strictly speaking, the EE for degenerate excited states is ill defined. We circumvent this problem by introducing a degeneracy breaking magnetic flux $\phi$ into Eq. (10). As long as the degeneracy is broken the EE of any excited state $|k_1, k_2\rangle$ is well defined and does not depend on $\phi$.

For two-particle states $|k_1, k_2\rangle$, the reduced density matrix is composed of three blocks: $\rho_A(0)(1, 1)$, $\rho_A(1)(i, j)$ (of size $N_A$) and $\rho_A(2)(i, j)$ (size $N_A(N_A - 1)/2$). For the zero particle block:
\[ \rho_A(0)(1, 1) = \frac{1}{N^2} \sum_{j_1, j_2 > N_A} |A(j_1, k_1, j_2, k_2)|^2 = (1 - x)^2 - y^2, \]

where $y = (\sin(\pi(k_2 - k_1)x)/(\pi(k_2 - k_1)))$. Thus the eigenvalue of this block is $(1 - x)^2 - y^2$. Using symmetry, one can immediately deduce the eigenvalues of the two-particle reduced density matrix, without actually diagonalizing the $N_A(N_A - 1)/2$ matrix. Since $S_A = S_B$, the contribution to the EE from $\rho_A(2)(i, j)$, must be equal to the contribution from $\rho_A(0)(1, 1)$. This infers that $\rho_A(2)(i, j)$ has only one non-zero eigenvalue. Seeing that region B’s
length is $N - N_A$, according to Eq. (11), the non-zero
eigenvalue of $\rho_A^{(2)}(i, j)$ is equal to $x^2 - y^2$.

The one-particle block density matrix is given by:

$$\rho_A^{(1)}(i, j) = \frac{1}{N^2} \sum_{j > N_A} A^*(j_1, k_1, i, k_2)A(j_1, k_1, j, k_2) =$$

$$\frac{e^{-i\rho_1(i-j)}}{N}(1-x)(1 + e^{-i(p_2-p_1)(i-j)}) + \frac{1}{iN(p_2-p_1)}\left[e^{-i(p_2-p_1)}(e^{i(p_2-p_1)N_A} - 1) - e^{i(p_2-p_1)j}e^{-i(p_2-p_1)N_A} - 1\right].$$

(12)

This cumbersome form is substantially simplified when
$k_2 - k_1$ is large. In that case the second term in Eq. (12)
may be neglected and the density matrix block has a Toeplitz form

$$\rho_A^{(1)}(i, j) = \frac{1-x}{N}\left(e^{-i\rho_1(i-j)} + e^{-i\rho_2(i-j)}\right),$$

with $N_A - 2$ zero eigenvalues, and two degenerate eigenvalues equal to $x(1-x)$. The second term is negligible also
when $x = N_A/N \sim 1/2$, and $k_2 - k_1$ is even, resulting
in the same eigenvalues. We do not have the general
solution, nevertheless, it can be shown numerically that
$\rho_A^{(1)}(i, j)$ has no more than two non-zero eigenvalues,
which depend only on the difference $k_2 - k_1$. Moreover,
since the sum of all eigenvectors of the density matrix
should be one, the sum of those two eigenvalues should be
$2x(1-x) + 2y^2$. For the ground state (and excitations
for which $k_2 - k_1 = 1$) the two eigenvalues are well
described by $2x(1-x) + (2-1/\pi)y^2$ and $y^2/\pi$.

Thus, the EE of two-particle states composed from two
single-particle states of significantly different wave
numbers which are the majority of the two-particle states, is

$$S_A(k_2 - k_1 \gg 1) = -2[(1-x)\ln(1-x) - x\ln(x)].$$

(14)

This is twice the EE of a single particle state (Eq. (11)).
Thus, as long as the two occupied states $|k_1\rangle$ and $|k_2\rangle$
are far enough from each other, the two-particle EE is
just the sum of the EE of each occupied state. In the opposite
limit

$$S_A(k_2 - k_1 = 1) \sim -(x^2 - y^2)\ln((1-x)^2 - y^2) - (x^2 - y^2)\ln(x^2 - y^2) - [y^2/\pi]\ln[y^2/\pi] - [2x(1-x) + (2-1/\pi)y^2]\ln[2x(1-x) + (2-1/\pi)y^2].$$

(15)

The EE curves for other values of $k_2 - k_1$ can be calculated
numerically by diagonalizing the $N_A \times N_A$ matrix
representing $\rho_A^{(1)}$ (the two other eigenvalues for $\rho_A^{(0)}$
and $\rho_A^{(2)}$ are given be Eq. (11)). The results are depicted in

**FIG. 1:** (Color online) The EE of a two particle state $|k_1, k_2\rangle$
of a clean system as function of region A’s size $x = N_A/N$ for
a system of length $N = 1000$. The Heavy lines correspond
to the analytic prediction, (dotted for $k_2 - k_1 = 1$, Eq. (13),
dashed for $k_2 - k_1 \gg 1$, Eq. (14)). The thin lines pertain to the
numerically calculated EE for all values of $k_2 - k_1$ between
$1 \ldots 30$, where odd values are depicted by red curves, and even
one by red curves. It is clear that for $k_2 - k_1$ larger than 5 the
numerical curves fit Eq. (14) quite well. It is also clear that
all even $k_2 - k_1$ reach the same EE value $S_A(x = 1/2) = \ln(4)$
once $N_A = N/2$.

**INTERACTING CLEAN RING**

Incorporating nearest neighbor electron-electron interactions into the system, results in adding an interaction
term given by

$$H_{\text{int}} = U \sum_{j=1}^{N} \hat{a}_j^\dagger \hat{a}_j \hat{a}_{j+1}^\dagger \hat{a}_{j+1}$$

(16)
to the Hamiltonian, $H$, depicted in Eq. (1). In a clean system it is well known that far from half-filling the system behaves as a Luttinger liquid for any value of $U$ [34]. For the ground state EE of a clean system at half-filling (and $U < 2$, i.e., a Luttinger liquid) the EE changes only by an overall constant [1 3], while retaining the same logarithmic dependence. Thus, we expect that the EE of the two-particle states in a clean system will not be essentially affected by the presence or absence of electron-electron interactions. Unfortunately, it is not possible to calculate analytically the two-particle states of the interacting system. Thus, we must rely on a numerical solution for the problem.

Exact diagonalization is used to calculate all the eigenvectors of $H + H_{\text{int}}$, represented by a $N(N - 1)/2$ matrix. We have chosen a 100 site system, resulting in a matrix of size 4950. A reduced density matrix $\rho_A$, of size $1 + N_A + N_A(N_A + 1)/2$ is then constructed and diagonalized for each eigenstate, and the EE is calculated using its eigenvectors according to Eq. (6). The results are shown in Fig. 2 where the EE of 31 states around the ground state (i.e. the ground state and 1st - 30th excitation), and at quarter of the two-particle band (1222th - 1252st excitation) are shown. In both cases the EE for the non-interacting ($U = 0$) as well as for the interacting ($U = 1$) cases are almost equal (the interacting case is larger by a minute constant (of order $10^{-4}$ which can not be resolved at the resolution of the figure). As expected around the ground-state the excitations belong to the low $k_2 - k_1$ sector while for the higher excitations most states corresponds to large values of $k_2 - k_1$, i.e., well described by Eq. (14).

\section*{INTERACTING DISORDERED RING}

When disorder is added to a non-interacting system, all single particle states become localized. For the many-particle states, the behavior is more involved. As long as no interaction is present, the many-particle states remain localized, both for the ground state [35] as well as for all the excited states. Once interaction is introduced, the ground-state as well as low lying excitations remain localized, while above a critical energy the many-particle excitations are predicted to delocalize [11 13]. This transition, termed the many-body or Fock space localization transition, stems from the interactions coupling excitations with a different number of electron-hole couples. This type of transition is irrelevant for two particle systems. Nevertheless, as argued by Shepelynsky and Imry [26, 27], interaction between the pair of particles should enhance the two particle localization length, compared to the single electron localization length, as long as the two-particle level spacing is significantly smaller than the single electron level spacing, i.e., for higher excitations.

Can we see any signature of the enhanced two-particle localization length in the EE behavior of the excited states? First we have to understand the influence of disorder on the EE. In Ref. 8 it has been shown that for the ground-state the EE saturates on the length scale of $\xi$, and does not continue to grow logarithmic as in a clean system. Thus, the EE of a disordered system is always lower than the EE of a clean system. One would expect this feature to hold also for excited states. We check this assumption by calculating the EE using the excitations of the Hamiltonian given in Eq. (1), where the disorder is represented by a random on-site energy, $\epsilon_j$ taken from a uniform distribution in the range $[-W/2, W/2]$. For $W = 3$, single electron states at the middle of the band are expected to have a localization length $\xi \sim 10$ [36], while close to the band edge the single electron states are supposed to be much more strongly localized (Lifshitz tails) [37].

The EE is calculated by exact diagonalization for systems of size $N = 100$ as described in the previous section. The results are presented in Fig. 3 where the median EE in the vicinity of the ground-state (1st - 30th excitation), at 1/16 of the band (294th - 324th excitation), at 1/8 of the band (603th - 633th excitation), and at 1/4 of the band (1222th - 1252th excitation). The median EE is taken across the 31 excitations in each segment and 50 different realizations of disorder. We calculate the EE in the absence ($U = 0$) and presence ($U = 1$, $U = 3$) of electron-electron interactions. Around the ground state, the interactions do not play a significant role, and for all cases the EE is strongly suppressed compared to typical
significant difference between entangled as interaction is present, although there is no localization of the two-particle states, which become more This is a clear signature for the effect of interactions on lo-

gation is predicted only when there are at least a couple

values for a clean system. This is expected, since as men-
tioned, at the bottom of the band the states are strongly
localized, and therefore the EE is low.

For the non-interacting case, the EE higher in the band
are less suppressed as the localization length grows. The EE for high excitations in the interacting case is always larger than for the corresponding non-interacting states. This is a clear signature for the effect of interactions on localization of the two-particle states, which become more entangled as interaction is present, although there is no significant difference between $U = 1$ and $U = 3$. It is also clear that for higher excitations (larger localization length) the enhancement of the EE becomes stronger.

This enhancement could be expected on physical grounds. As has been shown [26–31], the localization length associated with an interacting two-particle state is larger than for a non-interacting state with the same disorder. Thus, one expects that the EE will also be larger and closer to its clean system value.

We therefore also investigate the case of weaker disor-
der, which for the localization length is of order of the sys-

tem size ($W = 1, \xi \sim 100$). As can be seen in Fig. 4 for the non-interacting case a similar pattern to the one observed Fig. 3 remains, although the EE is less suppressed by the weaker disorder. As expected, the enhancement of the EE by interactions is stronger for the weaker disor-
der. Surprisingly, above 1/8 of the band (corresponding to an excitation energy of $t$), the EE of the disordered interacting system is significantly larger than the limit for a clean system ($\ln(4)$). Although, extrapolating from the results presented in Fig. 3 increasing the system size while keeping the disorder fixed will result in a decrease of the EE below the clean system values once $L \gg \xi$. The increase above the clean system excitation EE may stem from the fact that as long as the two particles are confined within a single localization length the particles can not avoid each other and spend much time close to each other, leading to an enhancement of the EE. When the system size is much larger than the localization length, the two particles can reside in different regions of the sample, and interactions will not play an important role. However, this hand waving picture requires further study.

At first glance, these results seem to indicate that although interactions may enhance the EE as long as $L < \xi$, they become irrelevant for $L \gg \xi$, showing no support for the many-particle delocalization scenario [11–13] which should occur for $L \gg \xi$. This interpretation is wrong, since the many-particle delocalization scenario deals with a constant density of particles, and delocalization is predicted only when there are at least a couple of particles in the range of a single particle localization length. Thus the observed two-particle EE enhancement when the two particles are within a distance of $\xi$, as well as the fact that the enhancement increases significantly when the excitation energy, fits nicely with the scenario promoted in Ref. [13]. Of course, coupling between states with a different number of electron-hole generation is crucial for the delocalization scenario, and therefore a full demonstration of the delocalization transition has to be performed for a finite electron density system. Never-theless, the fact that the two-particle behavior fits nicely
with the delocalization scenario is encouraging.

CONCLUSIONS

The properties of the EE of two particle excited states in a one-dimensional ring were studied. For a clean system, the EE depends only on the difference in momentum between the two particles. If the difference is large the EE corresponds to the EE of two independent single particle states, i.e., \( S_A = -2[x \ln(x) + (1-x) \ln(1-x)] \). On the other hand, if the momenta are close, the EE of the two particle state is reduced compared to this value.

One may extrapolate that for \( m \) particles on a \( N \) site ring, as long as the density is low \( (m/N \ll 1) \), the upper limit of the EE is \( S_A = -m[x \ln(x) + (1-x) \ln(1-x)] \), which is also the typical value. This will be valid if the difference between the momenta of all particles taking part in a particular many-particle excited state is large. If this is not the case we expect the EE of the excited state to be lower. Further investigation of these cases is underway.

We have verified numerically that disorder reduces the EE. Short range particle interaction leads to an enhancement of the excited state EE, which become very significant once the localization length is of order of the system size. For high excitations the median EE of a many particle interacting excitation is not only above the disordered state to be lower. Further investigation of these cases is underway.

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