Corrections to universal Rényi entropy in quasiparticle excited states of quantum chains

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Abstract

We investigate the energy eigenstate Rényi entropy of generic bipartition in the fermionic, bosonic, and spin-1/2 XY chains. When the gap of the theory is large or all the momenta of the excited quasiparticles are large, the Rényi entropy takes a universal form, which is independent of the model, the quasiparticle momenta, and the subsystem connectedness. We calculate analytically the Rényi entropy in the extremely gapped limit and find different additional contributions to the universal Rényi entropy in various models. The corrections to the universal Rényi entropy cannot be neglected when the momentum differences of the excited quasiparticles are small. The Rényi entropy derived in the extremely gapped limit is still valid in the slightly gapped and even critical chains as long as all the momenta of the excited quasiparticles are large. In the case of double interval in the XY chain we find new universal results and their corrections. We call the result universal even though it is only valid for double interval in the spin-1/2 XY chain. In the case of the bosonic chain in the extremely massive limit we find analytically a novel formula for the Rényi entropy written as the permanent of a certain matrix. We support all of our analytical results with numerical calculations.
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1 Introduction

In the last couple of decades different measures of quantum entanglement have been used extensively to study different phases of the matter [1–4]. For a pure state, a good measure of entanglement is the entanglement entropy, which is just the von Neumann entropy of the reduced density matrix (RDM) and can be calculated as the analytical continuation of the Rényi entropy. The entanglement and Rényi entropies have been studied for various models in different situations. In this paper we will focus on one-dimensional quantum chains, whose subsystems can be one single interval, double disjoint intervals, or more disjoint intervals. Most of the early studies of the entanglement and Rényi entropies were focused on the ground state, for the single-interval cases see [5–26] and for multi-interval cases see [27–47]. One can also find various studies of the excited state entanglement and Rényi entropies in [48–69]. The excited states are natural generalizations of the ground state and are interesting for their own rights. The study of the entanglement in the individual excited states can be helpful in better understanding the equilibrium and dynamical properties of many-body quantum systems that can be well approximated by collective excitations, known as quasiparticles. They can be also useful in investigating the thermal states especially in lower temperatures. Moreover, the excite state Rényi entropy can be also measured in experiments following the setup in [70,71].

It is usually more desirable to look into the universal behaviors of the entanglement and Rényi entropies. The ground state entanglement entropy in a gapped model is usually proportional to the area of the subsystem [2], while the ground sate entanglement entropy in a critical quantum chain whose continuum limit gives a two-dimensional conformal field theory takes a universal logarithmic formula [8,13,16,17,19]. In a highly excited state the entanglement entropy usually behaves like the thermal entropy and has the form of the volume law [72–75]. The average entanglement entropy in the fermionic chains is also conjectured to take a particular universal volume law [76–81]. Recently, a novel form of universal entanglement and Rényi entropies in the excited state of quasiparticles was discovered in [60,61,63,64], see also for earlier partial results [51,53,58], which we will revisit in this work. We
As in [49, 50], we will use $|A\rangle$ and $|B\rangle$ to denote the ground state and the momentum. This is different from the convention in [60, 61, 63, 64], where the total number of exited particles are $n$. In this paper we consider the Rényi entropy of a subsystem $A$ of $\ell$ sites on a circular chain of $L$ sites in the scaling limit $L \to +\infty$ and $\ell \to +\infty$ with finite ratio $x = \frac{\ell}{L}$. The subsystem can be consecutive or be composed of double or more disjoint intervals as shown in figure 1. The whole system has the density matrix $\rho_K = |K\rangle\langle K|$. Then one can integrate out the degrees of freedom of the complement of $A$, which we denote by $B = \bar{A}$, and obtain the RDM $\rho_{A,K} = \text{tr}_B \rho_K$. Finally, the Rényi entropy of the state $|K\rangle$ is

$$S_{A,K}^{(n)} = -\frac{1}{n-1} \log \text{tr}_A \rho_{A,K}^n.$$  \hspace{1cm} (1.1)

As in [49, 50], we will use $\mathcal{F}_{A,K}^{(n)}$ to denote the difference between $S_{A,K}^{(n)}$ and the Rényi entropy $S_{A,G}^{(n)}$ for the ground state $|G\rangle$ as

$$S_{A,K}^{(n)} = S_{A,G}^{(n)} - \frac{1}{n-1} \log \mathcal{F}_{A,K}^{(n)}.$$  \hspace{1cm} (1.2)

Explicitly, one can write

$$\mathcal{F}_{A,K}^{(n)} = \frac{\text{tr}_A \rho_{A,K}^n}{\text{tr}_A \rho_{A,G}^n}.$$  \hspace{1cm} (1.3)

In an integrable many-body quantum system, an excited state can be written in a simple form with respect to the excited quasiparticles. A general quasiparticle excited state takes the form $|K\rangle = |k_1^{r_1}k_2^{r_2} \cdots k_s^{r_s}\rangle$, where the quasiparticle with momentum $k_i$ is excited $r_i$ times with $i = 1, 2, \cdots, s$. The total number of exited particles are $R = \sum_{i=1}^s r_i$. We use $k_i$ which is an integer or a half-integer as the momentum. This is different from the convention in [60, 61, 63, 64], where $p_i = \frac{2\pi k_i}{L}$ is used as the momentum. Actually, $k_i$ is the total number of waves in the circular chain, and $p_i$ is the physical momentum. The universal Rényi entropy of the state $|k_1^{r_1}k_2^{r_2} \cdots k_s^{r_s}\rangle$ is [60, 61, 63, 64]

$$\mathcal{F}_{A,p_1^{r_1}p_2^{r_2} \cdots p_s^{r_s}}^{(n), \text{univ}} = \prod_{i=1}^s \left\{ \sum_{p=0}^{r_i} \binom{p}{r_i} x^p (1-x)^{r_i-p} \right\}^n,$$  \hspace{1cm} (1.4)

where $\binom{p}{r_i}$ is the binomial coefficient. The above equation is derived in the limit that $L \to +\infty$, $\ell \to +\infty$, $k_i \to +\infty$ with finite fixed $x = \frac{\ell}{L}$, $p_i = \frac{2\pi k_i}{L}$. \footnote{We thank Olalla Castro-Alvaredo, Cecilia De Fazio, Benjamin Doyon and István Szécsényi for explaining to us the precise limit they have used in [60, 61, 63].}

Figure 1: A subsystem made of a single interval (left) and a subsystem made of double disjoint intervals (right) on a circular chain of $L$ sites. For the single interval $A$ the length is $|A| = \ell$, and it is convenient to define $x = \frac{\ell}{L}$. For the double interval $A = A_1 \cup A_2$ the lengths are $|A_1| = \ell_1$, $|A_2| = \ell_2$, $|B_1| = d_1$, $|B_2| = d_2$, and one can define the parameters $x_1 = \frac{\ell_1}{L}$, $x_2 = \frac{\ell_2}{L}$, $y_1 = \frac{d_1}{L}$, $y_2 = \frac{d_2}{L}$, $x = x_1 + x_2$, $y = y_1 + y_2$. We have reported some of the results in the letter [82], and will present the details with additional novel results in this work.
to denote the universal Rényi entropy to emphasize the different limit that was used in [60,61,63]. The universal Rényi entropy is valid when either the correlation length $\frac{1}{\Delta}$ of the model or the maximal de Broglie wavelength of the quasiparticles is much smaller than the sizes of the subsystems but one does not need to require both, i.e. that it requires [60,61,63]

$$\min \left[ \frac{1}{\Delta}, \max_i \left( \frac{L}{|k_i|} \right) \right] \ll \min(\ell, L - \ell).$$

(1.5)

In other words, one needs either the gap $\Delta$ of the model is large or all the momenta of the excited quasiparticles are large. The universal Rényi entropy is independent of the model, the momenta of the quasiparticles, and the subsystem connectedness.

In this paper we will calculate the Rényi entropy of single and double intervals in the quasiparticle excited state $|K\rangle = |k_{r1} k_{r2} \cdots k_{rs}\rangle$ with general momenta $k_i$ in the fermionic, bosonic and XY chains. We calculate analytically the Rényi entropy in the single-particle, double-particle and triple-particle states in the extremely gapped limit by writing the excited states in terms of subsystem excitations, which we call subsystem mode method, and find different additional contributions to the universal Rényi entropy (1.4) in different models, and the new results with correction terms match perfectly with the numerical results calculated from other methods. The corrections to the universal Rényi entropy cannot be neglected when the momentum differences of the excited quasiparticles are small and are negligible when all the momentum differences are large

$$\min_{i_1 \neq i_2} |k_{i_1} - k_{i_2}| \gg 1.$$  

(1.6)

We also compare the Rényi entropy with additional correction terms derived in the extremely gapped limit with the numerical results in the corresponding slightly gapped and critical models and find that the new Rényi entropy is still valid as long as all the momenta of the excited quasiparticles are large. The validity of the universal Rényi entropy (1.4) found in [60,61,63,64] requires both (1.5) and (1.6), while the validity of the Rényi entropy with corrections we report in this paper only requires the condition (1.5). In a slightly gapped or critical model, the validity of the universal Rényi entropy requires that both all the quasiparticle momenta and all the momentum differences are large, while the validity of the Rényi entropy with additional corrections only requires all the momenta are large.

The remaining part of the paper is arranged as follows: In section 2 we summarize the main results of this paper. In section 3 we investigate the single-interval and double-interval Rényi entropies in the single-particle, double-particle, and triple-particle states in the fermionic chain. In section 4 we consider the Rényi entropies in the bosonic chain. In section 5 we consider the Rényi entropies in the XY chain. We conclude with discussions in section 6. In appendix A, we review the wave function method to calculate the Rényi entropy in the bosonic chain and we also further adapt the method to the extremely gapped limit.

## 2 Summary of results

In this section, we summarize the main results of this paper which will be presented in full detail in sections 3, 4 and 5.
In section 3, we investigate the Rényi entropy in the excited states of quasiparticles in the fermionic chain. We focus on the cases of the single interval and double interval. The generalization to multiple intervals is easy and we will not show details in this paper. We consider the single-particle state $|k\rangle$, double-particle state $|k_1k_2\rangle$ and triple-particle state $|k_1k_2k_3\rangle$. Analytically we calculate the Rényi entropy $\mathcal{F}_{A,K}^{(n)}$, and we find the additional corrections $\delta\mathcal{F}_{A,K}^{(n)}$ to the universal Rényi entropy $\mathcal{F}_{A,P}^{(n),\text{univ}}$.

\begin{equation}
\mathcal{F}_{A,K}^{(n)} = \mathcal{F}_{A,P}^{(n),\text{univ}} + \delta\mathcal{F}_{A,K}^{(n)}.
\end{equation}

Explicitly, we get $\mathcal{F}_{A,k}^{(n)} = \mathcal{F}_{A,p}^{(n),\text{univ}}$ with general $n$, for which there is no additional contribution. We also get the Rényi entropy $\mathcal{F}_{A,k_1k_2}^{(n)}$ with $n = 2,3,\cdots,7$ and $\mathcal{F}_{A,k_1k_2k_3}^{(n)}$ with $n = 2,3,4,5$. We compare the universal Rényi entropy and the corrected Rényi entropy with the numerical results calculated using the correlation functions [12–15,48–50]. We find perfect matches between the corrected Rényi entropy with the numerical results. In the limit of small momentum differences the additional terms are significant and cannot be neglected, while in the limit of large momentum differences the additional terms are negligible. We check that Rényi entropy with corrections is still valid for slightly gapped and even critical fermionic chains as long as all the quasiparticle momenta are large.

In section 4, we investigate the single-interval and double-interval Rényi entropies in the multi-particle state with the same momenta $|k^n\rangle$, double-particle state $|k_1k_2\rangle$, triple-particle state $|k_1^2k_2\rangle$ and triple-particle state $|k_1k_2k_3\rangle$ in the bosonic chain. In the extremely gapped limit, we calculate the analytical Rényi entropy using two different methods: one is by writing the excited states in terms of subsystem excitations, i.e. the subsystem mode method, similar to that in the fermionic chain, and the other is the wave function method. Explicitly, we get $\mathcal{F}_{A,k}^{(n)} = \mathcal{F}_{A,p}^{(n),\text{univ}}$ with general $n$, for which there is no additional contribution. We also get the analytical Rényi entropy $\mathcal{F}_{A,k_1k_2}^{(n)}$ with $n = 2,3,\cdots,7$, $\mathcal{F}_{A,k_1^2k_2}^{(n)}$ with $n = 2,3,\cdots,7$ and $\mathcal{F}_{A,k_1k_2k_3}^{(n)}$ with $n = 2,3,4,5$, which are still valid in the slightly gapped bosonic chains as long as all the quasiparticle momenta are large.

In section 5, we investigate the single-interval and double-interval Rényi entropies in the single-particle state $|k\rangle$ and double-particle state $|k_1k_2\rangle$ in the XY chain. The XY chain can be mapped to the fermionic chain that we investigate in section 3, but they have different local degrees of freedoms. The single-interval Rényi entropy in the XY chain is the same as that in the fermionic chain, while the double-interval Rényi entropy is very different. There is no additional contribution to the universal double-interval Rényi entropy in the single-particle state $|k\rangle$. It is remarkable that we find a new universal double-interval Rényi entropy in the double-particle state $|k_1k_2\rangle$, for which there are also additional corrections when the momentum difference $|k_1 - k_2|$ is small. We find that the analytical Rényi entropy, which is the new universal Rényi entropy plus the additional corrections terms, shows perfect match with the numerical results in the extremely gapped limit. When the momentum difference $|k_1 - k_2|$ is large, the Rényi entropy approaches the new universal Rényi entropy instead of the old one. The double-interval Rényi entropy is still valid in the slightly gapped XY chains as long as all the quasiparticle momenta are large. But in the critical XY chains we find that all the known analytical results do not match the numerical ones, for which we do not have a good explanation.

The derived corrected Rényi entropy depends on the model, the quasiparticle momenta, and the
subsystem connectedness. The corrected Rényi entropy depends on the momenta only through the momentum differences. It is exact in the extremely gapped limit of the fermionic, bosonic, and XY chains for arbitrary sizes of the whole system and the subsystem. In the fermionic and XY chains, the universal Rényi entropy derived in the extremely gapped limit is still exactly valid in the critical but non-relativistic model with $\gamma = 0$, $\lambda = 1$.

One highlight of the paper is that we establish the determinant formula (3.68) in the extremely gapped fermionic chain and the permanent formula (4.37) in the extremely gapped bosonic chain, which are very efficient for both analytical and numerical calculations of the Rényi entropy in the quasiparticle excited state.

3 Fermionic chain

We consider the Hamiltonian of fermionic chain of $L$ sites

$$H = \sum_{j=1}^{L} \left[ \lambda \left( a_j^\dagger a_j - \frac{1}{2} \right) - \frac{1}{2} \left( a_{j+1}^\dagger a_{j+1} + a_j^\dagger a_j \right) - \frac{\gamma}{2} \left( a_{j+1}^\dagger a_{j+1} + a_{j+1} a_j \right) \right],$$

with periodic or antiperiodic boundary conditions for the spinless fermions $a_j$, $a_j^\dagger$. It can be diagonalized as

$$H = \sum_k \varepsilon_k \left( c_k^\dagger c_k - \frac{1}{2} \right), \quad \varepsilon_k = \sqrt{\left( \lambda - \cos \frac{2\pi k}{L} \right)^2 + \gamma^2 \sin^2 \frac{2\pi k}{L}},$$

by the successive Fourier transformation and Bogoliubov transformation [83–85]

$$b_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ij\varphi_k} a_j, \quad b_k^\dagger = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ij\varphi_k} a_j^\dagger,$$

$$c_k = b_k \cos \frac{\theta_k}{2} + ib_{-k}^\dagger \sin \frac{\theta_k}{2}, \quad c_k^\dagger = b_k^\dagger \cos \frac{\theta_k}{2} - ib_{-k} \sin \frac{\theta_k}{2},$$

with the definitions

$$\varphi_k = \frac{2\pi k}{L}, \quad e^{i\theta_k} = \frac{\lambda - \cos \varphi_k + i\gamma \sin \varphi_k}{\varepsilon_k}.$$ (3.5)

In this paper we only consider the cases that $L$'s are even integers, and we also only consider the states in the Neveu-Schwarz (NS) sector, i.e. the antiperiodic boundary conditions for the fermionic modes $a_j$, $a_j^\dagger$. In fact, all the results we obtain in this paper are still valid for the states in the Ramond sector too. We have the half-integer momenta

$$k = \frac{1 - L}{2}, \cdots, -\frac{1}{2}, \frac{1}{2}, \cdots, \frac{L - 1}{2}.$$ (3.6)

The ground state $|G\rangle$ is annihilated by all the lowering operators

$$c_k |G\rangle = 0,$$ (3.7)

and the excited states are generated by applying the raising operators with different momenta on the ground state

$$|k_1 k_2 \cdots k_s\rangle = c_{k_1}^\dagger c_{k_2}^\dagger \cdots c_{k_s}^\dagger |G\rangle.$$ (3.8)
We consider the extremely gapped limit $\lambda \rightarrow +\infty$ of the fermionic chain. The Hamiltonian becomes

$$H = \lambda \sum_{j=1}^{L} \left( a_j^\dagger a_j - \frac{1}{2} \right),$$

(3.9)

and the fermions $a_j, a_j^\dagger$ at different positions decouple from each other. The Bogoliubov angle is vanishing $\theta_k = 0$, and we have

$$c_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ij\varphi_k} a_j, \quad c_k^\dagger = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ij\varphi_k} a_j^\dagger.$$  

(3.10)

The ground state is also annihilated by all the local lowering operators $a_j$

$$a_j |G\rangle = 0, \quad j = 1, 2, \ldots, L.$$  

(3.11)

### 3.1 Single interval

We consider an interval with $\ell$ consecutive sites $A = [1, \ell]$ on the periodic fermionic chain with $L$ sites. In the extremely gapped limit $\lambda \rightarrow +\infty$, the ground state is just a direct product state

$$|G\rangle = |G_A\rangle|G_B\rangle,$$

(3.12)

and the ground state Rényi entropy is vanishing

$$S_{A,G}^{(n)} = 0.$$  

(3.13)

In the limit $L \rightarrow +\infty, \ell \rightarrow +\infty, k_i \rightarrow +\infty$ with fixed $x = \frac{\ell}{L}, p_i = \frac{2\pi k_i}{L}$, the Rényi entropy for the excited state $|k_1 k_2 \cdots k_s\rangle$ takes the universal form [60,61,63,64]

$$F_{A,p_1 p_2 \cdots p_s}^{(n),\text{univ}} = \left[ x^n + (1-x)^n \right]^s.$$  

(3.14)

The universal Rényi entropy leads to the universal entanglement entropy

$$S_{A,p_1 p_2 \cdots p_s}^{\text{univ}} = s \left[ -x \log x - (1-x) \log(1-x) \right].$$  

(3.15)

In general this does not apply to an excited state with arbitrary $s$ as there is an upper bound for the entanglement entropy

$$S_{A,p_1 p_2 \cdots p_s}^{\text{univ}} \leq \min(\ell, L - \ell) \log 2.$$  

(3.16)

It gives an upper bound of the number of the excited quasiparticles

$$\frac{s}{L} \leq \frac{\min(x, 1-x) \log 2}{-x \log x - (1-x) \log(1-x)},$$  

(3.17)

which we show in figure 2. This is not surprising, since as stated in [60] there should be finite number of excited quasiparticles for the universal entanglement and Rényi entropies to be valid. In the following, we will relax the constraint for the momenta $k_i$ and find the nontrivial additional contributions $\delta F_{A,k_1 k_2 \cdots k_s}^{(n)}$ to the universal Rényi entropy

$$F_{A,k_1 k_2 \cdots k_s}^{(n)} = F_{A,p_1 p_2 \cdots p_s}^{(n),\text{univ}} + \delta F_{A,k_1 k_2 \cdots k_s}^{(n)}.$$  

(3.18)
The entanglement and Rényi entropies in the fermionic chain can be calculated numerically using the two-point correlation functions [12–15, 48–50]. We denote the general excited state $|k_1, k_2, \cdots, k_s\rangle$ by the set of excited momenta $K = \{k_1, k_2, \cdots, k_s\}$. One can define the Majorana modes as
\[d_{2j-1} = a_j + a_{j}^\dagger, \quad d_{2j} = i(a_j - a_{j}^\dagger).\] (3.19)

For the interval $A = [1, \ell]$ on the fermionic chain in excited state $|K\rangle$, one defines the $2\ell \times 2\ell$ correlation matrix
\[\langle d_{m_1} d_{m_2}\rangle_K = \delta_{m_1 m_2} + \Gamma^K_{m_1 m_2}, \quad m_1, m_2 = 1, 2, \cdots, 2\ell.\] (3.20)

The $\Gamma^K$ matrix which is antisymmetric and purely imaginary has entries
\[
\Gamma^K_{2j_1 - 1, 2j_2 - 1} = \Gamma^K_{2j_1, 2j_2} = f^K_{j_2 - j_1}, \quad \Gamma^K_{2j_1 - 1, 2j_2} = -\Gamma^K_{2j_2, 2j_1 - 1} = g^K_{j_2 - j_1},
\] (3.21)

where we defined the functions
\[
f^K_j = \frac{2i}{L} \sum_{k \in K} \sin(j\varphi_k), \quad g^K_j = -\frac{i}{L} \sum_{k \notin K} \cos(j\varphi_k - \theta_k) + \frac{i}{L} \sum_{k \in K} \cos(j\varphi_k - \theta_k).
\] (3.22)

In terms of the $2\ell$ eigenvalues $\pm \gamma^K_j$, $j = 1, 2, \cdots, \ell$, of the correlation matrix $\Gamma^K$, the entanglement and Rényi entropies of the length $\ell$ interval in state $K$ is
\[
S_{A,K} = \sum_{j=1}^{\ell} \left( -\frac{1 + \gamma^K_j}{2} \log_{2} \frac{1 + \gamma^K_j}{2} - \frac{1 - \gamma^K_j}{2} \log_{2} \frac{1 - \gamma^K_j}{2} \right), \quad S^{(n)}_{A,K} = -\frac{1}{n - 1} \sum_{j=1}^{\ell} \log \left[ \left( \frac{1 + \gamma^K_j}{2} \right)^n + \left( \frac{1 - \gamma^K_j}{2} \right)^n \right].
\] (3.23)

In the extremely gapped limit $\lambda \rightarrow +\infty$, there is vanishing Bogoliubov angle $\theta_k = 0$. One can also define the $\ell \times \ell$ correlation matrix $C^K_A$ with the entries
\[
[C^K_A]_{j_1 j_2} = \langle c_{j_1}^\dagger c_{j_2}\rangle_K = h^K_{j_2 - j_1}, \quad j_1, j_2 = 1, 2, \cdots, \ell,
\] (3.24)

and the function
\[
h^K_j = \frac{1}{L} \sum_{k \in K} e^{ij\varphi_k},
\] (3.25)
and calculate the entanglement and Rényi entropies from the eigenvalues \( \nu_j^K \), \( j = 1, 2, \cdots, \ell \), of the correlation matrix \( C^K_A \) as

\[
S_{A,K} = \sum_{j=1}^\ell \left[ -\nu_j^K \log \nu_j^K - (1 - \nu_j^K) \log(1 - \nu_j^K) \right],
\]

\[
S_{A,K}^{(n)} = -\frac{1}{n-1} \sum_{j=1}^\ell \log \left[ (\nu_j^K)^n + (1 - \nu_j^K)^n \right].
\]

For the following analytical calculations of the Rényi entropy it is convenient to define the subsystem modes in the extremely gapped limit

\[
c_{A,k} = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{i j \varphi_k} a_j, \quad c_{A,k}^\dagger = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{-i j \varphi_k} a_j^\dagger,
\]

\[
c_{B,k} = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{i j \varphi_k} a_j, \quad c_{B,k}^\dagger = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{-i j \varphi_k} a_j^\dagger.
\]

There are anti-commutation relations

\[\{c_{A,k}, c_{A,k}^\dagger\} = x, \quad \{c_{B,k}, c_{B,k}^\dagger\} = 1 - x,\]

and for \( k_1 \neq k_2 \) we have

\[\{c_{A,k_1}, c_{A,k_2}^\dagger\} = -\{c_{B,k_1}, c_{B,k_2}^\dagger\} = \alpha_{k_1-k_2},\]

with

\[\alpha_k = \frac{1}{L} \sum_{j=1}^\ell e^{2\pi i j k} \frac{e^{\frac{ni(L+1)k}{L}} - 1}{e^{\frac{\pi k}{L}} L \sin \frac{\pi k}{L}}.\]

3.1.1 Single-particle state \(|k\rangle\)

In the single-particle state \(|k\rangle\) of the extremely gapped fermionic chain, we write the density matrix of the whole system in terms of the subsystem modes

\[
\rho_k = (c_{A,k}^\dagger + c_{B,k}^\dagger)|G\rangle\langle G|(c_{A,k} + c_{B,k}).
\]

Tracing out the degrees of freedom of \( B \), we get the RDM

\[
\rho_{A,k} = c_{A,k}^\dagger|G_A\rangle\langle G_A|c_{A,k} + \langle c_{B,k} c_{B,k}^\dagger |G_A\rangle\langle G_A|.\]

We have used \( \text{tr}_B(c_{A,k}^\dagger |G\rangle\langle G|c_{B,k}) = \text{tr}_B(c_{B,k}^\dagger |G\rangle\langle G|c_{A,k}) = 0 \). Then we get

\[
\text{tr}_{A} \rho_{A,k}^n = \langle c_{A,k} c_{A,k}^\dagger \rangle^n_G + \langle c_{B,k} c_{B,k}^\dagger \rangle^n_G = x^n + (1 - x)^n.
\]

There is no additional contribution to the universal Rényi entropy in the single-particle state \(|k\rangle\). The analytical results match the numerical ones, which has been checked in [60,61], and we will not show the details here.

Since the subsystem modes play a crucial role in the analytical calculations we call the procedure the subsystem mode method.
3.1.2 Double-particle state $|k_1k_2\rangle$

In the double-particle state $|k_1k_2\rangle$ with general momenta $k_1, k_2$, we write the density matrix of the whole system as

$$\rho_{k_1k_2} = (c_{A,k_1}^\dagger + c_{B,k_1}^\dagger)(c_{A,k_2} + c_{B,k_2})|G\rangle\langle G|(c_{A,k_2} + c_{B,k_2})(c_{A,k_1} + c_{B,k_1}),$$

then we get the RDM

$$\rho_{A,k_1k_2} = c_{A,k_1}^\dagger c_{A,k_2}|G\rangle\langle G|c_{A,k_2} + c_{B,k_1}^\dagger c_{B,k_1}^\dagger G_{A,k_2} + c_{B,k_1}G_{A,k_1} - c_{B,k_1}c_{B,k_2}^\dagger G_{A,k_1} - G_{A,k_1}c_{A,k_2} - (c_{B,k_2}c_{B,k_1})^\dagger G_{A,k_1} - G_{A,k_1}c_{A,k_2}.$$  \hspace{1cm} (3.35)

The sign of each term can be determined by tr$\rho_{k_1k_2} = tr\rho_{A,k_1k_2}$. Note the minus signs due to the anti-commutation relations of the modes. Then one can calculate tr$\rho_{A,k_1k_2}^n$ with $n = 2, 3, 4, 5, 6, 7$. Explicitly, we get the nontrivial additional contributions to the universal Rényi entropy (3.14)

$$\delta F_{A,k_1k_2}^{(2)} = 8x(1 - x)\alpha^2_{12} + 4\alpha^4_{12},$$

$$\delta F_{A,k_1k_2}^{(3)} = -3(1 - 6x + 6x^2)\alpha^2_{12} + 9\alpha^4_{12},$$

$$\delta F_{A,k_1k_2}^{(4)} = -4(1 - 6x + 12x^2 - 16x^3 + 18x^4 - 12x^5 + 4x^6)\alpha^2_{12}$$

$$+ 8(1 + 3x - 2x^2 + 3x^3)\alpha^4_{12} + 8(1 + 2x - 2x^2)\alpha^6_{12} + 4\alpha^8_{12},$$

$$\delta F_{A,k_1k_2}^{(5)} = -5(1 - 8x + 28x^2 - 60x^3 + 80x^4 - 60x^5 + 20x^6)\alpha^2_{12}$$

$$+ 10(1 - 5x + 20x^2 - 30x^3 + 15x^4)\alpha^4_{12} + 100x(1 - x)\alpha^6_{12} + 25\alpha^8_{12},$$  \hspace{1cm} (3.39)

as well as $\delta F_{A,k_1k_2}^{(n)}$ with $n = 6, 7$ which we will not show in this paper. In the above expressions we have defined the shorthand $\alpha_{12} \equiv |\alpha_{k_1-k_2}|$ with the function $\alpha_k$ defined in (3.30). We see that the results become increasingly complex for higher Rényi indices $n$.

We plot the absolute value of the function $\alpha_k$ (3.30) in figure 3, and we see that it is nonnegligible for a small $k$ but it goes to zero rapidly by increasing the $k$. Note that we have already taken the limit $L \rightarrow +\infty$, $\ell \rightarrow +\infty$ with fixed $x = \ell / L$. We compare the results of the universal Rényi entropy, the analytical results with additional correction terms and the numerical results for the state $|k_1k_2\rangle$ in figure 4. We find perfect matches of the new Rényi entropy with additional corrections with the numerical results. For a small momentum difference $|k_1 - k_2|$ the additional terms are significant. For a large momentum difference $|k_1 - k_2|$ the additional terms can be neglected.

In fact, the result $F_{A,k_1k_2}^{(2)} = F_{A,p_1p_2}^{(2),\text{univ}} + \delta F_{A,k_1k_2}^{(2)}$ with the universal Rényi entropy (3.14) and the additional corrections (3.36) could be retrieved in the supplementary material of [60] by relaxing the constraint for the quasiparticle momenta. We identify the parameters $r, \varphi, p_1, p_2$ in the supplementary material of [60] as $r = x$, $\varphi = \pi$, $p_1 = \frac{2\pi k_1}{L}$, $p_2 = \frac{2\pi k_2}{L}$. Note that in our convention $k_1 - k_2$ is a general integer that can be either small or large. We get from Eq. (33) therein

$$N = L^2,$$  \hspace{1cm} (3.40)
Figure 3: The absolute value of the function $\alpha_k$ (3.30) decreases with the increase of $k$. We have set $L = 64$.

from Eq. (47) therein
\[
\frac{1}{N^2} \text{Tr} A((\rho_A^{(1)})^2) = (x^2 - \alpha_{12}^2)^2, \quad (3.41)
\]

from Eq. (49) therein
\[
\frac{1}{N^2} \text{Tr} A((\rho_A^{(2)})^2) = [(1 - x)^2 - \alpha_{12}^2]^2, \quad (3.42)
\]

and from Eq. (54) therein
\[
\frac{1}{N^2} \text{Tr} A((\rho_A^{(3)})^2) = 2x^2(1 - x)^2 + 2(1 + 2x - 2x^2)\alpha_{12}^2 + 2\alpha_{12}^4. \quad (3.43)
\]

Summing (3.41), (3.42), and (3.43) we get the Rényi entropy consistent with (3.36)
\[
\mathcal{F}_{A,k_1,k_2}^{(2)} = [x^2 + (1 - x)^2]^2 + 8x(1 - x)\alpha_{12}^2 + 4\alpha_{12}^4. \quad (3.44)
\]
For $k_1 - k_2$ being a fixed finite integer, $\alpha_{12}$ is not vanishing in the limit $L \to +\infty$, $\ell \to +\infty$ with fixed $x = \frac{\ell}{L}$
\[
\alpha_{12} \to \left| \frac{\sin[\pi(k_1 - k_2)x]}{\pi(k_1 - k_2)} \right|. \quad (3.45)
\]
So generally the additional terms cannot be neglected. On the other hand, for a large difference of the momenta $|k_1 - k_2| \to +\infty$ in the limit $L \to +\infty$, $\ell \to +\infty$ with fixed $x = \frac{\ell}{L}$,
\[
\alpha_{12} \to 0, \quad (3.46)
\]
and the universal entanglement and Rényi entropies in [60,61,63,64] are valid.

3.1.3 Triple-particle state $|k_1k_2k_3\rangle$

The calculations of the Rényi entropy in the triple-particle state $|k_1k_2k_3\rangle$ with general momenta $k_1, k_2, k_3$ are similar to the above. We will not show the details here. We get the additional contributions to the universal Rényi entropy
\[
\delta\mathcal{F}_{A,k_1,k_2,k_3}^{(2)} = 8x(1 - x)(1 - 2x + 2x^2)(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2) + 8(1 - 2x)(1 + 2x - 2x^2)\alpha_{12}\alpha_{13}\alpha_{23} + 4(1 - 2x + 2x^2)(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2)^2 + 16(1 - 2x)\alpha_{12}\alpha_{13}\alpha_{23}(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2) + 32\alpha_{12}^2\alpha_{13}^2\alpha_{23}^2. \quad (3.47)
\]
Figure 4: The universal Rényi entropy (“univ”, dotted lines), and the analytical (“ana”, solid lines) and numerical (“num”, empty circles) results of the single-interval Rényi entropy in the double-particle state $|k_1k_2\rangle$ in the extremely gapped fermionic chain. We use different colors to represent different Rényi indices $n$. We have set $\lambda = +\infty$, $L = 64$.

as well as $\delta F^{(n)}_{A,k_1k_2k_3}$ with $n = 3, 4, 5$ which we will not show in this paper. Note that we have defined the shorthand $\alpha_{i1i2} \equiv |\alpha_{k_1-i_2}|$ with the function (3.30). We compare the results of the universal Rényi entropy, the analytical results with additional corrections and the numerical results for the state $|k_1k_2k_3\rangle$ in the figure 5. We find perfect matches between the new analytical results and the numerical ones.

3.1.4 Slightly gapped and critical fermionic chains

We have calculated the analytical expressions of the Rényi entropy in the extremely gapped fermionic chain, and found a good matching with the numerical results. We wonder if the results apply to excited states of quasiparticles in the slightly gapped and even critical fermionic chains. We compare the results of the universal Rényi entropy, the results with additional corrections, and the numerical results in the double-particle state $|k_1k_2\rangle$ and the triple-particle state $|k_1k_2k_3\rangle$ in the slightly gapped and critical fermionic chains in the figures 6 and 7. We see that the results of the Rényi entropy with the additional corrections are universal in the sense that they are still valid as long as all the momenta of the excited quasiparticles and the size of the system $L$ are large.

Especially, for the special fermionic chain with $\gamma = 0, \lambda = 1$, which is critical but non-relativistic, the new Rényi entropy with additional terms is exact even for small $L$, $\ell$. This is because for $\gamma = 0, \lambda = 1$ the Bogoliubov angle defined in (3.5) is also vanishing $\theta_k = 0$, the same as that in the extremely gapped
fermionic chain.

In section 6 we will quantify the convergence of the results of slightly gapped cases to the extremely gapped cases in more detail.

3.2 Double interval

We consider the double interval on a circular fermionic chain as shown in figure 1. The universal Rényi entropy does not depend on the connectedness of the subsystem, and so the double-interval Rényi entropy in the quasiparticle excited states only depends on \( x = x_1 + x_2 \), not on \( x_1 - x_2 \) or \( y_1 \). We will show both analytically and numerically that generally the Rényi entropy would depend on all the independent parameters \( x_1, x_2, y_1 \) if one relaxes the constraints on the momenta \( k_i \).

For the double-interval with \( A = A_1 \cup A_2 \) and \( B = B_1 \cup B_2 \), in the extremely gapped limit we can still define the subsystem modes

\[
\begin{align*}
c_{A,k} & = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{i j \varphi_k} a_j, \quad c_{A,k}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{-i j \varphi_k} a_j^{\dagger}, \\
c_{B,k} & = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{i j \varphi_k} a_j, \quad c_{B,k}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{-i j \varphi_k} a_j^{\dagger}.
\end{align*}
\]

(3.48)

There are anti-commutation relations

\[
\{ c_{A,k}, c_{A,k}^{\dagger} \} = x, \quad \{ c_{B,k}, c_{B,k}^{\dagger} \} = y.
\]

(3.49)
Figure 6: The universal Rényi entropy (dotted lines), the analytical single-interval Rényi entropy in the extremely gapped fermionic chain (solid lines), and the numerical single-interval Rényi entropy in the slightly gapped and critical fermionic chains (symbols) in the double-particle state $|k_1k_2\rangle$. We have set the momenta $(k_1, k_2) = (\frac{1}{2}, \frac{3}{2}) + \frac{i}{L}$, so that $k_i \to +\infty$ in the limit $L \to +\infty$, which is essential for the critical chains but is not important for the slightly gapped chains. For the analytical Rényi entropy we have set $L = +\infty$. 

Figure 7: The universal Rényi entropy (dotted lines), the analytical single-interval Rényi entropy in the extremely gapped fermionic chain (solid lines), and the numerical single-interval Rényi entropy (symbols) in the slightly gapped and critical fermionic chains in the triple-particle state $|k_1 k_2 k_3\rangle$. We have set the momenta $(k_1, k_2, k_3) = (\frac{1}{2}, \frac{3}{2}, \frac{5}{2}) + \frac{L}{8}$. For the analytical Rényi entropy we have set $L = +\infty$. 
and for $k_1 \neq k_2$ we have
$$\{c_{A,k_1}, c_{A,k_2}^\dagger\} = -\{c_{B,k_1}, c_{B,k_2}^\dagger\} = \beta_{k_1-k_2},$$
where we have defined
$$\beta_k = \frac{1}{L} \sum_{j \in A_1 \cup A_2} e^{\frac{2\pi i j k}{L}} = e^{\frac{\pi i k(\ell_1+1)}{L}} \sin \frac{\pi k}{L} \sin \frac{\pi \ell_1}{L} + e^{\frac{\pi i k(\ell_1+2\ell_2 + \ell_2)}{L}} \sin \frac{\pi k}{L} \sin \frac{\pi \ell_2}{L}.$$  \tag{3.51}

### 3.2.1 Single-particle state $|k\rangle$

The calculations and the results are the same as those for the single-interval Rényi entropy in subsection (3.1.1). There is no additional contribution to the universal double-interval Rényi entropy in the single-particle state $|k\rangle$.

### 3.2.2 Double-particle state $|k_1k_2\rangle$

The calculations of the double-interval Rényi entropy in the double-particle state $|k_1k_2\rangle$ are similar to those for the single-interval Rényi entropy in subsection 3.1.2. The results are just the ones in subsection 3.1.2 after the following substitution
$$|\alpha_{k_1-k_2}| \rightarrow |\beta_{k_1-k_2}|,$$
where $\beta_k$ is defined in (3.51). For example, we have
$$\delta F^{(2)}_{A_1A_2,k_1k_2} = 8x(1-x)|\beta_{k_1-k_2}|^2 + 4|\beta_{k_1-k_2}|^4,$$
$$\delta F^{(3)}_{A_1A_2,k_1k_2} = -3(1-6x + 6x^2)|\beta_{k_1-k_2}|^2 + 9|\beta_{k_1-k_2}|^4.$$

We compare the analytical and numerical results in figure 8. We see the necessity of the additional correction terms when the momentum difference $|k_1 - k_2|$ is small.

### 3.2.3 Triple-particle state $|k_1k_2k_3\rangle$

The calculations of the double-interval Rényi entropy in the triple-particle state $|k_1k_2k_3\rangle$ are similar to those presented before. We get the additional contributions to the universal Rényi entropy
$$\delta F^{(2)}_{A_1A_2,k_1k_2k_3} = 8x(1-3x + 4x^2 - 2x^3)|\gamma_{k_1k_2k_3}| + 4(1-6x^2 + 4x^3)|\delta_{k_1k_2k_3}^2 + 4(1-2x + 2x^2)|\gamma_{k_1k_2k_3}| + 8(1-2x)|\gamma_{k_1k_2k_3}| \delta_{k_1k_2k_3} + 8\delta_{k_1k_2k_3}^2,$$
$$\delta F^{(3)}_{A_1A_2,k_1k_2k_3} = -3(1-9x + 27x^2 - 36x^3 + 18x^4)|\gamma_{k_1k_2k_3}| + 27x(1-3x + 2x^2)|\delta_{k_1k_2k_3} + 9(1-3x + 3x^2)|\gamma_{k_1k_2k_3}| + 27(1-2x)|\gamma_{k_1k_2k_3} \delta_{k_1k_2k_3} + 27\delta_{k_1k_2k_3}^2,$$
with the definitions
$$\gamma_{k_1k_2k_3} = |\beta_{k_1-k_2}|^2 + |\beta_{k_1-k_3}|^2 + |\beta_{k_2-k_3}|^2,$$
$$\delta_{k_1k_2k_3} = \beta_{k_1-k_2} \beta_{k_2-k_3} \beta_{k_3-k_1} + \beta_{k_1-k_3} \beta_{k_3-k_2} \beta_{k_2-k_1}.$$  \tag{3.57}

We also get $\delta F^{(n)}_{A_1A_2,k_1k_2k_3}$ with $n = 4,5$, which we will not show in this paper. We compare the analytical and numerical results in the figure 9. There are perfect matches between the results of the Rényi entropy with the numerical ones.
Figure 8: The universal Rényi entropy (dotted lines), and the analytical (solid lines) and numerical (empty circles) results of the double-interval Rényi entropy in the double-particle state $|k_1k_2\rangle$ in the extremely gapped fermionic chain. We have set $\lambda = +\infty$, $L = 64$. 

\[
\mathcal{F}_{A_1A_2,k_1k_2}(n) = \begin{cases} 
\frac{1}{2}, & n = 2, \\
\frac{3}{4}, & n = 3, \\
\frac{7}{8}, & n = 4, \\
\frac{1}{16}, & n = 5.
\end{cases}
\]
Figure 9: The universal Rényi entropy (dotted lines), and the analytical (solid lines) and numerical (empty circles) results of the double-interval Rényi entropy in the triple-particle state $|k_1k_2k_3\rangle$ in the extremely gapped fermionic chain. We have set $\lambda = +\infty, \ L = 64.$
3.2.4 Slightly gapped and critical fermionic chains

We calculate the double-interval Rényi entropy in the slightly gapped and critical fermionic chains, and find that the results with additional terms are still valid in the limit that all the quasiparticle momenta are large. The results are shown in the figures 10 and 11. As before, the universal Rényi entropy is exact for the fermionic chain with $\gamma = 0, \lambda = 1$.

3.3 Multiple intervals

The generalization from double interval to multiple intervals is easy. We just need to change $\beta_k$ defined in (3.51) to

$$\beta_k = \frac{1}{L} \sum_{j \in A} e^{2\pi i kj}, \quad (3.58)$$

where $A$ can be made of arbitrary number of disjoint intervals.

3.3.1 Rényi entropy

In the single-particle state $|k\rangle$, there is no additional contribution to the universal Rényi entropy. In the double-particle state $|k_1k_2\rangle$ and triple-particle state $|k_1k_2k_3\rangle$, the expressions of the Rényi entropy are the same as those in the subsection 3.2.2 and subsection 3.2.3, respectively, and we just need to use the definition of $\beta_k$ presented in (3.58). It is easy to compare the analytical and numerical results of the multi-interval Rényi entropy, but we will not show the details here.

3.3.2 Average Rényi entropy

In the extremely gapped limit, the interactions between the fermions at the neighboring sites could be omitted. We check that our results of the single-interval and double-interval Rényi entropies satisfy the position-momentum duality [86, 87]

$$S(n)_{A,K} = S(n)_{K,A}. \quad (3.59)$$

We have used integers to label the sites, while the momenta in the NS sector are half-integers. We can still change $A \leftrightarrow K$, because $S(n)_{A,K}$ only depend on the momentum differences rather than the momenta themselves. In other words, $S(n)_{A,K} = S(n)_{A,K+k_0}$ for an arbitrary constant $k_0$. When the momenta in the set $K$ are half-integers, the duality (3.59) can be understood as

$$S(n)_{A,K} = S(n)_{K+\frac{1}{2},A}. \quad (3.60)$$

Explicitly, we are able to check that

$$F(n)_{j,k_{12},j} = F(n)_{k_{12},j,k_{12}}, \quad n = 2, 3, \cdots, 7,$$

$$F(n)_{j_{12},k_1,k_2} = F(n)_{k_1,k_{12},j_{12}}, \quad n = 2, 3, \cdots, 7,$$

$$F(n)_{j,k_1,k_2,k_3} = F(n)_{k_1,k_2,k_3,j}, \quad n = 2, 3, 4, 5,$$

$$F(n)_{j_{12},k_1,k_2,k_3} = F(n)_{k_1,k_2,k_3,j_{12}}, \quad n = 2, 3, 4, 5. \quad (3.61)$$
Figure 10: The universal Rényi entropy (dotted lines), the analytical double-interval Rényi entropy in the extremely gapped fermionic chain (solid lines), and the numerical double-interval Rényi entropy in the slightly gapped and critical fermionic chains (symbols) in the double-particle state $|k_1 k_2\rangle$. We have set the momenta $(k_1, k_2) = \left(\frac{1}{2}, \frac{3}{2}\right) + \frac{L}{8}$, $x_1 = x_2 = \frac{1}{8}$. For the analytical Rényi entropy we have set $L = +\infty$. 

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Figure 11: The universal Rényi entropy (dotted lines), the analytical double-interval Rényi entropy in the extremely gapped fermionic chain (solid lines), and the numerical double-interval Rényi entropy in the slightly gapped and critical fermionic chains (symbols) in the triple-particle state $|k_1k_2k_3\rangle$. We have set the momenta $(k_1,k_2,k_3) = (\frac{1}{2}, \frac{3}{2}, \frac{5}{2}) + \frac{L}{\pi}, x_1 = x_2 = \frac{1}{\pi}$. For the analytical Rényi entropy we have set $L = +\infty$. 

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For example, we have
\[
\mathcal{F}^{(2)}_{j,k_1k_2} = \mathcal{F}^{(2)}_{k_1k_2,j} = \frac{L^2 - 4L + 8}{L^2},
\]
\[
\mathcal{F}^{(4)}_{j,k_1k_2k_3} = \mathcal{F}^{(4)}_{k_1k_2k_3,j} = \frac{L^4 - 12L^3 + 54L^2 - 108L + 162}{L^4}.
\] (3.62)

Using the duality (3.59), it is also convenient to calculate the average Rényi entropy [65, 76–78, 80, 81]
\[
\langle S_A^{(n)} \rangle = \frac{1}{2L} \sum_K S_A^{(n)} = \frac{1}{2L} \sum_K S_{K,A}^{(n)}.
\] (3.63)

For \( A \) consisting of one (general \( n \)), two (\( n = 2, 3, \cdots, 7 \)), and three (\( n = 2, 3, 4, 5 \)) successive sites, i.e. single interval \( A \) with \(|A| = \ell = 1, 2, 3\), we can check numerically the average Rényi entropy
\[
\lim_{L \to +\infty} \langle S_A^{(n)} \rangle = |A| \log 2.
\] (3.64)

This is just the finding in [77].

It is easy to check that the expression (1.4) does not satisfy the position-momentum duality (3.59). For example, there are
\[
\mathcal{F}^{(n)}_{j,p_1p_2} = \left[ \frac{1}{L^n} + \left( 1 - \frac{1}{L} \right)^n \right]^2 \neq \mathcal{F}^{(n)}_{k_1k_2,2\pi j / L} = \left( \frac{2}{L} \right)^n + \left( 1 - \frac{2}{L} \right)^n.
\] (3.65)

This is not surprising, as the universal Rényi entropy is expected to be valid only in the limit \( L \to +\infty \).

On the other hand, in the limit \( L \to +\infty \), the position-momentum duality is satisfied trivially for \( \mathcal{F}^{(n)}_{j,p_1p_2} \) and \( \mathcal{F}^{(n)}_{k_1k_2,2\pi j / L} \) in (3.65). As can be seen in figure 2, the universal Rényi entropy is not valid also when too many quasiparticles are excited. Moreover, the universal Rényi entropy is not valid when the momentum differences are small. So one cannot calculate the average Rényi entropy from the universal Rényi entropy.

3.4 Rényi entropy with general index \( n \) and entanglement entropy

One can use the result (3.26) from the correlation matrix method and the position-momentum duality (3.59) and calculate the excited state Rényi entropy analytically. For a subsystem \( A \) in the state \( |K\rangle = |k_1k_2 \cdots k_s\rangle \) with the excitations of \( |K| = s \) different quasiparticles, we define the \( |K| \times |K| \) matrix \( C_K^A \) with entries
\[
[C_K^A]_{i_1i_2} = h_{k_1}^{A} - k_{i_1}, \ \ i_1, i_2 = 1, 2, \cdots, s,
\] (3.66)
with the function
\[
h_k^A = \frac{1}{L} \sum_{j \in A} e^{2\pi i j k / L}.
\] (3.67)

Note that \( h_0^A = x \) and for \( k \neq 0 \) we have \( h_k^A = \beta_k \) that is defined in (3.58). The excited state Rényi entropy is just
\[
\mathcal{F}^{(n)}_{A,K} = \det[(C_K^A)^n + (1 - C_K^A)^n].
\] (3.68)

The formula is very efficient for both analytical and numerical calculations. We confirmed that it always leads to the same analytical results as we obtained by writing the excited states in terms of subsystem excitations.

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In the single-particle state $|k\rangle$ there is $C^A_k = x$, and we reproduce the universal Rényi entropy with no additional contribution $F^{(n)}_{A,k} = F^{(n),\text{univ}}_{A,p} = x^n + (1 - x)^n$. In a general multi-particle state $|k_1 k_2 \cdots k_s\rangle$ that all the momentum differences are large, $C^A_{k_1 k_2 \cdots k_s} = x I_s$ with $I_s$ being an $s \times s$ identity matrix, and we then get easily the most general universal Rényi entropy in the fermionic chain $F^{(n),\text{univ}}_{A,p_1 p_2 \cdots p_s} = [x^n + (1 - x)^n]^s$.

In the double-particle state $|k_1 k_2\rangle$ with general momenta $k_1, k_2$ there is

$$C^A_{k_1 k_2} = \begin{pmatrix} x & \beta_{k_2 - k_1} \\ \beta_{k_1 - k_2} & x \end{pmatrix},$$

(3.69)

whose eigenvalues are

$$\nu_1 = x + |\beta_{k_1 - k_2}|, \quad \nu_2 = x - |\beta_{k_1 - k_2}|.$$  

(3.70)

We get the double-particle state Rényi entropy with general index $n$

$$F^{(n)}_{A,k_1 k_2} = [(x + |\beta_{k_1 - k_2}|)^n + (1 - x - |\beta_{k_1 - k_2}|)^n][(x - |\beta_{k_1 - k_2}|)^n + (1 - x + |\beta_{k_1 - k_2}|)^n].$$  

(3.71)

We take the $n \to 1$ analytical continuation and get the entanglement entropy

$$S_{A,k_1 k_2} = -(x + |\beta_{k_1 - k_2}|) \log(x + |\beta_{k_1 - k_2}|) - (1 - x - |\beta_{k_1 - k_2}|) \log(1 - x - |\beta_{k_1 - k_2}|)
- (x - |\beta_{k_1 - k_2}|) \log(x - |\beta_{k_1 - k_2}|) - (1 - x + |\beta_{k_1 - k_2}|) \log(1 - x + |\beta_{k_1 - k_2}|).$$  

(3.72)

We see nontrivial additional contributions to the universal double-particle state Rényi entropy (3.15).

In the triple-particle state $|k_1 k_2 k_3\rangle$ with general momenta $k_1, k_2, k_3$ there is

$$C^A_{k_1 k_2 k_3} = \begin{pmatrix} x & \beta_{k_2 - k_1} & \beta_{k_3 - k_1} \\ \beta_{k_1 - k_2} & x & \beta_{k_3 - k_2} \\ \beta_{k_1 - k_3} & \beta_{k_2 - k_3} & x \end{pmatrix},$$

(3.73)

whose eigenvalues $\nu_i$ with $i = 1, 2, 3$ are solutions to the equation

$$\nu^3 - 3x\nu^2 + (3x^2 - \gamma_{k_1 k_2 k_3})\nu - (x^3 - \gamma_{k_1 k_2 k_3} x + \delta_{k_1 k_2 k_3}) = 0,$$  

(3.74)

with the definitions $\gamma_{k_1 k_2 k_3}$ and $\delta_{k_1 k_2 k_3}$ in (3.57). The Rényi entropy with general index $n$ and the entanglement entropy are just

$$F^{(n)}_{A,k_1 k_2 k_3} = \prod_{i=1}^3 [\nu_i^n + (1 - \nu_i)^n],$$

$$S_{A,k_1 k_2 k_3} = \sum_{i=1}^3 [-\nu_i \log \nu_i - (1 - \nu_i) \log(1 - \nu_i)].$$  

(3.75)

We compare the universal entanglement entropy, the analytical and numerical entanglement entropy in the double-particle state $|k_1 k_2\rangle$ and the triple-particle state $|k_1 k_2 k_3\rangle$ in the extremely gapped fermionic chain in figure 12.

The analytical entanglement and Rényi entropies in an excited state with a larger number of quasi-particles can be calculated similarly, but we will not report the results in this paper.
Figure 12: The universal entanglement entropy (dotted lines), and the analytical (solid lines) and numerical (circles) results of the entanglement entropy in the double-particle state $|k_1 k_2\rangle$ (left) and the triple-particle state $|k_1 k_2 k_3\rangle$ (right) in the extremely gapped fermionic chain. We use different colors for different momenta. We have set $\lambda = +\infty$, $L = 64$, $k_1 = \frac{1}{2}$.

4 Bosonic chain

We consider the circular bosonic chain

$$H = \frac{1}{2} \sum_{j=1}^{L} \left[ p_j^2 + m^2 q_j^2 + (q_j - q_{j+1})^2 \right],$$

(4.1)

which is just the locally coupled harmonic chain and is also the discretization of the two-dimensional massive scalar field theory. We have the periodic boundary condition $q_{L+1} = q_1$. The mass $m$ is just the gap of the model. We take the number of sites $L$ as an even integer. It can be diagonalized by the Fourier transformation

$$q_j = \frac{1}{\sqrt{L}} \sum_k e^{-2\pi ijk} \varphi_k, \quad p_j = \frac{1}{\sqrt{L}} \sum_k e^{-2\pi ijk} \pi_k,$$

(4.2)

with the momentum

$$k = 1 - \frac{L}{2}, \ldots, -1, 0, 1, \ldots, \frac{L}{2} - 1, \frac{L}{2}.$$  

(4.3)

The Hamiltonian becomes

$$H = \frac{1}{2} \sum_k (\pi_k^+ \pi_k + \varepsilon_k^2 \varphi_k^+ \varphi_k),$$

(4.4)

with the frequency

$$\varepsilon_k = \sqrt{m^2 + 4 \sin^2 \frac{\pi k}{L}}.$$  

(4.5)

One can define the ladder operators

$$b_k = \frac{\varepsilon_k}{2} \left( \varphi_k + \frac{i}{\varepsilon_k} \pi_k \right), \quad b_k^+ = \frac{\varepsilon_k}{2} \left( \varphi_k^+ - \frac{i}{\varepsilon_k} \pi_k \right).$$

(4.6)

The Hamiltonian becomes

$$H = \sum_k \varepsilon_k \left( b_k^+ b_k + \frac{1}{2} \right).$$  

(4.7)
The ground state $|G\rangle$ is annihilated by all the lowering operators

$$b_k|G\rangle = 0.$$  \hfill (4.8)

The excited states are constructed by applying various raising operators on the ground state

$$|k_1^{r_1}k_2^{r_2}\cdots k_s^{r_s}\rangle = \frac{(b^\dagger_{k_1})^{r_1}(b^\dagger_{k_2})^{r_2}\cdots (b^\dagger_{k_s})^{r_s}}{\sqrt{r_1!r_2!\cdots r_s!}}|G\rangle.$$  \hfill (4.9)

In the extremely massive limit $m \to +\infty$, the bosonic chain approaches $L$ decoupled oscillators

$$H = \frac{1}{2} \sum_{j=1}^{L} (p_j^2 + m^2x_j^2),$$  \hfill (4.10)

and for each oscillator one can define the local ladder operators

$$a_j = \sqrt{\frac{m}{2}} \left(q_j + i \frac{p_j}{m}\right), \quad a_j^\dagger = \sqrt{\frac{m}{2}} \left(q_j - i \frac{p_j}{m}\right).$$  \hfill (4.11)

In the limit $m \to +\infty$, the lowering and raising operators (4.6) become

$$b_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{2\pi i j k/L} a_j, \quad b_k^\dagger = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-2\pi i j k/L} a_j^\dagger.$$  \hfill (4.12)

The ground state is also annihilated by the lowering operators at each site

$$a_j|G\rangle = 0, \quad j = 1, 2, \cdots, L.$$  \hfill (4.13)

### 4.1 Single interval

We consider an interval with $\ell$ consecutive sites $A = [1, \ell]$ on the periodic bosonic chain with $L$ sites. In the extremely gapped limit $m \to +\infty$, the ground state is just a direct product state

$$|G\rangle = |G_A\rangle|G_B\rangle,$$  \hfill (4.14)

and the Rényi entropy is vanishing

$$S^{(n)}_{A,G} = 0.$$  \hfill (4.15)

In the excited state $|k_1^{r_1}k_2^{r_2}\cdots k_s^{r_s}\rangle$ with large $k_i$, the universal Rényi entropy discussed in [60,61,63,64] is just (1.4). We will relax the constraints for the momenta $k_i$ and show nontrivial additional contributions $\delta F^{(n)}_{A,k_1^{r_1}k_2^{r_2}\cdots k_s^{r_s}}$ to the universal Rényi entropy

$$F^{(n)}_{A,k_1^{r_1}k_2^{r_2}\cdots k_s^{r_s}} = F^{(n)\text{univ}}_{A,p_1^{r_1}p_2^{r_2}\cdots p_s^{r_s}} + \delta F^{(n)}_{A,k_1^{r_1}k_2^{r_2}\cdots k_s^{r_s}}.$$  \hfill (4.16)

For later analytical calculations, it is convenient to define in the extremely gapped limit

$$b_{A,k} = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{ij\varphi_k} a_j, \quad b_{A,k}^\dagger = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{-ij\varphi_k} a_j^\dagger,$$
$$b_{B,k} = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{ij\varphi_k} a_j, \quad b_{B,k}^\dagger = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{-ij\varphi_k} a_j^\dagger.$$  \hfill (4.17)
There are commutation relations

\[ [b_{A,k}, b_{A,k}^\dagger] = x, \quad [b_{B,k}, b_{B,k}^\dagger] = 1 - x, \quad (4.18) \]

and for \( k_1 \neq k_2 \) there are

\[ [b_{A,k_1}, b_{A,k_2}^\dagger] = -[b_{B,k_1}, b_{B,k_2}^\dagger] = \alpha_{k_1-k_2}. \quad (4.19) \]

with the definition of \( \alpha_k \) presented in (3.30). The following analytical calculations in the harmonic chain are similar to those in the fermionic chain, with the difference of changing the anti-commutation relations to the commutation ones.

For a general gap \( m \), the excited state Rényi entropy can be calculated numerically from the method of the wave function [60,61]. In the extremely gapped limit \( m \to +\infty \) the wave function method can be also used to calculate the analytical Rényi entropy. We will come back to this method at the end of this section. In the following in analogy with the fermionic calculations we calculate the Rényi entropies using the subsystem mode method.

### 4.1.1 Multi-particle state with equal momenta \(|k^r\rangle\)

For the state \(|k^r\rangle\) with \( r \) quasiparticles of equal momenta \( k \), we write the density matrix of the whole system as

\[ \rho_{k^r} = \frac{1}{r!} (b_{A,k}^\dagger + b_{B,k}^\dagger)^r |G\rangle \langle G|(b_{A,k} + b_{B,k})^r, \quad (4.20) \]

then we get the RDM

\[ \rho_{A,k^r} = \frac{1}{r!} \sum_{p=0}^r C_r^p \langle (b_{B,k})^{r-p} (b_{A,k}^{\dagger})^p |G\rangle \langle G|(b_{A,k}^{\dagger})^p |A\rangle \langle A|(b_{A,k})^p. \quad (4.21) \]

where \( C_r^p \) is the binomial coefficient. Then we obtain

\[ \text{tr}_{A} \rho_{A,k^r}^n = \frac{r}{r!} \sum_{p=0}^r \left[ \langle (b_{A,k})^p (b_{A,k}^{\dagger})^p |G\rangle \langle G|(b_{A,k}^{\dagger})^p |A\rangle \langle A|(b_{A,k})^p \right] = \sum_{p=0}^r C_r^p x^p (1 - x)^{r-p}. \quad (4.22) \]

There is no additional contribution to the universal Rényi entropy in the state \(|k^r\rangle\).

### 4.1.2 Double-particle state \(|k_1k_2\rangle\)

For the excited state with two different quasiparticles \(|k_1k_2\rangle\) with general nonequal \( k_1, k_2 \), we write the density matrix of the whole system as

\[ \rho_{k_1k_2} = (b_{A,k_1}^\dagger + b_{B,k_1}^\dagger)(b_{A,k_2} + b_{B,k_2}) |G\rangle \langle G|(b_{A,k_2} + b_{B,k_2})(b_{A,k_1} + b_{B,k_1}), \quad (4.23) \]

and then we get the RDM\(^2\)

\[ \rho_{A,k_1k_2} = b_{A,k_1}^\dagger b_{A,k_2}^\dagger |A\rangle \langle A|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_1}b_{B,k_2}^\dagger |G\rangle \langle G|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_2}b_{B,k_1}^\dagger |G\rangle \langle G|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_1}b_{B,k_2} |G\rangle \langle G|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_1}b_{B,k_2}^\dagger |G\rangle \langle G|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_1}b_{B,k_2} |G\rangle \langle G|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_2}b_{B,k_1} |G\rangle \langle G|b_{A,k_2}b_{A,k_1} + \langle b_{B,k_2}b_{B,k_1} |G\rangle \langle G|b_{A,k_2}b_{A,k_1}. \quad (4.24) \]

\(^2\)It is interesting to compare the double-particle state RDMs in the fermionic chain (3.35) and the bosonic chain (4.24). Note the sign differences due to the difference of the anti-commutation and commutation relations.
Finally we get the nontrivial additional contributions to the universal Rényi entropy

\[
\delta \mathcal{F}_{A,k_1 k_2}^{(2)} = 4(1 - 2x)^2 \alpha_{12}^2 + 4\alpha_{12}^4,
\]

(4.25)

\[
\delta \mathcal{F}_{A,k_1 k_2}^{(3)} = 3(1 - 2x)^2(1 + 2x - 2x^2)\alpha_{12}^2 - 3(1 - 8x + 8x^2)\alpha_{12}^4,
\]

(4.26)

\[
\delta \mathcal{F}_{A,k_1 k_2}^{(4)} = 4(1 - 2x)^2(1 - 2x + 6x^2 - 8x^3 + 4x^4)\alpha_{12}^2
\]

\[
+ 8(1 - 8x + 27x^2 - 38x^3 + 19x^4)\alpha_{12}^4 + 16(1 - 2x)^2\alpha_{12}^6 + 4\alpha_{12}^8,
\]

(4.27)

as well as \(\delta \mathcal{F}_{A,k_1 k_2}^{(n)}\) with \(n = 5, 6, 7\) which we will not show in this paper. Note that \(\alpha_{12} = |\alpha_{k_1 k_2}|\) is defined in (3.30). We get the same analytical results using the wave function method in the extremely gapped limit. We compare the results of the universal Rényi entropy and the analytical results with additional terms for the state \(|k_1 k_2\rangle\) in the figure 13. For a small momentum difference \(|k_1 - k_2|\), the additional terms cannot be neglected, while for a large momentum difference, the additional terms are negligible.

### 4.1.3 Triple-particle state \(|k_1^2 k_2\rangle\)

In the triple-particle state \(|k_1^2 k_2\rangle\) with general nonequal momenta \(k_1, k_2\), the calculations are similar and we will not show the details here. We get the additional contributions to the universal Rényi entropy

\[
\delta \mathcal{F}_{A,k_1^2 k_2}^{(2)} = 8(1 - 2x)^2(1 - 3x + 3x^2)\alpha_{12}^2 + 4(5 - 18x + 18x^2)\alpha_{12}^4,
\]

(4.28)
Figure 14: The universal Rényi entropy (dotted lines) and the single-interval Rényi entropy with corrections (solid lines) in the triple-particle state $|k_1^2 k_2^2 k_3^2\rangle$ in the extremely gapped bosonic chain. We have set $m = +\infty$, $L = 64$.

\[
\delta F^{(3)}_{A,k_1^2 k_2^2} = 6(1 - 2x)^2(1 - 15x^2 + 30x^3 - 15x^4)\alpha_{12}^2 - 6(2 - 33x + 132x^2 - 198x^3 + 99x^4)\alpha_{12}^4 - 12(2 - 3x)(1 - 3x)\alpha_{12}^6, \quad (4.29)
\]

as well as $\delta F^{(n)}_{A,k_1^2 k_2^2}$ with $n = 4, 5, 6, 7$ which we will not show in this paper. We get the same analytical results using the wave function method in the extremely gapped limit. We compared the results of the universal Rényi entropy and the results with additional terms for the state $|k_1^2 k_2^2\rangle$ in the figure 14.

### 4.1.4 Triple-particle state $|k_1 k_2 k_3\rangle$

In the triple-particle state $|k_1 k_2 k_3\rangle$ with general nonequal $k_1, k_2, k_3$, we get the additional contributions to the universal Rényi entropy

\[
\delta F^{(2)}_{A,k_1 k_2 k_3} = 4(1 - 2x)^2(1 - 2x + 2x^2)(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2) - 16(1 - 2x)^3\alpha_{12}\alpha_{13}\alpha_{23}
\]

\[
+ 16(1 - 2x)^2(\alpha_{12}\alpha_{13}^2 + \alpha_{12}^2\alpha_{23} + \alpha_{13}\alpha_{23}^2) + 4(1 - 2x + 2x^2)(\alpha_{12}^4 + \alpha_{13}^4 + \alpha_{23}^4)
\]

\[
- 32(1 - 2x)\alpha_{12}\alpha_{13}\alpha_{23}(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2) + 80\alpha_{12}\alpha_{13}\alpha_{23}^2, \quad (4.30)
\]
Figure 15: The universal Rényi entropy (dotted lines) and the single-interval Rényi entropy with corrections (solid lines) in the triple-particle state $|k_1k_2k_3\rangle$ in the extremely gapped bosonic chain. We have set $m = +\infty$, $L = 64$.

\[
\delta F^{(3)}_{A,k_1k_2k_3} = 3(1 - 2x)^2(1 + 2x - 2x^2)(1 - 3x + 3x^2)(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2)
- 54x(1 - x)(1 - 2x)^3\alpha_{12}\alpha_{13}\alpha_{23} - 6(1 - 2x)^2(1 - 13x + 13x^2)(\alpha_{12}^2\alpha_{13}^2
+ \alpha_{12}^2\alpha_{23}^2 + \alpha_{13}^2\alpha_{23}^2) - 3(1 - 3x + 3x^2)(1 - 8x + 8x^2)(\alpha_{12}^4 + \alpha_{13}^4 + \alpha_{23}^4)
+ 6(1 - 2x)(7 - 40x + 40x^2)\alpha_{12}\alpha_{13}\alpha_{23}(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2) - 144(1 - 5x
+ 5x^2)\alpha_{12}^2\alpha_{13}^2\alpha_{23}^2 - 24(1 - 2x)^2(\alpha_{12}^4\alpha_{13}^2 + \alpha_{12}^2\alpha_{13}^4 + \alpha_{12}^4\alpha_{23}^2 + \alpha_{13}^4\alpha_{23}^2
+ \alpha_{12}^2\alpha_{23}^4 + \alpha_{13}^2\alpha_{23}^4) + 96(1 - 2x)\alpha_{12}\alpha_{13}\alpha_{23}(\alpha_{12}^2\alpha_{13}^2 + \alpha_{12}^2\alpha_{23}^2 + \alpha_{13}^2\alpha_{23}^2)
- 24\alpha_{12}^2\alpha_{13}^2\alpha_{23}^2(\alpha_{12}^2 + \alpha_{13}^2 + \alpha_{23}^2),
\]

as well as $\delta F^{(n)}_{A,k_1k_2k_3}$ with $n = 4, 5$ which we will not show the details here. We get the same analytical results using the wave function method in the extremely gapped limit. We compare the results of the universal Rényi entropy and the results with additional contributions for the state $|k_1k_2k_3\rangle$ in the figure 15.

### 4.1.5 Slightly gapped bosonic chain

We have calculated the analytical expressions of the Rényi entropy in the extremely gapped harmonic chain. We compare the results of the universal Rényi entropy, the results with additional corrections in the extremely gapped bosonic chain, and the numerical results in the double-particle state $|k_1k_2\rangle$, the triple-particle state $|k_1^2k_2\rangle$ and the triple-particle state $|k_1k_2k_3\rangle$ in the slightly gapped harmonic chain.
4.2.1 Multi-particle state with equal momenta $|k^r\rangle$

There is no additional contribution to the universal double-interval Rényi entropy in the multi-particle state with equal momenta $|k^r\rangle$.

4.2.2 Double-particle state $|k_1k_2\rangle$

We get analytically the additional contributions $\delta F_{A_1A_2,k_1k_2}^{(n)}$ with $n = 2, 3, \cdots, 7$ to the universal double-interval Rényi entropy $F_{A_1A_2,p_1p_2}^{(n),\text{univ}}$, in the double-particle state $|k_1k_2\rangle$, in the extremely gapped bosonic chain. The results are just the expressions $\delta F_{A,k_1k_2}^{(n)}$ presented in the subsection 4.1.2 after the following substitution

$$|\alpha_{k_1-k_2}| \to |\beta_{k_1-k_2}|.$$  \hspace{1cm} (4.32)

We compare the universal double-interval Rényi entropy and the Rényi entropy with corrections in the figure 17.
Figure 17: The universal Rényi entropy (dotted lines) and the double-interval Rényi entropy with corrections (solid lines) in the double-particle state $|k_1 k_2\rangle$ in the extremely gapped bosonic chain. We have set $m = +\infty$, $L = 64$. 
4.2.3 Triple-particle state $|k_1^2 k_2^2\rangle$

We calculate analytically the additional terms $\delta F_{A_1 A_2, k_1^2 k_2^2}^{(n)}$ with $n = 2, 3, \cdots , 7$ in the triple-particle state $|k_1^2 k_2^2\rangle$. The expressions are just the results $\delta F_{A, k_1^2 k_2^2}^{(n)}$ in subsection 4.1.3 by sending

$$|\alpha_{k_1-k_2}| \rightarrow |\beta_{k_1-k_2}|.$$ \hspace{1cm} (4.33)

We compare the universal double-interval Rényi entropy and the universal Rényi entropy in figure 18.

4.2.4 Triple-particle state $|k_1 k_2 k_3^2\rangle$

We calculate the additional contributions to the universal double-interval Rényi entropy in the triple-particle state $|k_1 k_2 k_3^2\rangle$ as

$$\delta F_{A_1 A_2, k_1 k_2 k_3^2}^{(2)} = 4(1-2x)^2(1-2x+2x^2)\gamma_{k_1 k_2 k_3} - 8(1-2x)^3\delta_{k_1 k_2 k_3}$$

$$+ 4(1-2x+2x^2)\gamma_{k_1 k_2 k_3}^2 + 8(1-6x+6x^2)\epsilon_{k_1 k_2 k_3}$$

$$- 16(1-2x)\gamma_{k_1 k_2 k_3}^3 \delta_{k_1 k_2 k_3} + 8\delta_{k_1 k_2 k_3}^2 + 48\zeta_{k_1 k_2 k_3},$$ \hspace{1cm} (4.34)

$$\delta F_{A_1 A_2, k_1 k_2 k_3^2}^{(3)} = 3(1-2x)^2(1+2x-2x^2)(1-3x+3x^2)\gamma_{k_1 k_2 k_3} - 27x(1-x)(1-2x)^3\delta_{k_1 k_2 k_3}$$

$$- 3(1-11x+35x^2-48x^3+24x^4)\gamma_{k_1 k_2 k_3}^2 + 12x(1-x)(3-14x+14x^2)\epsilon_{k_1 k_2 k_3}$$

$$+ 3(1-2x)(7-40x+40x^2)\gamma_{k_1 k_2 k_3}^3 - 24(1-2x)^2\gamma_{k_1 k_2 k_3}\epsilon_{k_1 k_2 k_3}$$

$$- 3(5-24x+24x^2)\delta_{k_1 k_2 k_3}^2 - 12(1-12x+12x^2)\zeta_{k_1 k_2 k_3}$$

$$- 12(1-12x+12x^2)\zeta_{k_1 k_2 k_3}^2,$$ \hspace{1cm} (4.35)

with $\gamma_{k_1 k_2 k_3}$ and $\delta_{k_1 k_2 k_3}$ defined in (3.57) and

$$\epsilon_{k_1 k_2 k_3} = |\beta_{k_1-k_2}|^2 |\beta_{k_1-k_3}|^2 + |\beta_{k_1-k_2}|^2 |\beta_{k_2-k_3}|^2 + |\beta_{k_1-k_3}|^2 |\beta_{k_2-k_3}|^2,$$

$$\zeta_{k_1 k_2 k_3} = |\beta_{k_1-k_2}|^2 |\beta_{k_1-k_3}|^2 |\beta_{k_2-k_3}|^2.$$ \hspace{1cm} (4.36)

We also calculate analytically $\delta F_{A_1 A_2, k_1 k_2 k_3^2}^{(n)}$ with $n = 4, 5$ which we will not show in this paper. We compare the universal double-interval Rényi entropy and the Rényi entropy with corrections in figure 19.

4.2.5 Slightly gapped bosonic chain

In the slightly gapped bosonic chain, we can calculate the double-interval Rényi entropy numerically in the double-particle state $|k_1 k_2\rangle$, triple-particle state $|k_1^2 k_2^2\rangle$ and triple-particle state $|k_1 k_2 k_3^2\rangle$. We compare the numerical results with the universal double-interval Rényi entropy and the Rényi entropy with corrections in the extremely gapped bosonic chain in figure 20. We see that the new Rényi entropy with additional corrections in the extremely gapped bosonic chain is still valid in the limit of large momenta.

4.3 Multiple intervals

Similar to the extremely gapped fermionic chain, the generalization from double interval to multiple intervals is easy. We will not show the details here.
Figure 18: The universal Rényi entropy (dotted lines) and the double-interval Rényi entropy with corrections (solid lines) in the triple-particle state $|k_1^2 k_2^2\rangle$ in the extremely gapped bosonic chain. We have set $m = +\infty$, $L = 64$. 
Figure 19: The universal Rényi entropy (dotted lines) and the double-interval Rényi entropy with corrections (solid lines) in the triple-particle state $|k_1 k_2 k_3\rangle$ in the extremely gapped bosonic chain. We have set $m = +\infty$, $L = 64$. 
Figure 20: The universal Rényi entropy (dotted lines), the analytical double-interval Rényi entropy in the extremely gapped bosonic chain (solid lines), and the numerical Rényi entropy in the slightly gapped bosonic chain (symbols) in the double-particle state $|k_1 k_2\rangle$ (left), the triple-particle state $|k_1^2 k_2\rangle$ (middle) and the triple-particle state $|k_1 k_2 k_3\rangle$ (right). We have set $m = 10^{-4}$, $(k_1, k_2, k_3) = (1, 2, 3) + \frac{L}{8}$, $x_1 = x_2 = \frac{1}{8}$. For the analytical results we have set $L = +\infty$.

4.4 A permanent formula in the extremely gapped limit

For the general excited state $|K\rangle = |k_1^{i_1} k_2^{i_2} \cdots k_s^{i_s}\rangle$, there are totally $|K\rangle = R = \sum_{i=1}^8 r_i$ number of excited quasiparticles. In the extremely gapped limit of the bosonic chain, using the wave function method, in the appendix A, we show that the excited state Rényi entropy of a subsystem $A$, which could be either a single interval or general multiple intervals, is just the permanent of a certain matrix as follows:

$$F^{(n)}_{A,k} = \frac{\text{per} \Omega^{(n)}_{A,k}}{\prod_{i=1}^8 (r_i)!^n},$$

(4.37)

where the definition of the $n|K| \times n|K|$ matrix $\Omega^{(n)}_{A,k}$ can be found in (A.20) and (A.15). We show the details of the wave function method and the proof of the formula (4.37), i.e. (A.22), in appendix A.

For example, to calculate $F^{(n)}_{A,k} = F^{(n)\text{, univ}}_{A,p} = x^n + (1 - x)^n$ with a general integer $n \geq 2$ we need the $n \times n$ matrix

$$\Omega^{(n)}_{A,k} = \begin{pmatrix}
1 - x & x & & & & \\
x & 1 - x & x & & & \\
& \ddots & \ddots & \ddots & & \\
& & 1 - x & x & & \\
x & & & 1 - x & & 
\end{pmatrix},$$

(4.38)

to calculate $F^{(3)}_{A,k^2} = F^{(3)\text{, univ}}_{A,p^2} = x^6 + [2x(1-x)]^3 + (1-x)^6$ we need the $6 \times 6$ matrix

$$\Omega^{(3)}_{A,k^2} = \begin{pmatrix}
1 - x & x & 0 & 1 - x & x & 0 \\
0 & 1 - x & x & 0 & 1 - x & x \\
x & 0 & 1 - x & x & 0 & 1 - x \\
1 - x & x & 0 & 1 - x & x & 0 \\
0 & 1 - x & x & 0 & 1 - x & x \\
x & 0 & 1 - x & x & 0 & 1 - x 
\end{pmatrix},$$

(4.39)
and to calculate $J_{A,k_1k_2}^{(3)}$ (4.26) with general momenta $k_1 \neq k_2$ we need the $6 \times 6$ matrix

$$
\Omega_{A,k_1k_2}^{(3)} = 
\begin{pmatrix}
1 - x & x & 0 & -\beta_{k_1-k_2} & \beta_{k_1-k_2} & 0 \\
0 & 1 - x & x & 0 & -\beta_{k_1-k_2} & \beta_{k_1-k_2} \\
x & 0 & 1 - x & \beta_{k_1-k_2} & 0 & -\beta_{k_1-k_2} \\
-\beta_{k_2-k_1} & \beta_{k_2-k_1} & 0 & 1 - x & x & 0 \\
0 & -\beta_{k_2-k_1} & \beta_{k_2-k_1} & 0 & 1 - x & x \\
\beta_{k_2-k_1} & 0 & -\beta_{k_2-k_1} & x & 0 & 1 - x \\
\end{pmatrix},
$$

(4.40)

with the definition of $\beta_k$ (3.58). Note that these examples of $\Omega_{A,K}^{(n)}$ apply to not only single-interval but also multi-interval cases.

In the limit that all the momentum differences are large, i.e. $|k_i - k_j| \to +\infty$ for all $i_1 \neq i_2$, we have $\beta_{k_i-k_j} \to 0$, and the excited state Rényi entropy should approach the universal Rényi entropy (1.4). One can use this idea to prove the existence of the most general universal term as follows: We first note that for the state $|k^r\rangle$ there is the $nr \times nr$ matrix $\Omega_{A,k^r}^{(n)}$ written in the form of $r \times r$ blocks

$$
\Omega_{A,k^r}^{(n)} = 
\begin{pmatrix}
\Omega_{A,k}^{(n)} & \Omega_{A,k}^{(n)} & \cdots & \Omega_{A,k}^{(n)} \\
\Omega_{A,k}^{(n)} & \Omega_{A,k}^{(n)} & \cdots & \Omega_{A,k}^{(n)} \\
\vdots & \vdots & \ddots & \vdots \\
\Omega_{A,k}^{(n)} & \Omega_{A,k}^{(n)} & \cdots & \Omega_{A,k}^{(n)} \\
\end{pmatrix} = J_r \otimes \Omega_{A,k}^{(n)},
$$

(4.41)

with the $n \times n$ matrix $\Omega_{A,k}^{(n)}$ (4.38) and the $r \times r$ matrix $J_r$ all of whose entries are 1. There is the permanent

$$
\text{per} \ \Omega_{A,k^r}^{(n)} = (r!)^n \sum_{p=0}^r [C_p^r p^r (1-x)^{r-p}]^n.
$$

(4.42)

Since in the large momentum difference limit we already have $\beta_{k_i-k_j} \to 0$ for all $i_1 \neq i_2$, there is the $n|K| \times n|K|$ matrix for the general state in the form of a direct sum

$$
\Omega_{A,k_1^{r_1}k_2^{r_2}\ldots k_s^{r_s}}^{(n)} = \bigoplus_{i=1}^s \Omega_{A,k_i^{r_i}}^{(n)},
$$

(4.43)

with the $nr_i \times nr_i$ matrix $\Omega_{A,k_i^{r_i}}^{(n)}$, for each $i$ defined as (4.41). It is easy to get the permanent

$$
\text{per} \ \Omega_{A,k_1^{r_1}k_2^{r_2}\ldots k_s^{r_s}}^{(n)} = \prod_{i=1}^s \text{per} \ \Omega_{A,k_i^{r_i}}^{(n)}.
$$

(4.44)

This just leads to the universal Rényi entropy (1.4).

It would be interesting to find the permanent of the matrix $\Omega_{A,K}^{(n)}$ without the large momentum difference limit and calculate the Rényi entropy for general $n$ and then take the $n \to 1$ limit to calculate the von Neumann entropy. In this respect the block circulant structure of the matrix $\Omega_{A,K}^{(n)}$ might be useful.
5  XY chain

We consider the transverse field XY chain of \( L \) sites

\[
H = -\sum_{j=1}^{L} \left( \frac{1 + \gamma}{4} \sigma_{j}^{x} \sigma_{j+1}^{x} + \frac{1 - \gamma}{4} \sigma_{j}^{y} \sigma_{j+1}^{y} + \frac{\lambda}{2} \sigma_{j}^{z} \right),
\]

with periodic or antiperiodic boundary conditions for the Pauli matrices \( \sigma_{j}^{x,y,z} \). The XY chain can be mapped to the fermionic chain by some nonlocal transformations, but they have different local degrees of freedom. It can be diagonalized as

\[
H = \sum_{k} \varepsilon_{k} \left( c_{k}^{\dagger} c_{k} - \frac{1}{2} \right), \quad \varepsilon_{k} = \sqrt{\left( \lambda - \cos \frac{2\pi k}{L} \right)^{2} + \gamma^{2} \sin^{2} \frac{2\pi k}{L}},
\]

by successive Jordan-Wigner transformation, Fourier transformation and Bogoliubov transformation [83–85]

\[
a_{j} = \left( \prod_{i=1}^{j-1} \sigma_{i}^{z} \right) \sigma_{j}^{+}, \quad a_{j}^{\dagger} = \left( \prod_{i=1}^{j-1} \sigma_{i}^{z} \right) \sigma_{j}^{-},
\]

\[
b_{k} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ij\varphi_{k}} a_{j}, \quad b_{k}^{\dagger} = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ij\varphi_{k}} a_{j}^{\dagger},
\]

\[
c_{k} = b_{k} \cos \frac{\theta_{k}}{2} + ib_{-k}^{\dagger} \sin \frac{\theta_{k}}{2}, \quad c_{k}^{\dagger} = b_{k}^{\dagger} \cos \frac{\theta_{k}}{2} - ib_{-k} \sin \frac{\theta_{k}}{2},
\]

with the definitions

\[
\sigma_{j}^{\pm} = \frac{1}{2} (\sigma_{j}^{x} \pm i\sigma_{j}^{y}), \quad \varphi_{k} = \frac{2\pi k}{L}, \quad e^{i\theta_{k}} = \frac{\lambda - \cos \varphi_{k} + i\gamma \sin \varphi_{k}}{\varepsilon_{k}}.
\]

In this paper we only consider the cases that \( L \) is an even integer, and we only consider the states in the NS sector. We have the momenta

\[
k = \frac{1 - L}{2}, \ldots, \frac{1}{2}, \frac{1}{2}, \ldots, \frac{L - 1}{2}.
\]

The ground state \(|G\rangle\) is annihilated by all the lowering operators

\[
c_{k}|G\rangle = 0,
\]

and the excited states are generated by applying the raising operators with different momenta on the ground state

\[
|k_{1}k_{2} \cdots k_{s}\rangle = c_{k_{1}}^{\dagger} c_{k_{2}}^{\dagger} \cdots c_{k_{s}}^{\dagger}|G\rangle.
\]

When \( s \) is an even integer it is an excited state in the periodic XY chain in terms of the Pauli matrices, and when \( s \) is an odd integer it is an excited state in the antiperiodic chain.

We consider the extremely gapped limit \( \lambda \to +\infty \) of the XY chain. The Hamiltonian is

\[
H = -\frac{\lambda}{2} \sum_{j=1}^{L} \sigma_{j}^{z},
\]
in which the spins decouple from each other. The ground state is just the state with spin up at each site in the $\sigma_j^z$ basis

$$|G\rangle = |\uparrow\uparrow\cdots\uparrow\rangle$$  \hspace{1cm} (5.11)

The Bogoliubov angle is vanishing $\theta_k = 0$, and we have

$$c_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ij\varphi_k} a_j, \quad c_k^\dagger = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ij\varphi_k} a_j^\dagger.$$  \hspace{1cm} (5.12)

Note that the ladder operators $a_j$, $a_j^\dagger$ are not actually local modes, although $\sigma_j^+$, $\sigma_j^-$ are. The ground state is also annihilated by all the lowering operators $a_j$, $\sigma_j^+$

$$a_j|G\rangle = \sigma_j^+|G\rangle = 0, \quad j = 1, 2, \cdots, L.$$  \hspace{1cm} (5.13)

5.1 Single interval

We consider an interval with $\ell$ consecutive sites $A = [1, \ell]$ and its complement $B = [\ell + 1, L]$ on the circular XY chain of $L$ sites. For the analytical calculations of the Rényi entropy, it is convenient to define the subsystem modes in the extremely gapped limit

$$c_{A,k} = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{ij\varphi_k} a_j, \quad c_{A,k}^\dagger = \frac{1}{\sqrt{L}} \sum_{j \in A} e^{-ij\varphi_k} a_j^\dagger,$$

$$c_{B,k} = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{ij\varphi_k} a_j, \quad c_{B,k}^\dagger = \frac{1}{\sqrt{L}} \sum_{j \in B} e^{-ij\varphi_k} a_j^\dagger.$$  \hspace{1cm} (5.14)

There are anti-commutation relations

$$\{c_{A,k}, c_{A,k}^\dagger\} = x, \quad \{c_{B,k}, c_{B,k}^\dagger\} = 1 - x, \hspace{1cm} (5.15)$$

and for $k_1 \neq k_2$ we have

$$\{c_{A,k_1}, c_{A,k_2}^\dagger\} = -\{c_{B,k_1}, c_{B,k_2}^\dagger\} = \alpha_k,$$  \hspace{1cm} (5.16)

with the definition of $\alpha_k$ presented in (3.30). We define the string

$$S_A = \prod_{j \in A} \sigma_j^z,$$  \hspace{1cm} (5.17)

and the operators

$$\tilde{c}_{B,k} = S_A c_{B,k}, \quad \tilde{c}_{B,k}^\dagger = S_A c_{B,k}^\dagger.$$  \hspace{1cm} (5.18)

Note that $\tilde{c}_{B,k}$, $\tilde{c}_{B,k}^\dagger$ are defined locally in $B$, while $c_{B,k}$, $c_{B,k}^\dagger$ are not. Of course, $c_{A,k}$, $c_{A,k}^\dagger$ are defined locally in $A$.

5.1.1 Single-particle state $|k\rangle$

In the single-particle state $|k\rangle$, we write the density matrix of the whole system as

$$\rho_k = (c_{A,k}^\dagger + c_{B,k}^\dagger)|G\rangle\langle G| (c_{A,k} + c_{B,k}).$$  \hspace{1cm} (5.19)
5.1.3 Triple-particle state

The analytical calculations of the Rényi entropy in the triple-particle state are similar to the above. The results are the same as those in the fermionic chain in subsection 3.1.3. We will not show the details here.

There is no additional contribution to the Rényi entropy in the single-particle state $|k\rangle$.

5.1.2 Double-particle state $|k_1k_2\rangle$

In the double-particle state $|k_1k_2\rangle$ with general $k_1, k_2$, we write the density matrix of the whole system as

$$
\rho_{k_1k_2} = (c_{A,k_1}^\dagger + c_{B,k_1}^\dagger)(c_{A,k_2}^\dagger + c_{B,k_2}^\dagger)|G\rangle\langle G|(c_{A,k_1} + c_{B,k_1})(c_{A,k_2} + c_{B,k_2},
$$

and we get the RDM

$$
\rho_{A,k_1k_2} = \langle c_{A,k_1}^\dagger + c_{B,k_1}^\dagger\rangle\langle c_{A,k_2}^\dagger + c_{B,k_2}^\dagger\rangle|G\rangle\langle G|(c_{A,k_1} + c_{B,k_1})(c_{A,k_2} + c_{B,k_2}),
$$

and

$$
\rho_{A,k_1k_2} = \langle c_{A,k_1}c_{A,k_2}\rangle|G\rangle\langle G|\langle c_{A,k_1}c_{A,k_2}\rangle + \langle c_{B,k_1}c_{B,k_2}\rangle|G\rangle\langle G|\langle c_{B,k_1}c_{B,k_2}\rangle + \langle c_{A,k_1}c_{B,k_2}\rangle|G\rangle\langle G|\langle c_{A,k_1}c_{B,k_2}\rangle
$$

We have used for example:

$$
\text{tr}_B(c_{B,k_1}^\dagger c_{B,k_2}^\dagger|G\rangle\langle G|c_{B,k_2}c_{B,k_1}) = \text{tr}_B(S_{A,B,k_1}S_{A,B,k_2}|G\rangle\langle G|S_{A,B,k_2}S_{A,B,k_1}) = \langle \hat{c}_{B,k_1}\hat{c}_{B,k_2}\rangle|G\rangle\langle G|\langle \hat{c}_{B,k_1}\hat{c}_{B,k_2}\rangle,
$$

and

$$
\text{tr}_B(c_{B,k_1}^\dagger c_{B,k_2}^\dagger|G\rangle\langle G|c_{B,k_2}c_{B,k_1}) = \text{tr}_B(c_{A,k_1}^\dagger S_{A,B,k_2}|G\rangle\langle G|S_{A,B,k_2}c_{A,k_1}) = -\langle \hat{c}_{B,k_1}\hat{c}_{B,k_2}\rangle|G\rangle\langle G|\langle \hat{c}_{B,k_1}\hat{c}_{B,k_2}\rangle.
$$

Note the minus signs due to the anti-commutation relations. Then one can calculate $\text{tr}_A\rho_{A,k_1k_2}^n$ with $n = 2, 3, 4, 5, 6, 7$. They are the same as those in the fermionic chain presented in the subsection 3.1.2.

5.1.3 Triple-particle state $|k_1k_2k_3\rangle$

The analytical calculations of the Rényi entropy in the triple-particle state $|k_1k_2k_3\rangle$ with general $k_1, k_2, k_3$ are similar to the above. The results are the same as those in the fermionic chain in subsection 3.1.3. We will not show the details here.
5.2 Double interval

The double-interval Rényi entropies in the XY chain were calculated numerically in [28,30,34–36]. Here we will adopt the efficient method presented in [36] for the numerical calculations.

For the analytical calculations of the double-interval Rényi entropy, we define for \( i = 1,2 \)

\[
c_{A_i,k} = \frac{1}{\sqrt{L}} \sum_{j \in A_i} e^{ij\varphi_k} a_j, \quad c^\dagger_{A_i,k} = \frac{1}{\sqrt{L}} \sum_{j \in A_i} e^{-ij\varphi_k} a_j^\dagger,
\]

\[
c_{B_i,k} = \frac{1}{\sqrt{L}} \sum_{j \in B_i} e^{ij\varphi_k} a_j, \quad c^\dagger_{B_i,k} = \frac{1}{\sqrt{L}} \sum_{j \in B_i} e^{-ij\varphi_k} a_j^\dagger.
\]

We define the strings for \( X = A_1, A_2, B_1, B_2 \)

\[
S_X = \prod_{j \in X} \sigma_j^z.
\]

Then we define

\[
\tilde{c}_{A_i,k} = c_{A_i,k}, \quad \tilde{c}_{A_2,k} = S_{B_i} c_{A_2,k}, \quad \tilde{c}_{B_1,k} = S_{A_1} c_{B_1,k}, \quad \tilde{c}_{B_2,k} = S_{A_1} S_{A_2} c_{B_2,k},
\]

\[
\tilde{c}^\dagger_{A_i,k} = c^\dagger_{A_i,k}, \quad \tilde{c}^\dagger_{A_2,k} = S_{B_i} c^\dagger_{A_2,k}, \quad \tilde{c}^\dagger_{B_1,k} = S_{A_1} c^\dagger_{B_1,k}, \quad \tilde{c}^\dagger_{B_2,k} = S_{A_1} S_{A_2} c^\dagger_{B_2,k}.
\]

Note that \( \tilde{c}_{A_i,k}, \tilde{c}^\dagger_{A_i,k} \) are defined locally in \( A = A_1 \cup A_2 \), and \( \tilde{c}_{B_i,k}, \tilde{c}^\dagger_{B_i,k} \) are defined locally in \( B = B_1 \cup B_2 \). The operators \( \tilde{c}_{A_i,k}, \tilde{c}^\dagger_{A_i,k} \) commute with the operators \( \tilde{c}_{B_i,k}, \tilde{c}^\dagger_{B_i,k} \). For later convenience, we define for \( X = A_1, A_2, A, B_1, B_2, B \) the factors

\[
\beta_{X,k} = \frac{1}{L} \sum_{j \in X} e^{2\pi i j k}.
\]

5.2.1 Single-particle state \(|k\rangle\)

The single-particle state can be written as

\[
|k\rangle = (c^\dagger_{A_1,k} + c^\dagger_{A_2,k} + c_{B_1,k} + c_{B_2,k})|G\rangle = (c^\dagger_{A_1,k} + c^\dagger_{A_2,k} + c^\dagger_{B_1,k} + c^\dagger_{B_2,k})|G\rangle,
\]

and then we get the RDM

\[
\rho_{A_1A_2,k} = (c^\dagger_{A_1,k} + c^\dagger_{A_2,k})|G\rangle \langle G| \langle \tilde{c}_{A_1,k} + \tilde{c}_{A_2,k} + (\tilde{c}_{B_1,k} + \tilde{c}_{B_2,k})(\tilde{c}^\dagger_{B_1,k} + \tilde{c}^\dagger_{B_2,k})G |G\rangle,
\]

and finally we have

\[
\text{tr}_{A_1A_2} \rho_{A_1A_2,k} = x^n + y^n.
\]

There are no additional contributions to the universal Rényi entropy.

5.2.2 Double-particle state \(|k_1k_2\rangle\)

The double-particle state can be written as

\[
|k_1k_2\rangle = (c^\dagger_{A_1,k_1} + c^\dagger_{A_2,k_1} + c_{B_1,k_1} + c_{B_2,k_1})(c^\dagger_{A_1,k_2} + c^\dagger_{A_2,k_2} + c_{B_1,k_2} + c_{B_2,k_2})|G\rangle
\]

\[
= ([c^\dagger_{A_1,k_1} + c^\dagger_{A_2,k_1} + c^\dagger_{A_2,k_2} + c^\dagger_{B_1,k_2} + c_{B_1,k_1} + c_{B_2,k_2} + c_{B_1,k_1} + c_{B_2,k_2}]|G\rangle
\]

\[
+ c^\dagger_{B_1,k_1} (c^\dagger_{A_2,k_1} + c^\dagger_{A_2,k_2}) + c^\dagger_{B_1,k_1} + c_{B_1,k_1} c^\dagger_{B_2,k_2}
\]

\[
+ c_{B_2,k_1} (c^\dagger_{A_2,k_1} - c_{A_2,k_2}) + (c^\dagger_{B_1,k_1} + c_{B_2,k_1}) (c^\dagger_{B_1,k_2} + c_{B_2,k_2}) |G\rangle.
\]

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We get the RDM

\[
\rho_{A_1 A_2 k_1 k_2} = (\hat{c}_{A_1 k_1}^\dagger + \hat{c}_{A_2 k_2}^\dagger)(\hat{c}_{A_1 k_1} + \hat{c}_{A_2 k_2})|G_A\rangle \langle G_A| (\hat{c}_{A_1 k_1} + \hat{c}_{A_2 k_2}) (\hat{c}_{A_1 k_1}^\dagger + \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_1 k_1} \hat{c}_{B_1 k_1}^\dagger \rangle |G_B\rangle \langle G_B| (\hat{c}_{A_1 k_1} - \hat{c}_{A_2 k_2}) (\hat{c}_{A_1 k_1}^\dagger - \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_1 k_1} \hat{c}_{B_1 k_1}^\dagger \rangle |G_B\rangle \langle G_B| (-\hat{c}_{A_1 k_2}^\dagger + \hat{c}_{A_2 k_2}^\dagger) (\hat{c}_{A_1 k_2} \hat{c}_{A_1 k_2}^\dagger - \hat{c}_{A_2 k_2} \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_1 k_1} \hat{c}_{B_1 k_1}^\dagger \rangle |G_B\rangle \langle G_B| (-\hat{c}_{A_1 k_2} \hat{c}_{A_1 k_2}^\dagger + \hat{c}_{A_2 k_2} \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_2 k_2} \hat{c}_{B_2 k_2}^\dagger \rangle |G_B\rangle \langle G_B| (\hat{c}_{A_1 k_1} + \hat{c}_{A_2 k_2}) (\hat{c}_{A_1 k_1}^\dagger + \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_2 k_2} \hat{c}_{B_2 k_2}^\dagger \rangle |G_B\rangle \langle G_B| (-\hat{c}_{A_1 k_2}^\dagger - \hat{c}_{A_2 k_2}^\dagger) (\hat{c}_{A_1 k_2} \hat{c}_{A_1 k_2}^\dagger - \hat{c}_{A_2 k_2} \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_2 k_2} \hat{c}_{B_2 k_2}^\dagger \rangle |G_B\rangle \langle G_B| (-\hat{c}_{A_1 k_2} \hat{c}_{A_1 k_2}^\dagger - \hat{c}_{A_2 k_2} \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle \hat{c}_{B_2 k_2} \hat{c}_{B_2 k_2}^\dagger \rangle |G_B\rangle \langle G_B| (-\hat{c}_{A_1 k_2} \hat{c}_{A_1 k_2}^\dagger + \hat{c}_{A_2 k_2} \hat{c}_{A_2 k_2}^\dagger)
\]

\[
+ \langle (\hat{c}_{B_1 k_1} + \hat{c}_{B_2 k_2})(\hat{c}_{B_1 k_1}^\dagger + \hat{c}_{B_2 k_2}^\dagger)(\hat{c}_{B_1 k_1} \hat{c}_{A_1 k_1} + \hat{c}_{B_2 k_2} \hat{c}_{A_2 k_2})|G_B\rangle \langle G_A|.
\]

(5.36)

In the limit of large momentum difference $|k_1 - k_2| = +\infty$, we obtain the new universal Rényi entropies

\[
\mathcal{F}_{A_1 A_2 p_1 p_2}^{(2),\text{univ}} = (x^2 + y^2)^2 - 16x_1 x_2 y_1 y_2,
\]

\[
\mathcal{F}_{A_1 A_2 p_1 p_2}^{(3),\text{univ}} = (x^3 + y^3)^2 - 24x_1 x_2 y_1 y_2 x y,
\]

\[
\mathcal{F}_{A_1 A_2 p_1 p_2}^{(4),\text{univ}} = (x^4 + y^4)^2 - 32x_1 x_2 y_1 y_2 x^2 y^2 + 64x_1^2 x_2^2 y_1^2 y_2^2,
\]

\[
\mathcal{F}_{A_1 A_2 p_1 p_2}^{(5),\text{univ}} = (x^5 + y^5)^2 - 40x_1 x_2 y_1 y_2 x^3 y^3 + 160x_1^2 x_2^2 y_1^2 y_2^2 x y,
\]

\[
\mathcal{F}_{A_1 A_2 p_1 p_2}^{(6),\text{univ}} = (x^6 + y^6)^2 - 48x_1 x_2 y_1 y_2 x^4 y^4 + 288x_1^2 x_2^2 y_1^2 y_2^2 x^2 y^2 - 256x_1^3 x_2^3 y_1^3 y_2^3.
\]

(5.37)

Although quite remarkable, this is not surprising, and, in fact as stated in [60, 61], the validity of the universal Rényi entropy therein requires that the quasiparticles are localized quantum excitations, while in the XY chain the spinless fermions are not localized excitations. We also get $\mathcal{F}_{A_1 A_2 p_1 p_2}^{(n),\text{univ}}$ for larger $n$, but we will not show the results in this paper. Though the results are only for double interval in the XY chain, we still call them universal in the sense that they are not dependent on the explicit values.
of the momenta. Moreover, we get the additional contributions to the new universal Rényi entropy

\[ \delta F^{(2)}_{A_1A_2k_1k_2} = -2(x-y)(|\beta_{A_1,k_1-k_2}|^2 + |\beta_{A_2,k_1-k_2}|^2 - |\beta_{B_1,k_1-k_2}|^2 - |\beta_{B_2,k_1-k_2}|^2) - 2[x^2 - (y_1 - y_2)^2](\beta_{A_1,k_1-k_2}\beta_{A_2,k_2-k_1} + cc) - 2[y^2 - (x_1 - x_2)^2](\beta_{B_1,k_1-k_2}\beta_{B_2,k_2-k_1} + cc) - 4(xy - 2x_1y_1)(\beta_{A_1,k_1-k_2}\beta_{B_1,k_2-k_1} + cc) - 4(xy - 2x_1y_2)(\beta_{A_2,k_1-k_2}\beta_{B_1,k_2-k_1} + cc) - 4(xy - 2x_2y_1)(\beta_{A_1,k_1-k_2}\beta_{B_2,k_2-k_1} + cc) + (\beta_{A_1,k_1-k_2} + \beta_{B_1,k_1-k_2})^2 + (\beta_{A_2,k_2-k_1} + \beta_{B_2,k_2-k_1})^2 - 8(\beta_{A_1,k_1-k_2}\beta_{A_2,k_1-k_2}\beta_{B_1,k_2-k_1}\beta_{B_2,k_2-k_1} + cc), \]  

where we use “cc” to denote the complex conjugate terms. We also get \( \delta F^{(n)}_{A_1A_2k_1k_2} \) with \( n = 3, 4 \), whose forms are too complicated and we will not present them in this paper. We compare the analytical and numerical results in the figure 21. We see that the results with additional correction terms match perfectly with the numerical results, and in the limit of the large momentum difference the numerical results approach the new universal Rényi entropies instead of the old ones.

5.2.3 Slightly gapped and critical XY chains

We calculate the double-interval Rényi entropy in the single-particle state \(|k\rangle \) and the double-particle state \(|k_1k_2\rangle \) in the slightly gapped and critical XY chains, as shown respectively in the figures 22 and 23. In the slightly gapped XY chains, the results with additional correction terms are still valid in the limit of large momenta. As in the fermionic chain, the Rényi entropy is exact in the XY chain with \((\gamma, \lambda) = (0, 1)\), and this is because the Bogoliubov angle \( \theta_k \) defined in (5.6) is vanishing. However, in the critical XY chains with \((\gamma, \lambda) = (0, 0), (\gamma, \lambda) = (0, 0.5), (\gamma, \lambda) = (0.5, 1), (\gamma, \lambda) = (1, 1) \) and \((\gamma, \lambda) = (+\infty, \text{finite}) \) there are significant mismatches, for which we do not have a good understanding.

5.3 Multiple intervals

Unlike those in the extremely gapped fermionic and bosonic chains, the generalization to multiple intervals in the extremely gapped XY chain is more complicated. The analytical and numerical calculations of the multi-interval Rényi entropy in the extremely gapped XY chain are straightforward but tedious. We will not consider them in this paper.

6 Discussions

The main results that we have obtained in this paper are summarized in the section 2. We have calculated the Rényi entropies in single-particle, double-particle and triple-particle excited states of fermionic, bosonic, and XY models that depend on the model, momenta of the excited quasiparticles, and the connectedness of the subsystem. Although they are derived in the extremely gapped limit they are still valid in the slightly gapped and critical models as long as all the momenta of the excited quasiparticles are large. The Rényi entropy approaches the universal Rényi entropy in the limit that all the momentum differences among the excited quasiparticles are large.
Figure 21: The old universal Rényi entropy (red dotted lines), the new universal Rényi entropy (blue dashed lines), and the analytical (solid lines) and numerical (empty circles) results of the double-interval Rényi entropy in the double-particle state $|k_1 k_2\rangle$ of the extremely gapped XY chain. We have set $\lambda = +\infty$, $L = 64$, $k_1 = \frac{1}{2}$.
Figure 22: The universal Rényi entropy (dotted lines) and the numerical double-interval Rényi entropy in the slightly gapped and critical XY chains (symbols) in the single-particle state $|k\rangle$. We have set the momenta $k = \frac{1}{2} + \frac{L}{N}$, $x_1 = x_2 = \frac{1}{2}$. For the analytical results with additional terms we have set $L = +\infty$. 

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Figure 23: The old universal Rényi entropy (red dotted lines), the new universal Rényi entropy (blue dashed lines), the analytical Rényi entropy in the extremely gapped XY chain (solid lines), and the numerical Rényi entropy in the slightly gapped and critical XY chains (symbols) in the double-particle state $|k_1k_2\rangle$. We have set the momenta $(k_1, k_2) = (\frac{1}{2}, \frac{3}{2}) + \frac{L}{5}$, $x_1 = x_2 = \frac{1}{5}$. For the analytical results with additional terms we have set $L = +\infty$. 

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In figures 6, 7, 10, 11, 16, 20, 22, 23 we showed that the Rényi entropy in the slightly gapped fermionic, bosonic and XY chains approach to the results in the extremely gapped chain in the large system size and the large momentum limit, i.e. $L \to +\infty$ and $k_i \to +\infty$. It is interesting to quantify the convergence using numerical calculations.\(^3\) We show the result of the fermionic chain in the first row of figure 24 and find

$$
\left| 1 - \frac{F_{A,K}^{(2)}(\text{finite } \lambda)}{F_{A,K}^{(2)}(\lambda = +\infty)} \right| \sim \frac{1}{L}.
$$

We show the result of the bosonic chain in the first row of figure 25 and find

$$
\left| 1 - \frac{F_{A,K}^{(2)}(\text{finite } m)}{F_{A,K}^{(2)}(m = +\infty)} \right| \sim \frac{1}{L^2}.
$$

We show the result of the XY chain in the left two panels of figure 26 and find

$$
\left| 1 - \frac{F_{A,K}^{(2)}(\text{finite } \lambda)}{F_{A,K}^{(2)}(\lambda = +\infty)} \right| \sim \frac{1}{L}.
$$

It is also interesting to see how the Rényi entropy approaches to the expected analytical result with the increase of the gap $\Delta \to +\infty$. In the fermionic chain (3.1) with fixed $\gamma = 1$, the gap is $\Delta = \lambda - 1$ and in the bosonic chain (4.1) the gap is $\Delta = m$. We show the results of the fermionic chain in the second row of figure 24 and find

$$
\left| 1 - \frac{F_{A,K}^{(2)}(\text{finite } \lambda)}{F_{A,K}^{(2)}(\lambda = +\infty)} \right| \sim \frac{1}{(\lambda - 1)^2}.
$$

We show the results of the bosonic chain in the second row of figure 25 and find

$$
\left| 1 - \frac{F_{A,K}^{(2)}(\text{finite } m)}{F_{A,K}^{(2)}(m = +\infty)} \right| \sim \frac{1}{m^4}.
$$

We show the results of the XY chain in the right two panels of figure 26 and find

$$
\left| 1 - \frac{F_{A,K}^{(2)}(\text{finite } \lambda)}{F_{A,K}^{(2)}(\lambda = +\infty)} \right| \sim \frac{1}{(\lambda - 1)^2}.
$$

It is interesting to note the different scaling behaviors in different models. We get the same results for other values of the Rényi index $n$.

It is remarkable, though not surprising, that exact calculations reveals a new universal double-interval double-particle state Rényi entropy in the XY chain, which does not depend on the values of the momenta. In the limit of large gap and large momentum difference, the double-interval double-particle state Rényi entropies approach to the new universal Rényi entropies, instead of the old ones. The analytical double-interval double-particle state Rényi entropy we have obtained in XY chain is exact in the extremely gapped limit, i.e. that $\gamma$ is finite and $\lambda \to +\infty$, as well as at the critical and non-relativistic point $\gamma = 0, \lambda = 1$. We checked that it is still valid in the nearly gapped XY chains as long as all the momenta of the quasiparticles are large. However, it is not valid in the critical chains

\(^3\)We thank the anonymous referee for stimulating the discussions in this paragraph.
Figure 24: The ratio \(1 - \frac{\mathcal{F}^{(2)}_{\lambda,k}(\text{finite } \lambda)}{\mathcal{F}^{(2)}_{\lambda,k}(\lambda = +\infty)}\) in the fermionic chain (joined empty circles). For single interval we set \(x = \frac{1}{\gamma}\) and for double interval we set \(x_1 = x_2 = y_1 = \frac{1}{5}\). We have set the momenta \((k_1, k_2, k_3) = (\frac{1}{2}, \frac{3}{2}, \frac{5}{2}) + \frac{L}{8}\). We add red straight lines in each figure serving as guidance to the eye to demonstrate the asymptotic behaviors of the Rényi entropy. In the first row the red lines are proportional to \(\frac{1}{L}\), and in the second row the red lines are proportional to \(\frac{1}{(\lambda - 1)^2}\).

even when all the momenta of the quasiparticles are large (except at the special non-relativistic point \(\gamma = 0, \lambda = 1\)), for which we do not have a good explanation. We hope to come back to the problem in the future.

We calculated analytically the Rényi entropy with a relatively small Rényi index \(n\) in an excited state with a rather small number of quasiparticles in the extremely gapped fermionic, bosonic, and XY chains by writing the excited states in terms of local excitations. In the extremely gapped fermionic and bosonic chains, we established respectively the formulas (3.68) and (4.37), which are much more efficient in the analytical calculations. These formulas are also very efficient in numerical calculations. We anticipate that they would be useful to calculate the Rényi entropy for generic \(n\), make the analytical continuation \(n \to 1\), and get the entanglement entropy. In subsection (3.4) we have made some preliminary investigations and obtained the entanglement entropy in the double-particle and triple-particle states in the extremely gapped fermionic chain. This is especially intriguing for the excited state Rényi entropy in the bosonic chain, for which as far as we know there is no even a numerical method to calculate the excited state entanglement entropy.

In this paper we have only considered the models where there are only one kind of quasiparticles, and the “interactions” between quasiparticles of different momenta lead to the additional contributions
Figure 25: The ratio \(1 - \frac{x_A^{(2)}(\text{finite } m)}{x_A^{(2)}(m=+\infty)}\) in the bosonic chain (joined empty circles). For single interval we set \(x = \frac{1}{4}\) and for double interval we set \(x_1 = x_2 = y_1 = \frac{1}{5}\). We have set the momenta \((k_1, k_2, k_3) = (1, 2, 3) + \frac{L}{8}\). We add the red straight lines as guidance to the eye. In the panels (a), (b), (d), (e) and (f) there are oscillations, and we add multiple red straight lines. In the first row the red lines are proportional to \(\frac{1}{L^2}\), and in the second row the red lines are proportional to \(\frac{1}{m^2}\).

Figure 26: The ratio \(1 - \frac{x_A^{(2)}(\text{finite } \lambda)}{x_A^{(2)}(\lambda=+\infty)}\) in the XY chain (joined empty circles). For single interval we set \(x = \frac{1}{4}\) and for double interval we set \(x_1 = x_2 = y_1 = \frac{1}{8}\). We have set the momenta \(k = \frac{1}{2} + \frac{L}{8}\) and \((k_1, k_2) = (\frac{1}{2}, \frac{3}{2}) + \frac{L}{8}\). The red straight lines are guidance to the eye. In the left two panels the red lines are proportional to \(\frac{1}{L}\), and in the right two panels the red lines are proportional to \(\frac{1}{(\lambda-1)^2}\).
to the universal Rényi entropy. It would be interesting to consider the excited state Rényi entropy in the models with more than one kind of quasiparticles, and the interactions between different kinds of quasiparticles can in principle lead to the additional terms.

It would be interesting to compare quantitatively the difference of a subsystem density matrices of two different quasiparticle excited states. The Schatten and trace distances between the two RDMs can do this job. Then one expects the universal subsystem Schatten and trace distances and their corrections, similar to the universal Rényi and entanglement entropies whose validity requires both large momenta and large momentum difference and their corrections that are valid in the limit of large momenta. We have reported some preliminary results in [88,89], and we will report more details in [90].

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A Wave function method in bosonic chain

We review the method of wave function to calculate the excited state Rényi entropy in the bosonic chain [60,61], and especially we also show how it can be used to calculate analytically the Rényi entropy in the extremely massive limit. We only give the formulas we used to calculate numerically and analytically the Rényi entropy. One can see more details in [61], as well as in [89]. We follow the convention in [89].

We focus on the case of one single interval \( A = [1, \ell] \) and its complement \( B = [\ell + 1, L] \). It is similar for the double-interval and multi-interval cases, one just needs to relabel the sites. We will not show the details here.

A.1 General gapped bosonic chain

The ground state wave function is related to the \( L \times L \) matrix

\[
W_{j_1 j_2} = w_{j_1 - j_2}, \quad w_j = \frac{1}{L} \sum_{k=1-L^2}^{L^2} \varepsilon_k e^{2\pi i j k / L},
\]

(A.1)

where \( \varepsilon_k \) is the single-particle energy (4.5). One can write the above matrix as a \( 2 \times 2 \) block matrix as follows:

\[
W = \begin{pmatrix}
A & B \\
C & D
\end{pmatrix},
\]

(A.2)
with the matrices $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\mathcal{D}$ of respectively $\ell \times \ell$, $\ell \times (L - \ell)$, $(L - \ell) \times \ell$, $(L - \ell) \times (L - \ell)$ entries. By replica trick, one can construct the $nL \times nL$ matrix $\mathcal{M}$ with $2n \times 2n$ blocks

$$
\mathcal{M} = \begin{pmatrix}
\begin{array}{ccc}
2\mathcal{A} & \mathcal{B} & C \\
C & 2\mathcal{D} & C \\
C & 2\mathcal{D} & C \\
\mathcal{B} & 2\mathcal{A} & \mathcal{B} \\
\mathcal{B} & 2\mathcal{A} & \mathcal{B} \\
\mathcal{B} & 2\mathcal{A} & \mathcal{B} \\
C & 2\mathcal{D} & C \\
C & 2\mathcal{D} & C \\
C & 2\mathcal{D} & C \\
\hline 
B & \cdots & \cdots \\
\cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots \\
\end{array}
\end{pmatrix}.

$$

(A.3)

We consider a general excited state $|K\rangle$, and its wave function is related to a function $f_K(\{u_k\})$ that depends on

$$
u_k = \sqrt{\frac{2\varepsilon_k}{L}} \sum_{j=1}^{L} e^{-\frac{2\pi i j k}{L}} q_{a,j}. \quad \text{(A.4)}$$

The wave functions $f_K(\{u_{a,k}\})$ and $f_K(\{v_{a,k}\})$ of the replicated ket state $|K\rangle$ and bra state $\langle K|$ depend respectively on

$$
u_{a,k} = \sqrt{\frac{2\varepsilon_k}{L}} \sum_{j=1}^{L} e^{-\frac{2\pi i j k}{L}} q_{a,j},

\quad \text{and}

$$
v_{a,k} = \sqrt{\frac{2\varepsilon_k}{L}} \left( \sum_{j=1}^{\ell} e^{-\frac{2\pi i j k}{L}} q_{a+1,j} + \sum_{j=\ell+1}^{L} e^{-\frac{2\pi i j k}{L}} q_{a,j} \right).

$$

(A.5)

with $q_{a,j}$ being the replicated coordinates and $a = 1, 2, \cdots, n$ being the replica indices. It is understood that $q_{a+1,j} = q_{1,j}$.

The Rényi entropy in the state $|K\rangle$ can be written as the expectation value

$$
\mathcal{F}_{A,K}^{(n)} = \left\langle \prod_{a=1}^{n} [f_K(\{u_{a,k}\})f_K(\{v_{a,k}\})] \right\rangle.

$$

(A.6)

The definition of $\langle \cdots \rangle$ could be found in Eq. (3.30) of [89] and it could be evaluated by the bosonic Wick contractions

$$
\begin{align*}
\sqrt{u_{a_1,k_1}u_{a_2,k_2}} &= U_{a_1,k_1}^T \mathcal{M}^{-1} U_{a_2,k_2}, \\
\sqrt{v_{a_1,k_1}v_{a_2,k_2}} &= V_{a_1,k_1}^T \mathcal{M}^{-1} V_{a_2,k_2}, \\
\sqrt{v_{a_1,k_1}v_{a_2,k_2}} &= V_{a_1,k_1}^T \mathcal{M}^{-1} V_{a_2,k_2}.
\end{align*}

$$

(A.7)

The vectors $U_{a,k}$, $V_{a,k}$ with $nL$ components have the nonvanishing entries

$$
\begin{align*}
[U_{a,k}]_{(a-1)L+j} &= \sqrt{\frac{2\varepsilon_k}{L}} e^{-\frac{2\pi i j k}{L}}, \quad a = 1, \cdots, n, \quad j = 1, \cdots, L, \\
[V_{a,k}]_{(a-1)L+j} &= \sqrt{\frac{2\varepsilon_k}{L}} e^{\frac{2\pi i j k}{L}}, \quad a = 1, \cdots, n, \quad j = \ell + 1, \cdots, L, \\
[V_{a,k}]_{aL+j} &= \sqrt{\frac{2\varepsilon_k}{L}} e^{\frac{2\pi i j k}{L}}, \quad a = 1, \cdots, n-1, \quad j = 1, \cdots, \ell, \\
[V_{n,k}]_{j} &= \sqrt{\frac{2\varepsilon_k}{L}} e^{\frac{2\pi i j k}{L}}, \quad j = 1, \cdots, \ell.
\end{align*}

$$

(A.8)
A.2 Extremely gapped bosonic chain

In the extremely gapped limit \( m \to +\infty \), it is convenient to rescale the matrix (A.3), the coordinates (A.5), and the vectors (A.8) as

\[
\tilde{\mathcal{M}} = \frac{\mathcal{M}}{2m}, \quad \tilde{u}_{a,k} = \frac{u_{a,k}}{\sqrt{2m}}, \quad \tilde{v}_{a,k} = \frac{v_{a,k}}{\sqrt{2m}}, \quad \tilde{U}_{a,k} = \frac{U_{a,k}}{\sqrt{2m}}, \quad \tilde{V}_{a,k} = \frac{V_{a,k}}{\sqrt{2m}}. \tag{A.9}
\]

The function \( w_j \) defined in (A.1) becomes trivially

\[
w_j = m\delta_j, \tag{A.10}
\]

and then the matrix \( \tilde{\mathcal{M}} = I_{nL} \) is just the \( nL \times nL \) identity matrix. We obtain the vectors

\[
\begin{align*}
[\tilde{U}_{a,k}]_{(a-1)L+j} &= \frac{1}{\sqrt{L}} e^{-\frac{2\pi i j k}{L}}, \ a = 1, \cdots, n, \ j = 1, \cdots, L, \\
[\tilde{V}_{a,k}]_{(a-1)L+j} &= \frac{1}{\sqrt{L}} e^{\frac{2\pi i j k}{L}}, \ a = 1, \cdots, n, \ j = 1, \cdots, L, \\
[\tilde{V}_{a,k}]_{aL+j} &= \frac{1}{\sqrt{L}} e^{\frac{2\pi i j k}{L}}, \ a = 1, \cdots, n - 1, \ j = 1, \cdots, \ell, \\
[\tilde{V}_{n,k}]_{j} &= \frac{1}{\sqrt{L}} e^{\frac{2\pi i j k}{L}}, \ j = 1, \cdots, \ell. \tag{A.11}
\end{align*}
\]

Then we get the Rényi entropy in the extremely gapped bosonic chain

\[
\mathcal{F}_{n,k}^{(n)} = \left\langle \prod_{a=1}^{n} f_K(\{\tilde{u}_{a,k}\}) f_K(\{\tilde{v}_{a,k}\}) \right\rangle, \tag{A.12}
\]

which is evaluated by the bosonic Wick contractions

\[
\begin{align*}
\tilde{u}_{a_1,k_1} \tilde{u}_{a_2,k_2} &= \tilde{U}_{a_1,k_1}^{T} \tilde{U}_{a_2,k_2}, \\
\tilde{v}_{a_1,k_1} \tilde{v}_{a_2,k_2} &= \tilde{V}_{a_1,k_1}^{T} \tilde{V}_{a_2,k_2}, \\
\tilde{v}_{a_1,k_1} \tilde{u}_{a_2,k_2} &= \tilde{V}_{a_1,k_1}^{T} \tilde{U}_{a_2,k_2}. \tag{A.13}
\end{align*}
\]

Note that

\[
\tilde{U}_{a_1,k_1}^{T} \tilde{U}_{a_2,k_2} = \tilde{V}_{a_1,k_1}^{T} \tilde{V}_{a_2,k_2} = \delta_{a_1 a_2} \delta_{k_1 + k_2}, \tag{A.14}
\]

with \( \delta_{k_1 + k_2} = 1 \) for \( k_1 + k_2 = 0 \) and \( k_1 = k_2 = \frac{L}{2} \) and \( \delta_{k_1 + k_2} = 0 \) otherwise. We get the product

\[
\tilde{V}_{a_1,k_1}^{T} \tilde{U}_{a_2,k_2} = \left\{ \begin{array}{ll}
1 - x & k_1 = k_2 \\
-\alpha_{k_1 - k_2} & k_1 \neq k_2, \quad a_1 = a_2 \\
x & k_1 = k_2, \quad a_1 = a_2 - 1 \mod n' \\
\alpha_{k_1 - k_2} & k_1 \neq k_2, \quad a_1 = a_2 \\
0 & \text{otherwise}
\end{array} \right. \tag{A.15}
\]

with the definition of the function \( \alpha_k \) given in (3.30).

We consider a special state \( |k_1^{r_1} k_2^{r_2} \cdots k_s^{r_s}\rangle \) that only the modes with momenta \( k_1, k_2, \cdots, k_s \in \{1, 2, \cdots, \frac{L}{2} - 1\} \) are excited. We have

\[
f_K(\{\tilde{u}_{a,k}\}) = \prod_{i=1}^{s} \frac{\tilde{u}_{a,k}}{\sqrt{r_i}}, \quad f_K(\{\tilde{v}_{a,k}\}) = \prod_{i=1}^{s} \frac{\tilde{v}_{a,k}}{\sqrt{r_i}}. \tag{A.16}
\]
Then we get the Rényi entropy

\[ \mathcal{F}_{A,K}^{(n)} = \frac{1}{\prod_{i=1}^{n}(r_i)!} \langle \prod_{a=1}^{n} \prod_{i=1}^{s} [u_{a,k_i}^T v_{a,k_i}] \rangle, \]  

(A.17)

with the only non-vanishing contractions

\[ \tilde{v}_{a_1,k_1} u_{a_2,k_2} = \tilde{V}_{a_1,k_1}^{T} \tilde{U}_{a_2,k_2}, \]  

(A.18)

which is just (A.15). The total number of excited modes is

\[ R = \sum_{i=1}^{s} r_i, \]  

(A.19)

and in replica trick it becomes \( nR \). On the RHS of (A.17) there are \( nR \) number of \( \tilde{u}_{a,k} \) and \( nR \) number of \( v_{a,k} \), and we organize them as \( \tilde{u}_I, \tilde{v}_I \) with \( I = 1, 2, \cdots, nR \). Note that each of \( \tilde{u}_{a,k_i} \) and \( \tilde{v}_{a,k_i} \) has a repetition of \( r_i \) times. For \( \tilde{u}_I, \tilde{v}_I \), there are corresponding vectors \( \tilde{U}_I, \tilde{V}_I \). We define the \( nR \times nR \) matrix \( \Omega_{A,K}^{(n)} \) with entries

\[ [\Omega_{A,K}^{(n)}]_{IJ} = \tilde{V}_I^{T} \tilde{U}_J. \]  

(A.20)

The excited state Rényi entropy in the extremely gapped bosonic chain (A.17) is just the permanent\(^4\)

\[ \mathcal{F}_{A,K}^{(n)} = \frac{\text{per} \Omega_{A,K}^{(n)}}{\prod_{i=1}^{n}(r_i)!}. \]  

(A.22)

Although we have derived the final formula (A.22) for the special state \( |K\rangle = |k_1^{r_1} k_2^{r_2} \cdots k_s^{r_s}\rangle \) that only the modes with momenta \( k_1, k_2, \cdots, k_s \in \{1, 2, \cdots, \frac{L}{2} - 1\} \) are excited, it can be shown that the formula applies to a general excited state \( |k_1^{r_1} k_2^{r_2} \cdots k_s^{r_s}\rangle \) with momenta \( k_1, k_2, \cdots, k_s \in \{-\frac{L}{2} + 1, \cdots, -1, 0, 1, \cdots, \frac{L}{2}\} \) as long as a property of the Hermite polynomials and the complex Hermite polynomials, which we elaborate below, is correct.

As it is already shown in [80], in the wave function with the modes \( k = 0, \frac{L}{2} \), appear the Hermite polynomials

\[ H_r(x) = e^{\frac{x^2}{2}}(x - \partial_x)^r e^{-\frac{x^2}{2}} = (-)^r e^{2x^2} \partial_x^r e^{-2x^2}, \]  

(A.23)

and for other modes there appear the complex Hermite polynomials

\[ H_{r,s}(z, \bar{z}) = e^{z\bar{z}}(z - \partial_z)^r (\bar{z} - \partial_{\bar{z}})^s e^{-z\bar{z}} = (-)^{r+s} e^{2z\bar{z}} \partial_z^r \partial_{\bar{z}}^s e^{-2z\bar{z}}. \]  

(A.24)

The Hermite polynomials are orthogonal

\[ \langle H_r(x) H_s(x) \rangle = \delta_{rs} 2^r r!, \]  

(A.25)

\(^4\)Naively, we would expect that the formula

\[ \mathcal{F}_{A,K}^{(n)} = \det \Omega_{A,K}^{(n)}, \]  

(A.21)

applies to a general excited state \( |K\rangle = |k_1 k_2 \cdots k_s\rangle \) in the extremely gapped fermionic chain. We compared the analytical results coming from (A.21) with the results we get by writing the excited states in terms of local excitations in the section 3, and found that (A.21) leads to a correct result for an odd integer \( n = 3, 5, \cdots \) but leads to a wrong result when \( n \) is an even integer. In fact for an even integer \( n \) the formula (A.21) cannot even give the correct universal part of the Rényi entropy let alone the additional part. It would be interesting to have a better understanding of the formula (A.21) in the extremely gapped fermionic chain and the formula (A.22) in the extremely gapped bosonic chain.

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with the expectation value evaluated by the bosonic Wick contraction

$$\prod_{xx} = \frac{1}{2}.$$  \hspace{1cm} (A.26)

Note that $H_0(x) = 1$ and $H_1(x) = 2x$. We claim that

$$\langle H_r(x)H_s(x) \rangle = \langle \overset{r}{(2x)^r} H_s(x) \rangle,$$  \hspace{1cm} (A.27)

where we impose the rule that the Wick contractions between the variables under the same curly bracket are not allowed. Using the recursive formula for $s \geq 1$

$$H_s(x) = 2xH_{s-1}(x) - H'_{s-1}(x),$$  \hspace{1cm} (A.28)

we get for $r \geq 1$

$$\langle (2x)^r H_s(x) \rangle = 2r \langle (2x)^{r-1} H_{s-1}(x) \rangle,$$  \hspace{1cm} (A.29)

which proves the claim (A.27). As the Hermite polynomials are complete, we get

$$\langle H_r(x)P(x) \rangle = \langle (2x)^r P(x) \rangle,$$  \hspace{1cm} (A.30)

for an arbitrary polynomial $P(x)$ of $x$.

The complex Hermite polynomials are also complete and orthogonal

$$\langle H_{r,s}(z,\bar{z})H_{p,q}(z,\bar{z}) \rangle = \delta_{rq}\delta_{sp}2^{r+s}r!s!, \hspace{1cm} (A.31)$$

with the expectation value evaluated by the bosonic Wick contractions

$$\prod_{z\bar{z}} = \prod_{\bar{z}z} = 0, \hspace{0.5cm} \prod_{z\bar{z}} = \frac{1}{2}.$$  \hspace{1cm} (A.32)

Note that $H_{0,0}(z,\bar{z}) = 1$, $H_{1,0}(z,\bar{z}) = 2z$, $H_{0,1}(z,\bar{z}) = 2\bar{z}$. Note also $[H_{r,s}(z,\bar{z})]^* = H_{s,r}(z,\bar{z})$. From the recursive formulas

\[ H_{r,s}(z,\bar{z}) = 2zH_{r-1,s}(z,\bar{z}) - \partial_z H_{r-1,s}(z,\bar{z}), \quad r \geq 1, \]
\[ H_{r,s}(z,\bar{z}) = 2\bar{z}H_{r,s-1}(z,\bar{z}) - \partial_\bar{z} H_{r,s-1}(z,\bar{z}), \quad s \geq 1, \]  \hspace{1cm} (A.33)

we get

\[ \langle (2z)^r(2\bar{z})^s H_{p,q}(z,\bar{z}) \rangle = 2r \langle (2z)^{r-1}(2\bar{z})^s H_{p,q-1}(z,\bar{z}) \rangle, \quad r, q \geq 1, \]
\[ \langle (2z)^r(2\bar{z})^s H_{p,q}(z,\bar{z}) \rangle = 2s \langle (2z)^r(2\bar{z})^{s-1} H_{p-1,q}(z,\bar{z}) \rangle, \quad s, p \geq 1. \]  \hspace{1cm} (A.34)

This leads to

$$\langle H_{r,s}(z,\bar{z})H_{p,q}(z,\bar{z}) \rangle = \langle (2z)^r(2\bar{z})^s H_{p,q}(z,\bar{z}) \rangle,$$  \hspace{1cm} (A.35)

and then for an arbitrary polynomial $P(z,\bar{z})$ of $z,\bar{z}$ we further get

$$\langle H_{r,s}(z,\bar{z})P(z,\bar{z}) \rangle = \langle (2z)^r(2\bar{z})^s P(z,\bar{z}) \rangle.$$  \hspace{1cm} (A.36)
This proves the formula (A.22) with (A.15), which applies to a general excited state \(|k_1 k_2 \cdots k_s\rangle\) in the extremely gapped bosonic chain. It can be used to calculate analytically the Rényi entropy in the extremely gapped bosonic chain when the number of excited quasiparticles \(R\) is small. We check that the analytical calculations with the wave function method always lead to the same results as we get by the subsystem mode method in the section 4, but unfortunately, we cannot prove the equivalence of the two methods for general states. When \(R\) is large, although the analytical calculations are cumbersome, the numerical calculations are still very efficient.

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