Particle partition entanglement of one dimensional spinless fermions

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Abstract. We investigate the scaling of the Rényi entanglement entropies for a particle bipartition of interacting spinless fermions in one spatial dimension. In the Tomonaga-Luttinger liquid regime, we calculate the second Rényi entanglement entropy and show that the leading order finite-size scaling is equal to a universal logarithm of the system size plus a non-universal constant. Higher-order corrections decay as power-laws in the system size with exponents that depend only on the Luttinger parameter. We confirm the universality of our results by investigating the one dimensional $t - V$ model of interacting spinless fermions via exact-diagonalization techniques. The resulting sensitivity of the particle partition entanglement to boundary conditions and statistics supports its utility as a probe of quantum liquids.

1. Introduction

Identical particles are fundamentally indistinguishable in quantum mechanics, unlike their classical counterparts that can always be discriminated due to an infinite set of observable properties. While this indistinguishability allows for the power provided by the second quantization formalism, it can also lead to ambiguity [1, 2, 3] when considering another defining property of composite quantum systems: entanglement. A pure state representing N quantum particles $|\Psi\rangle \in \mathcal{H}$ in Hilbert space $\mathcal{H}$ is said to be bipartite entangled if it cannot be written in a simple tensor product form $|\Psi\rangle \neq |\Psi_A\rangle \otimes |\Psi_B\rangle$ where A and B are vector spaces with $|\Psi_A\rangle \in A$ and $|\Psi_B\rangle \in B$ such that $A \otimes B = \mathcal{H}$. Conventionally, A and B correspond to a set of distinguishable single-particle modes whose occupation numbers are physical observables, i.e., spatial or momentum modes. However, for indistinguishable itinerant particles, there is no natural tensor product decomposition into single-particle modes due to the symmetrization or anti-symmetrization of the wavefunction with respect to the interchange of first quantized particle coordinates for bosons and fermions, respectively. Thus, the *mode entanglement* may depend on the choice of single-particle modes, leading to questions as to which (if any) are preferred and moreover, if these quantum correlations are even physically meaningful [4, 5, 6, 7, 8, 9, 10, 11]. For example, even in the absence of interactions, a system of N free itinerant bosons [12, 13] or fermions [14, 15, 16] is always entangled under a spatial biparition as a result of all allowed states being normalized linear combinations of Slater determinants or permanents.

Insights into these issues can be gained by considering the N-body wavefunction in first quantized form where a bipartition can be made in terms of identical particle labels. The resulting *n-particle partition entanglement* is a measure of quantum correlations between the subsets of n and $N - n$ particles. As individual (or groups of) identical particles are not operationally distinguishable, there have been claims that this type of entanglement is not useful as a resource for quantum information processing [4, 17, 10]. However, schemes have been recently proposed to transfer it to experimentally addressable modes [18]. In a foundational series of papers, Haque *et al.* explored the particle partition entanglement in fractional quantum hall [19, 20] and itinerant bosonic, fermionic and anyonic lattice gases in one spatial dimension [21, 22]. This type of particle partition entanglement has since been investigated in other one dimensional systems including the fermionic Calogero-Sutherland [23], anyonic hard-core [24] and bosonic Lieb-Liniger [25, 26] models as well as rotating bose and fermi gases in two dimensions [27]. In analogy to the universal finite size scaling behavior of the entanglement entropy of one dimensional quantum gases under a spatial mode bipartition [28, 29, 30], a leading order scaling form for the particle partition entanglement entropy S supported by exact diagonalization on small lattice models was proposed in Ref. [21] which is linear in the subsystem size n and logarithmic in the system size N: $S \sim n \ln N$.

Motivated by this empirical prediction, in this paper, we investigate the particle

partition entanglement for itinerant interacting spinless fermions in one spatial dimension. For Galilean invariant systems in the spatial continuum, we confirm the scaling form proposed in Ref. [21] within the Tomonaga-Luttinger liquid framework [31, 32] and determine how the leading order power-law corrections to the asymptotic scaling depend on the strength of the interactions between particles for $n = 1$. By exploiting symmetries of the n-particle reduced density matrix, we are able to measure the particle entanglement entropy in the one dimensional fermionic $t - V$ model for systems composed of up to $M = 28$ lattice sites at half filling, allowing us to confirm our predictions from continuum field theory.

The rest of this paper is organized as follows. We introduce a quantitative measure of entanglement, the Rényi entanglement entropy and discuss some known results for interacting spinless fermions. We then derive the 1-particle entanglement entropy in the low energy limit and compare with exact diagonalization results on a lattice. We conclude with a discussion of the role of boundary conditions, degeneracy and implications for future studies of models with generalized statistics. All numerical data and code necessary to reproduce the results and figures in this paper can be found in Ref. [33].

2. Particle Partition Entanglement

The entanglement of the pure state $|\Psi\rangle$ under a general bipartition into A and B can be quantified via the Rényi entanglement entropy:

$$S_\alpha\left[\rho_A\right] \equiv \frac{1}{1-\alpha} \ln\left(\mathrm{Tr}\rho_A^\alpha\right), \tag{1}$$

where α is the Rényi index and ρ_A is the reduced density matrix obtained by tracing out all degrees of freedom in B

$$\rho_A \equiv \mathrm{Tr}_B \left|\Psi\right\rangle\!\left\langle\Psi\right|. \tag{2}$$

For $\alpha = 1$ the Rényi entropy is equivalent to the von Neumann entropy: $-\mathrm{Tr}\,\rho_A \ln \rho_A$. While it is common for A and B to be defined by some set of observable modes, for a many-body system consisting of N itinerant particles they can refer to subsystems of particles. As depicted in Fig. 1, such a bipartition of indistinguishable particles (in this case spinless fermions) is completely specified by the number of particles in the subsystem, n. The entanglement entropy under a particle bipartition is then a function of the familiar n-body reduced density matrix ρ_n, (n-RDM) defined in first quantized notation in one spatial dimension as:

$$\rho_n \equiv \int dx_{n+1} \cdots \int dx_N \left\langle x_{n+1} \cdots x_N |\Psi\right\rangle \left\langle \Psi| x_{n+1} \cdots x_N\right\rangle \tag{3}$$

where we have taken the normalization $\mathrm{Tr}\rho_n = 1$. From this form, it is clear that the particle partition Rényi entropies $S_\alpha[\rho_n] \equiv S_\alpha(n)$ only vanish when the N-body ground
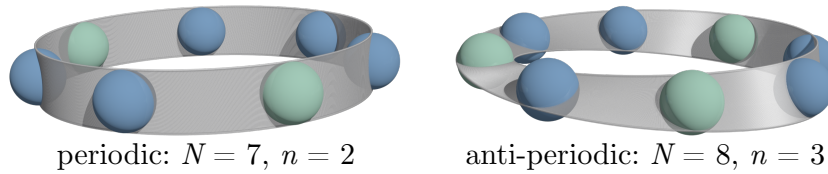
periodic: $N = 7$, $n = 2$ anti-periodic: $N = 8$, $n = 3$

Figure 1. A schematic of $N = 7$ fermions in one spatial dimension subject to periodic boundary conditions under a n-particle partition with $n = 2$ (left) and anti-periodic boundary conditions with $N = 8$ and $n = 3$ (right). All fermions are identical, while the partitions A and B are distinguished via their first quantized labels.

state $|\Psi\rangle$ can be written as a general tensor product state in first quantized notation. This immediately implies that $S_\alpha(n) = 0$ when all particles are condensed into a single mode, and thus the particle partition entanglement of the non-interacting Bose gas is identically zero, in contrast to non-zero results for its spatial mode entanglement [12, 13]. This is not the case for many-fermion systems, which always have non-zero particle entanglement, even in the absence of interactions [15]. Particle entanglement entropy is sensitive to both interactions and statistics, and as ρ_n is free of any length scale, it can capture non-local effects making it complimentary to the more conventionally studied spatial mode entanglement entropy.

As described in the introduction, Zozulya et al. [21] first proposed a "standard" finite-size scaling form for the particle entanglement entropy of fermions:

$$S(n, N) = \ln \binom{N}{n} + a + \mathcal{O}\left(\frac{1}{N^\gamma}\right) \tag{4}$$

where a and γ are non-universal dimensionless numbers that can depend on n. These coefficients are known for the case of non-interacting fermions where $a = 0$ [22] and for the Laughlin state with filling fraction ν: $a = -n \ln \nu$, $\gamma = 2$ when $n \ll N$ [19].

Recently, a general scaling form like Eq. (4) was investigated for a system of interacting bosons in the spatial continuum with $n = 1$ [26] where it was found that the pre-factor of the leading order logarithm is non-universal, depending on the interaction strength. In this paper, we apply extensions of these methods to interacting Galilean invariant one dimensional fermions and are able to systematically derive Eq. (4) while presenting results for both a and γ as a function of the interaction strength.

3. One-particle entanglement in fermionic Tomonaga-Luttinger liquids

We are interested in the asymptotic finite size scaling of the entanglement entropy (EE) as defined in Eq. (1) which can be investigated for any Rényi index α. Here we focus on the special case of $\alpha = 2$ as (i) the calculation will turn out to be analytically tractable and (ii) as it can be related to the expectation value of a local observable, it has proved to be the most direct numerical [34, 35, 36, 37] and even experimental [38, 39] route to its measurement. We begin by considering a system of N one-dimensional interacting

spinless fermions with density $\rho_0 = N/L$ (where L is the length of the system) whose low energy properties can be described in terms of the universal quantum hydrodynamics of Tomonaga-Luttinger liquid (TLL) theory [31, 32]. Within this framework, at zero temperature in the thermodynamic limit, any n-body reduced density matrix can in principle be computed [40] and in particular for $n = 1$ [41]

$$\rho_1\left(x, x'\right) = \frac{\sin(\pi \rho_0 |x - x'|)}{\pi \rho_0 L |x - x'| (1 + |x - x'|^2 \Lambda^2)^{(K + K^{-1} - 2)/4}}, \tag{5}$$

where $\text{Tr}\,\rho_1 = 1$ and both the ultraviolet (inverse short-distance) cutoff Λ and TLL parameter K depend on the microscopic details of the interaction between particles. Specifically, K characterizes the nature of the interaction, where $0 < K < 1$ ($K > 1$) corresponds to repulsive (attractive) interactions with free fermions having $K = 1$. For ease of notation, we will replace the non-negative K-dependent exponent in Eq. (5) with $g \equiv (K + K^{-1} - 2)/4$.

The one-particle partition second Rényi entanglement entropy can be computed by using ρ_1 in Eq. (1)

$$S_2(n = 1) = -\ln\left(\text{Tr}\left[\rho_1^2\right]\right) = -\ln\left(\int_{-L/2}^{L/2} dx \int_{-L/2}^{L/2} dx' \rho_1\left(x, x'\right) \rho_1\left(x', x\right)\right)$$
$$= \ln(N) - \ln(f(N, g, \Lambda/\rho_0)), \tag{6}$$

where we have used translational invariance of the system and

$$f(N, g, \Lambda/\rho_0) = \int_0^\infty dy \frac{2 \sin^2(\pi y)}{\pi^2 y^2 (1 + y^2 \Lambda^2/\rho_0^2)^{2g}}$$
$$- \int_{N/2}^\infty dy \frac{2 \sin^2(\pi y)}{\pi^2 y^2 (1 + y^2 \Lambda^2/\rho_0^2)^{2g}}. \tag{7}$$

The first integral can be evaluated exactly in terms of special functions:

$$A(g, \Lambda/\rho_0) = \int_0^\infty dy \frac{2 \sin^2(\pi y)}{\pi^2 y^2 (1 + y^2 \Lambda^2/\rho_0^2)^{2g}}$$
$$= \frac{\pi^{4g + \frac{1}{2}} \rho_0^{4g} \sec(2\pi g) \, {}_1F_2\left(2g; 2g + 1, 2g + \frac{3}{2}; \pi^2 \Lambda^{-2} \rho_0^2\right)}{2 \Lambda^{4g} \Gamma(2g + 1) \Gamma(2g + \frac{3}{2})}$$
$$+ \frac{\Lambda \Gamma\left(2g + \frac{1}{2}\right) \left[{}_1F_2\left(-\frac{1}{2}; \frac{1}{2}, \frac{1}{2} - 2g; \pi^2 \Lambda^{-2} \rho_0^2\right) - 1\right]}{\pi^{3/2} \rho_0 \Gamma(2g)}. \tag{8}$$

where ${}_1F_2(q; c, d; z)$ is the generalized hypergeometric and $\Gamma(z)$ the Gamma function. The leading order N dependence of the second integral in Eq. (7) can be extracted by replacing the highly oscillating periodic function $\sin^2(\pi y)$, in the large N limit, by its average over one period, i.e., $\sin^2(\pi y) \approx 1/2$ and expanding the rest of the integrand for large y. We find

$$f(N, g, \Lambda/\rho_0) \simeq A(g, \Lambda/\rho_0) - \frac{2^{4g+1}}{\pi^2 (4g + 1)(\Lambda/\rho_0)^{4g}} \frac{1}{N^{4g+1}} \tag{9}$$

and thus the second Rényi EE for $n = 1$ has the asymptotic form

$$S_2(n = 1) = \ln(N) - \ln\left[A(g, \Lambda/\rho_0)\right] + \frac{b(g, \Lambda/\rho_0)}{N^{4g+1}} + \mathcal{O}\left(\frac{1}{N^{4g+2}}\right) \qquad (10)$$

where

$$b(g, \Lambda/\rho_0) = \frac{2^{4g+1}}{\pi^2(4g+1)(\Lambda/\rho_0)^{4g}A(g, \Lambda/\rho_0)}. \qquad (11)$$

This result constitutes an analytical confirmation of the empirical scaling form in Eq. (4) first proposed by Haque *et al.* [21, 22], with $n = 1$, where

$$a = -\ln\left[A(g, \Lambda/\rho_0)\right], \ \gamma = 4g + 1. \qquad (12)$$

3.1. Non-interacting spinless fermions

In the non-interacting limit when $K = 1$ ($g = 0$), Eq. (8) yields $A(0, \Lambda/\rho_0) = 1$ and thus $a = 0$ in agreement with previous calculations of the particle partition EE for free fermions (FF) on a lattice [21] where it was found that $S_{2,FF}(n = 1) = \ln N$. However, combining Eqs. (10)-(11) for $g = 0$ yields

$$S_2(n = 1) \simeq \ln(N) + \frac{2}{\pi^2 N}. \qquad (13)$$

in disagreement with the lattice result by a factor of $\mathcal{O}(N^{-1})$. To ensure that this discrepancy does not arise from the approximations made in expanding the integral in Eq. (7) we can return to the exact expression for the 1-RDM for non-interacting spinless fermions:

$$\rho_{1,FF}(x, x') = \frac{\sin(\pi\rho_0|x - x'|)}{\pi\rho_0 L|x - x'|}, \qquad (14)$$

which leads to a soluble integral and analytic form for the EE in the spatial continuum:

$$S_{2,FF}(n = 1) = \ln(N) - \ln\left\{\frac{2\left[N\pi\text{Si}(N\pi) + \cos(\pi N) - 1\right]}{\pi^2 N}\right\} \qquad (15)$$

where $\text{Si}(z)$ is the sine integral. Expanding for large N recovers the asymptotic form in Eq. (13) which differs from the known lattice result.

3.2. Effects of boundary conditions

The origin of this $1/N$ difference between free spinless fermions in the continuum vs. the lattice is related to our neglect of finite-size boundary conditions when studying the asymptotic behavior of the second Rényi EE. To properly capture the finite-size effects of periodic boundary conditions we replace separations $|x - x'|$ with the chord length between two points on a ring of circumference L [42]:

$$|x - x'| \to \frac{L}{\pi}\sin\left(\frac{\pi}{L}|x - x'|\right). \qquad (16)$$

Using the finite-size corrected 1-RDM, the integral in Eq. (7) takes the form

$$f(N, g, \Lambda/\rho_0) = \frac{2}{N^2} \int_0^{N/2} dy \frac{\sin^2(\pi y)}{\sin^2(\frac{\pi y}{N}) \left[1 + \frac{N^2 \Lambda^2}{\pi^2 \rho_0^2} \sin^2(\frac{\pi y}{N})\right]^{2g}}. \tag{17}$$

where the effects of finite L will appear only in the prefactors of decaying terms in an asymptotic expansion. Employing Eq. (17) for free fermions with $g = 0$ we recover the known lattice result $S_{2,FF}(n = 1) = \ln(N)$. For all subsequent comparisons with numerical data at finite g we employ the appropriately finite size corrected form of the 1-RDM when computing the Rényi entanglement entropy.

4. Exact diagonalization of the $t - V$ chain of spinless fermions

In order to test the validity of our main result in Eq. (10) for the $n = 1$ particle partition EE, we consider the $t - V$ model of N spinless fermions on a chain with M sites defined by the Hamiltonian

$$H = -t \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) + V \sum_i n_i n_{i+1} \tag{18}$$

where $c_i^\dagger$ and c_i are the fermionic creation and annihilation operators at site i and $n_i = c_i^\dagger c_i$ is the occupation number. The model is parameterized by the nearest-neighbor hopping amplitude $t > 0$, and interaction strength V. We consider only the half-filled case ($M = 2N$) with periodic boundary conditions (PBC) for odd number of fermions N, while for even N we use antiperiodic boundary conditions (APBC) to avoid the otherwise degenerate ground state [42] (See Fig. 1). In order to make connection with the general TLL theory described above, we require a method to determine the parameter K from the microscopic $t - V$ model. This can be accomplished via the Jordan–Wigner transformation [43] which maps the $t - V$ model onto the XXZ spin-1/2 chain that is exactly solvable [44, 45]. In the range $|V/t| < 2$, the system is known to be in the TLL phase, where the analytical form of K is given by

$$K = \frac{\pi}{2 \cos^{-1}(-V/2t)}. \tag{19}$$

By increasing the repulsive interaction across $V/t = 2$ ($K = 1/2$), the system undergoes a continuous phase transition to a charge-density wave (CDW) phase. In contrast, the transition across $V/t = -2$ ($K \to \infty$) is a discrete one, where the fermions tend to form a single cluster.

Beginning with the non-interacting case ($V/t = 0$), the free fermionic Hamiltonian is diagonal in the momentum-space representation leading to a ground state that is a Slater determinant of the N lowest energy modes. The rank of the resulting n-RDM is $\binom{N}{n}$ and with equal eigenvalues [21], it follows (as introduced above) that all the Rényi EEs are equal to

$$S_{\alpha,FF}(n) = \ln \binom{N}{n}. \tag{20}$$

In the presence of interactions, we calculate the von Neumann ($\alpha = 1$) and the second ($\alpha = 2$) Rényi EEs from the ground state of Eq. (18) which we obtain via numerical exact diagonalization. The resulting n-RDM has maximum possible rank $\binom{M}{n}$ due to the indistinguishability of the $n < N$ particles in the partition, as opposed to $n!\binom{M}{n}$, the full dimension of the Hilbert space in the first quantized basis. Exploiting this symmetry, (for details, see Appendix A) we are able to study systems up to $M = 28$ sites, a considerable advancement over previous work [22]. The results are shown in Fig. 2 which demonstrates that the entanglement entropy $S_\alpha(n = 1)$ increases with increasing
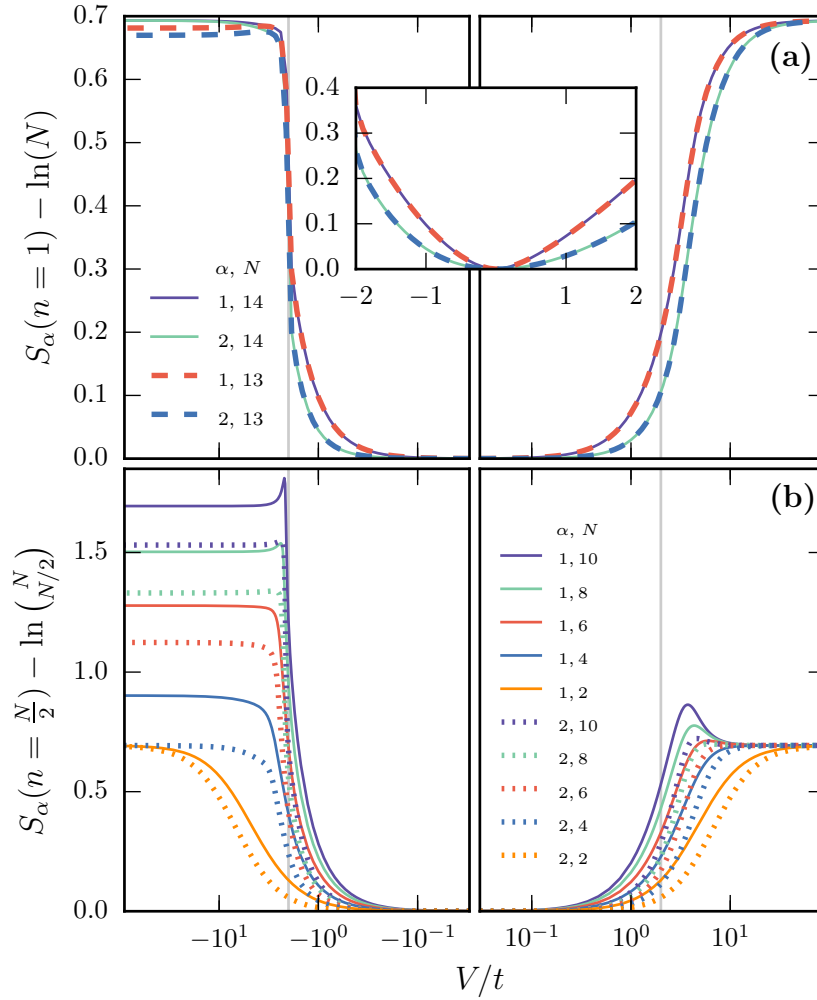

Figure 2. Interaction effects on the n-particle entanglement entropy $S_\alpha(n)$ for $\alpha = 1, 2$ in the ground state of the $t - V$ model. (a) $S_\alpha(n = 1) - \ln N$ vs V/t for $N = 13$ and 14 with periodic and anti-periodic boundary conditions, respectively. The light gray vertical lines mark the location of the known phase transitions at $V/t = \pm 2$. The subtracted $\ln(N)$ term is the one-particle entanglement entropy for free fermions. Inset: the Tomonaga-Luttinger liquid region where we expect the continuum theory to apply. (b) $S_\alpha(n = N/2) - \ln\binom{N}{N/2}$ vs V/t for *macroscpic* partitions with $1 \leq n \leq 5$ and anti-periodic boundary conditions. As $n \to N/2$, features appear near the phase transitions for $\alpha = 1$.

interaction strength $|V/t|$ up to a maximum of $S_{\alpha,FF}(n=1)+\ln 2$ (for even N) in the limit $|V/t|\to\infty$ [21, 22]. For attractive interactions, $S_\alpha(n=1)$ displays a sharp increase around the first-order transition point $V/t=-2$. In contrast, $S_\alpha(n=1)$ does not seem to be sensitive to the continuous transition at $V/t=2$ [21]. However, when considering a macroscopic partition size $n=N/2$, we observe that $S_\alpha(n=N/2)$ develops a peak near $V/t=2$ which appears to approach the critical point as we increase N (Fig. 2 (b)). Eventually, $S_\alpha(n=N/2)$ saturates to $\ln\binom{N}{N/2}+\ln 2$ in the limit $V/t\to\infty$, with details given in Appendix B.

We now turn to the TLL region $|V/t|<2$, where we expect the scaling of the interaction contribution to the EE: $S_2(n=1)-\ln(N)$, to be linear in $1/N^{4g+1}$ with corrections of $\mathcal{O}(1/N^{4g+2})$ as in Eq. (10). To test this prediction, we rearrange Eq. (10) as:

$$\frac{S_2(n=1)-\ln(N)-a}{b}=N^{-(4g+1)}+\mathcal{O}\left(N^{-(4g+2)}\right). \tag{21}$$

and calculate $S_2(n=1)$ as a function of N using the ground state of $t-V$ model for different values of the interaction strength V/t, deep in the TLL phase (away from the phase transitions). For each interaction strength V/t, we compute $g=(K+K^{-1}-2)/4$ using Eq. (19) and extract a and b from a linear fit to the $S_2(n=1)-\ln(N)$ vs $N^{-(4g+1)}$ data set. Next, we use the extracted coefficients to rescale $S_2(n=1)-\ln(N)$ according to Eq. (21). The results are illustrated in Fig. 3, where, for suitably large N, the data follows the straight line predicted by Eq. (21) with unit slope, verifying the TLL scaling form in Eq. (10). Deviations from linearity for smaller N arise due to finite size corrections of $\mathcal{O}(1/N^{4g+2})$.
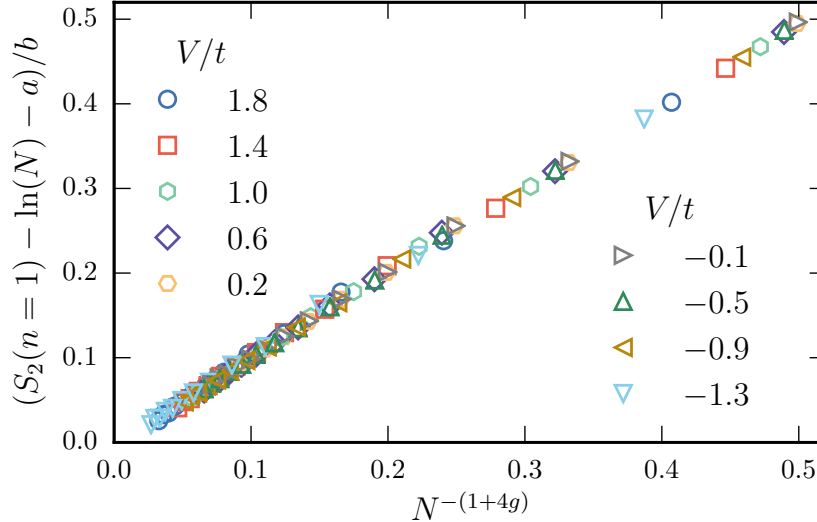

Figure 3. Finite size scaling of $S_2(n=1)-\ln(N)$ with $N^{-(4g+1)}$ for $2\leq N\leq 14$ confirming the empirical asymptotic scaling predicted by Zozulya *et al.* [19] and identifying the power of the leading finite size correction as $\gamma=4g+1$. The coefficients a and b depend on the interaction strength V/t and are calculated from a linear fit of the exact diagonalization data according to Eq. (10).

Having understood the asymptotic scaling of the 1-particle partition Rényi EE with N, we now consider its dependence on the interaction strength g. This amounts to asking if the g-dependence of the scaling coefficients a and b for the $t - V$ model can be predicted from our continuum theory. To answer this question we calculate the second Rényi EE for $|V/t| < 2$ in the liquid phase at fixed N by evaluating the full integral in Eq. (17) numerically including all contributions from finite N. However, in order to compare the resulting particle EE with that obtained from the exact diagonalization, we need to identify the corresponding non-universal value of the ratio Λ/ρ_0 in the $t - V$ model. At half filling, the average particle density is $\rho_0 = 1/2x_0$ where x_0 is the lattice separation, while one estimates the ultraviolet cutoff Λ to be of the order of $1/x_0$, yielding $\Lambda/\rho_0 \approx 2$. The open and closed symbols in Fig. 4 show the exact diagonalization results for $S_2(n = 1) - \ln(N)$ as a function of g for $N = 13$. The three lines correspond
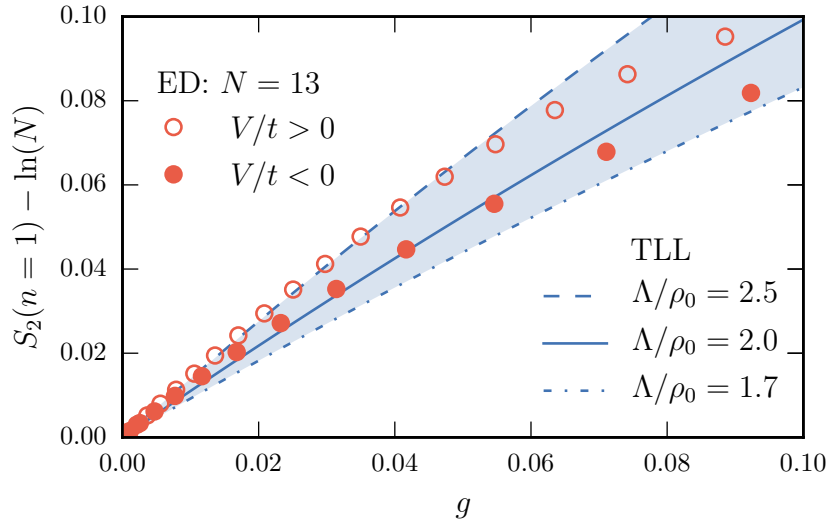

Figure 4. The effective interaction dependence of the 1-particle partition second Rényi entanglement entropy $S_2(n = 1) - \ln(N)$. Open (closed) points were computed via exact diagonalization of the $t - V$ model for $N = 13$ with repulsive (attractive) interactions. The lines show the prediction from the Tomonaga-Luttinger liquid theory for three different values of the ultraviolet cutoff Λ measured in units of the density ρ_0.

to the prediction from the TLL theory for slightly different values of the UV cutoff Λ. Due to the highly non-linear relationship between the interaction strength V/t and the TLL parameter K (Eq. 19), in combination with the sensitivity of the particle partition entanglement to the strength and nature of inter-particle interactions, it is no surprise that the EE in the $t - V$ model is a multi-valued function of the effective interaction parameter g for attractive and repulsive interactions. Clearly, high energy lattice-scale physics, not captured within the low energy TLL theory is responsible for this behavior. Moreover, recall that the ultraviolet cutoff, Λ, in Eq. (5), is proportional to the inverse of the effective range of the interaction [41]. Therefore, we expect Λ

to exhibit a dependence on the nature and strength of the interaction, i.e., have K-dependence [26]. Considering such a dependence, we find that the $t-V$ model results for $S_2(n=1)-\ln(N)$ are bounded by the theoretically calculated ones using $\Lambda/\rho_0 = 1.7$ and 2.5 (Fig. 4). Note that both ratios are of order 2.

Testing the proposed leading order scaling of the particle partition EE in Eq. (4) with the partition size n in the TLL phase, requires the calculation of n-RDM with $n > 1$. While this can be done in principle using standard techniques [40], the resulting evaluation of $S_2(n)$ requires performing $2n$ non-separable integrals. Even for the $n=2$ we were not able to analytically extract the asymptotic scaling of Tr ρ_2^2. However, from numerical exact diagonalization of the $t-V$ model in the in the TLL phase we were able to calculate the Rényi EEs for partitions up to $n = N/2 = 5$ for $N = 10$ as seen in Fig. 5. Our results are in agreement with previous calculations of $N = 6, n = 3$ [21] and
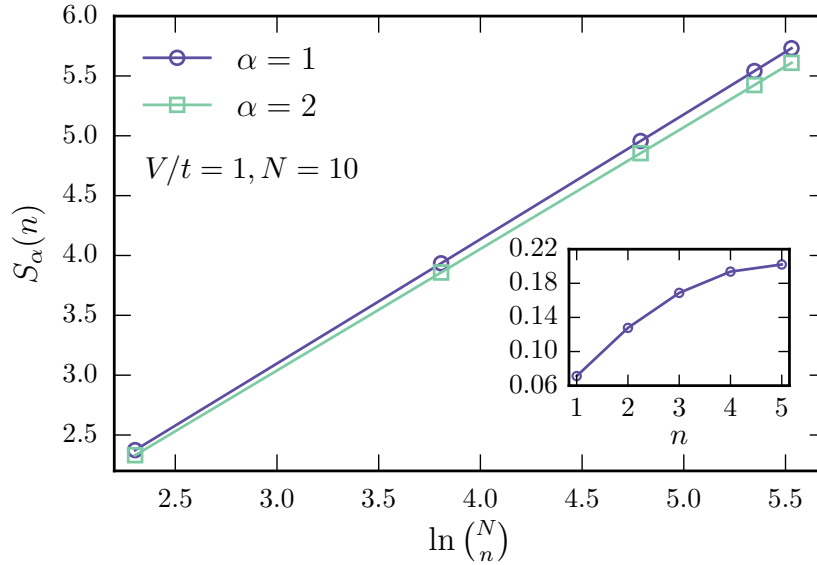

Figure 5. Scaling of $S_\alpha(n)$ with $\ln \binom{N}{n}$ for $\alpha = 1, 2$ in the ground state of the $t-V$ model with $V/t = 1$, $N = 10$, and for partition sizes $1 \le n \le 5$. Inset: Interaction contribution to the EE $(S_1(n) - \ln \binom{N}{n})$ vs n.

strongly suggest that the leading term in the scaling of the Rényi EEs with n is indeed equal to the Rényi EE of free fermions, i.e., $\ln \binom{N}{n}$. Interactions introduce a correction term that increases with the partition size with a negative curvature (see Fig. 5 inset) such that both the leading order constant and finite-size power-law corrections to scaling both depend on n.

Finally we investigate the question of whether particle bipartition EE is sensitive to the ground state degeneracy known to occur in the $t-V$ model with periodic boundary conditions and an even number of sites. Introducing the inversion operator P [46] defined by

$$Pc_i^\dagger P^\dagger = c_{M-i+1}^\dagger, \quad i = 1, \cdots, M. \tag{22}$$

where P commutes with the Hamiltonian of the $t-V$ model in Eq. (18) for PBC, we can write the degenerate ground state as a superposition of the eigenstates of the inversion operator: $P|\Phi_\pm\rangle = \pm|\Phi_\pm\rangle$, i.e.,

$$|\Psi\rangle = \cos(\theta)|\Phi_+\rangle + \sin(\theta)|\Phi_-\rangle. \tag{23}$$

Here, we only consider a superposition with real coefficients that can be varied through the parameter $0 \le \theta \le \pi$ and study the dependence of the Rényi EEs on θ as seen in Fig. 6. Our numerical results for repulsive interactions with $N = 10$ show that
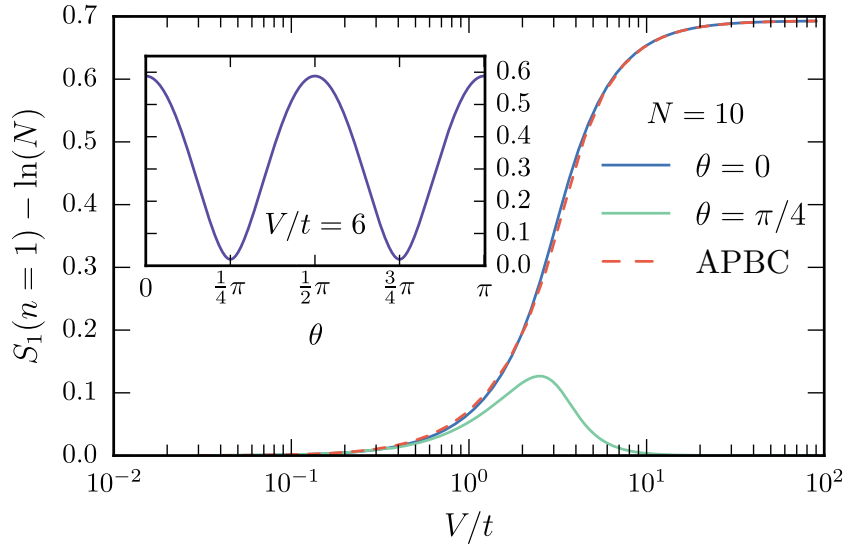

Figure 6. Effects of ground state degeneracy. The $S_2(n=1) - \ln(N)$ dependence on V/t in the ground state of the $t-V$ model for $N = 10$. Solid lines represent results obtained from the degenerate ground state in Eq. (23) using PBC and $\theta = 0, \pi/4$ (see the text for details). The dashed line corresponds to the non-degenerate ground state for APBC. Inset: $S_2(n=1) - \ln(N)$ vs θ for $V/t = 6$.

$S_1(n=1)$ oscillates with θ (Fig. 6 inset), where the maximum EE corresponds to $|\Psi\rangle$ being an eigenstate of P, i.e., $\theta = 0$ or $\theta = \pi/2$, and the minimum EE is obtained when both eigenstates $|\Phi_\pm\rangle$ contribute equally to $|\Psi\rangle$ (maximum uncertainty in P, $\theta = \pi/4, 3\pi/4$). Moreover, the difference between the lower and upper bound vanishes in the non-interacting limit and widens with increasing interaction strength up to $\ln 2$ in the limit $V/t \to \infty$ (see Appendix B). Interestingly, Fig. 6 shows that for $\theta = \pi/4$, $S_1(n=1)$ exhibits a peak near the critical point ($V/t = 2$), while the $S_1(n=1)$ dependence on V/t for $\theta = 0$ is very similar to that obtained from the non-degenerate ground state using APBC.

5. Conclusions

In this paper we have studied the finite size and interaction dependence of the particle partition Rényi entanglement entropies of a fermionic Tomonaga-Luttinger liquid and

find that:

$$S_\alpha(n, N) = \ln \binom{N}{n} + a_\alpha(n) + \mathcal{O}\left(\frac{1}{N^{\gamma_\alpha(n)}}\right) \tag{24}$$

where n is the number of particles in the subsystem and α the Rényi index. This result is in agreement with the empirical prediction made in Ref. [19]. For the special case $n = 1$, $\alpha = 2$ we have determined the power of the finite size correction to the leading logarithm to be $\gamma_2(1) = K + K^{-1} - 1$ where K is the Luttinger parameter and confirmed this interaction dependence for the $t - V$ model by mapping it to the exactly solvable XXZ chain. The more general result for $n > 1$, $\alpha \neq 2$ in Eq. (24) is supported by extensive exact diagonalization results on the lattice $t - V$ model of spinless fermions obtained on systems with up to $M = 28$ sites. This general scaling form can be contrasted with a bosonic Tomonaga-Luttinger liquid, where it was found [26] that $S_2(n, N) \simeq (n/K) \ln N + a_2'(n) + \mathcal{O}(1/N^{1-K^{-1}})$ which asymptotically recovers the free fermion result in the limit of hard-core bosons $(K \to 1^+)$ using the fact that $\binom{N}{n} \approx N^n/n!$ for $N \gg n$.

The universality of the prefactor of the leading order logarithm in Eq. (24) demonstrates that due to the required anti-symmetrization of the N-particle wavefunction, fermions are always more entangled than bosons under a particle partition. This is consistent with what was numerically found for hard-core particles with variable anyonic statistics [24]. Such sensitivity to particle statistics and interaction dependence is absent in the asymptotic scaling of the spatial mode entanglement entropy for critical (1+1)-dimensional systems where the prefactor is universal and related to the central charge of the underlying conformal field theory [28]. Thus, the particle partition entanglement appears to be a useful diagnostic of quantum correlations in many-body systems, and its logarithmic scaling with the total number of particles N highlights the potential utility of protocols [18] that aim to transfer it to experimentally accessible mode entanglement.

An interesting open question remains on the origin and development with system size of the peak in the entanglement entropy in the ground state of the $t - V$ model near the continuous phase transition at $V/t = 2$ for macroscopic particle partitions with $n = N/2$ (Fig. 2 (b)). A careful finite-size analysis of this unexpected feature (due to the lack of any natural length scale describing the partition) would require moving beyond exact diagonalization and employing recently adapted hybrid Monte Carlo methods [37, 47, 48].

Acknowledgments

Appendix A. Evaluating the n-particle partition entanglement

In this appendix, we show that the n-RDM of spinless hardcore particles on a lattice can be written as a tensor product of two lower-rank matrices. This simplification significantly reduces the numerical cost for calculating n-RDM for such quantum systems.

In general, for a pure quantum state $|\Psi\rangle$ in some Hilbert space $\mathcal{H}$ that can be written as the tensor product space $A \otimes B$, we can write

$$|\Psi\rangle = \sum_{i,j} C_{i,j} |\psi_i^A\rangle |\psi_j^B\rangle, \tag{A.1}$$

where $\{|\psi_i^A\rangle\}$ and $\{|\psi_j^B\rangle\}$ are orthonormal bases in the two Hilbert spaces A and B, respectively. Accordingly, the system degrees of freedom are bipartitioned between the two subsets $\{|\psi_i^A\rangle\}$ and $\{|\psi_j^B\rangle\}$. Using the product basis $\{|\psi_i^A\rangle|\psi_j^B\rangle\}$, the full density matrix can be written as

$$\rho = |\Psi\rangle\langle\Psi| = \sum_{i,j,i',j'} |\psi_i^A\rangle |\psi_j^B\rangle C_{i,j} C_{i',j'}^* \langle\psi_{i'}^A| \langle\psi_{j'}^B|. \tag{A.2}$$

The reduced density matrix ρ_A (ρ_B) of subspace A (B), is obtained from ρ by tracing out the degrees of freedom of subspace B (A),

$$\rho_A = \sum_m \langle\psi_m^B|\rho|\psi_m^B\rangle = \sum_{i,j} |\psi_i^A\rangle \left(\sum_m C_{i,m} C_{j,m}^* \right) \langle\psi_j^A|, \tag{A.3}$$

$$\rho_B = \sum_m \langle\psi_m^A|\rho|\psi_m^A\rangle = \sum_{i,j} |\psi_i^B\rangle \left(\sum_m C_{m,i} C_{m,j}^* \right) \langle\psi_j^B|. \tag{A.4}$$

Moreover, the reduced density matrices can be generated using the linear maps G_{AB} : $S_B \to S_A$ as $\rho_A = G_{AB} G_{AB}^\dagger$ and $\rho_B = (G_{AB}^\dagger G_{AB})^T$ where

$$G_{AB} = \sum_{i,j} C_{i,j} |\psi_i^A\rangle\langle\psi_j^B|. \tag{A.5}$$

Note that, in general, the matrix representing the linear maps G_{AB} is rectangular since the dimensions of the Hilbert spaces A and B can differ.

A.1. Particle bipartition

Let us now consider a quantum system of N spinless hardcore particles in a state $|\Psi\rangle = \sum_i \chi_i |\psi_i^N\rangle$, where $\{|\psi_i^N\rangle\}$ are the N particle second-quantization basis states, where each basis state corresponds to a single, possible, occupation number configuration (ONC). Now we recall that each ONC state is a linear combination of the distinguished particles states $\{|\psi_{i,j}^N\rangle\}$ as $|\psi_i^N\rangle = \sum_j \frac{f_j}{\sqrt{N!}} |\psi_{i,j}^N\rangle$, where j runs over all possible particle

permutations (PPs) and $f_j = e^{-i\phi_j}$ is the corresponding phase factor. Accordingly, we can write

$$|\Psi\rangle = \sum_{i,j} \frac{\chi_i f_j}{\sqrt{N!}} |\psi_{i,j}^N\rangle. \tag{A.6}$$

Now we partition N into two sets of particles: n_A and the remainder $n_B = N - n_A$. The distinguished particles basis $\{|\psi_{i,j}^N\rangle\}$ can be written as a tensor product of the two partitions basis

$$|\psi_{i,j}^N\rangle = |\psi_{i_A,j_A}^{n_A}\rangle |\psi_{i_B,j_B}^{n_B}\rangle, \tag{A.7}$$

where each ONC (labelled by i) of the N particles corresponds to a unique pair of ONCs i_A and i_B of the n_A and n_B particles, respectively. Similarly, each PP j of the N particles corresponds to a unique pair of PPs: j_A and j_B of the n_A and n_B particles.

$$|\Psi\rangle = \sum_{i_A,i_B,j_A,j_B} C_{i_A,i_B,j_A,j_B} |\psi_{i_A,j_A}^{n_A}\rangle |\psi_{i_B,j_B}^{n_B}\rangle, \tag{A.8}$$

with

$$C_{i_A,i_B,j_A,j_B} = \frac{\chi_i f_j}{\sqrt{N!}}. \tag{A.9}$$

The C_{i_A,i_B,j_A,j_B} depends on the indices i and j through the multiplication of χ_i and f_j, and without loss of generality, we can take

$$C_{i_A,i_B,j_A,j_B} = \tilde{C}_{i_A,i_B} \Phi_{j_A,j_B}. \tag{A.10}$$

Moreover, the dependence of Φ_{j_A,j_B} on the PP indices only guarantees that $|\Phi_{j_A,j_B}|^2 = $ *constant* that can be absorbed in $\tilde{C}_{i_A,i_B}$. Thus, we can set $|\Phi_{j_A,j_B}|^2 = 1$. Based on the fact that applying a particle permutation two one group of particles results in an overall phase factor that does not depend on the permutation of the other group of particles, we write

$$\Phi_{j_A,j_B} = F_{j_A}^{(A)} F_{j_B}^{(B)}, \tag{A.11}$$

with $|F_{j_A}^{(A)}|^2 = |F_{j_B}^{(B)}|^2 = 1$. Substituting in Eq. (A.8) we find

$$|\Psi\rangle = \sum_{i_A,i_B,j_A,j_B} \tilde{C}_{i_A,i_B} F_{j_A}^{(A)} F_{j_B}^{(B)} |\psi_{i_A,j_A}^{n_A}\rangle |\psi_{i_B,j_B}^{n_B}\rangle, \tag{A.12}$$

Let us now calculate the reduced density matrix of ρ_A using

$$G_{n_A n_B} = \sum_{i_A,i_B,j_A,j_B} \tilde{C}_{i_A,i_B} F_{j_A}^{(A)} F_{j_B}^{(B)} |\psi_{i_A,j_A}^{n_A}\rangle \langle\psi_{i_B,j_B}^{n_B}|, \tag{A.13}$$

as

$$\rho_A = G_{n_A n_B} G_{n_A n_B}^\dagger \tag{A.14}$$

$$= \sum_{i_A,j_A,i_A',j_A'} |\psi_{i_A,j_A}^{n_A}\rangle \sum_{i_B} \left(\tilde{C}_{i_A,i_B} \tilde{C}_{i_A',i_B}^* \right) F_{j_A}^{(A)} F_{j_A'}^{*(A)} \sum_{j_B} \left| F_{j_B}^{(B)} \right|^2 \langle\psi_{i_A',j_A'}^{n_A}|$$

$$= n_B! \sum_{i_A,j_A,i_A',j_A'} |\psi_{i_A,j_A}^{n_A}\rangle D_{i_A,i_A'} \Phi_{j_A,j_A'} \langle\psi_{i_A',j_A'}^{n_A}|, \tag{A.15}$$

with $D_{i_A,i'_A} = \sum_{i_B} \tilde{C}_{i_A,i_B} \tilde{C}^*_{i'_A,i_B}$ and $\Phi_{j_A,j'_A} = F^{(A)}_{j_A} F^{*(A)}_{j'_A}$. From Eq. (A.15) we see that ρ_A is a Kronecker product (tensor product) of the lower-rank Hermitian matrices D and Φ. where D can be calculated considering a single PP for each particle partition and the elements of Φ are the product of the relative phases of the chosen partitions (A.11)

A.2. Eigenvalues

Let V_D and V_Φ be two unitary transformations that diagonalize the sub matrices D and Φ, respectively. Such that $V_D^\dagger D V_D = \Lambda$ and $V_\Phi^\dagger \Phi V_\Phi = W$, where Λ and W are diagonal matrices with eigenvalues $\{\lambda_k\}$ and $\{w_l\}$. If we construct the unitary transformation U as

$$U = V_D \otimes V_\Phi, \tag{A.16}$$

and calculate $U^\dagger(\rho_A/n_B!)U$ we find

$$U^\dagger \left(\frac{\rho_A}{n_B!} \right) U = \sum_{k,l} |\psi^{n_1}_{k,l}\rangle \lambda_k w_l \langle \psi^{n_1}_{k,l}|. \tag{A.17}$$

Accordingly, the unitary transformation U diagonalizes ρ_A and the eigenvalues of ρ_A are $n_B!\lambda_k w_l$. Moreover, Φ has the structure of a simple projection operator onto the non-normalized state $|F^{(A)}\rangle = \sum_j^{n_A!} F^{(A)}_j |j\rangle = \sum_j^{n_A!} e^{i\phi_j}|j\rangle$ as $\Phi = |F^{(A)}\rangle\langle F^{(A)}|$. The only eigenstate of Φ with a nonzero eigenvalue is $|F^{(A)}\rangle$, where $\Phi|F^{(A)}\rangle = |F^{(A)}\rangle\langle F^{(A)}|F^{(A)}\rangle = n_A!|F^{(A)}\rangle$.

Therefore, we conclude that the nonzero eigenvalues of ρ_A are $n_A!n_B!\lambda_k$, where λ_k are the eigenvalues of the matrix D that is constructed using only one PP of each of the sets $\{|\psi^{n_A}_{i_A,j_A}\rangle\}$ and $\{|\psi^{n_B}_{i_B,j_B}\rangle\}$. As the rank of D is smaller than that of the n-RDM by a factor of $n_A!n_B!$ the numerical effort involved in calculating the eigenvalues of the n-RDM is enormously reduced.

Appendix B. n-particle partition entanglement in the $V/t \to \infty$ limit

Here we calculate the n-particle partition entanglement of the one-dimensional fermionic $t - V$ model at half filling ($N = M/2$) in the infinite repulsion limit ($V/t \to \infty$). In this limit, the Hamiltonian of the model (Eq. (18)) is reduced to

$$H = V \sum_i n_i n_{i+1} \tag{B.1}$$

which is diagonal in the occupation number representation with a two-fold degenerate ground state, where, at half filling, the fermions can avoid having any nearest neighbors by occupying sites with only odd indices ($|\psi_{\text{odd}}\rangle = |1010\cdots10\rangle$) or only even indices ($|\psi_{\text{even}}\rangle = |0101\cdots01\rangle$). Thus, one can write the ground state in this limit, as a superposition of $|\psi_{\text{odd}}\rangle$ and $|\psi_{\text{even}}\rangle$:

$$|\Psi\rangle = \cos(\Theta)e^{i\delta}|\psi_{\text{odd}}\rangle + \sin(\Theta)|\psi_{\text{even}}\rangle, \tag{B.2}$$

where we parametrize the amplitudes and the relative phase of the odd/even states using Θ and δ. Note that for $\delta = 0$ and $\Theta = \pi/4$ ($\Theta = 3\pi/4$), the ground state $|\Psi\rangle$ is also an eigenstate of the inversion operator P (Eq. (22)) with eigenvalue ± 1 where

$$P|\Phi_\pm\rangle = \pm|\Phi_\pm\rangle = \pm \left(\frac{1}{\sqrt{2}}|\psi_{\text{odd}}\rangle \pm \frac{1}{\sqrt{2}}|\psi_{\text{even}}\rangle \right). \tag{B.3}$$

The degeneracy persists in the case of finite interaction V/t for even/odd N with PBC/APBC. The degeneracy is lifted for odd/even N with APBC/PBC with the resulting ground state in the infinite repulsion limit approaching an eigenstate of P:

$$|\Psi\rangle = |\Phi_+\rangle = \frac{1}{\sqrt{2}}|\psi_{\text{odd}}\rangle + \frac{1}{\sqrt{2}}|\psi_{\text{even}}\rangle. \tag{B.4}$$

We now consider the n-particle partition entanglement of the degenerate ground state $|\Psi\rangle$ defined in Eq. (B.2), where we can write the corresponding full density matrix ρ as

$$\begin{aligned}\rho = {} & \cos^2(\Theta)|\psi_{\text{odd}}\rangle\langle\psi_{\text{odd}}| + \sin^2(\Theta)|\psi_{\text{even}}\rangle\langle\psi_{\text{even}}| \\ & + \sin(\Theta)\cos(\Theta)e^{i\delta}|\psi_{\text{odd}}\rangle\langle\psi_{\text{even}}| + \sin(\Theta)\cos(\Theta)e^{-i\delta}|\psi_{\text{even}}\rangle\langle\psi_{\text{odd}}|, \end{aligned} \tag{B.5}$$

If we partition the N particles into two distinguishable sets of $n_A = n$ and $n_B = N - n$ particles, we can write the states $|\psi_{odd}\rangle$ and $|\psi_{even}\rangle$ in terms of the first-quantized basis states of the two partitions as

$$|\psi_{\text{odd}}\rangle = \sum_{i_A, i_B, j_A, j_B} \frac{f^{\text{odd}}_{i_A, i_B, j_A, j_B}}{\sqrt{N!}} |\psi^{n_A, \text{odd}}_{i_A, j_A}\rangle |\psi^{n_B, \text{odd}}_{i_B, j_B}\rangle, \tag{B.6}$$

$$|\psi_{\text{even}}\rangle = \sum_{i_A, i_B, j_A, j_B} \frac{f^{\text{even}}_{i_A, i_B, j_A, j_B}}{\sqrt{N!}} |\psi^{n_A, \text{even}}_{i_A, j_A}\rangle |\psi^{n_B, \text{even}}_{i_B, j_B}\rangle, \tag{B.7}$$

where the indices i_A and i_B label possible occupation number configurations (ONCs) in both partitions A and B while j_A and j_B label different particle permutations (PPs). Also, $f^{\text{odd}}_{i_A, i_B, j_A, j_B}$ and $f^{\text{even}}_{i_A, i_B, j_A, j_B}$ are overall phase factors, where the superscript odd (even) is to indicate that only sites with odd (even) indices are occupied. We note that in this decomposition the states $|\psi_{\text{even}}\rangle$ and $|\psi_{\text{odd}}\rangle$ are constructed from non-overlapping subspaces (even/odd) of partition B. Similarly for partition A. By tracing out all degrees of freedom in B from ρ (Eq. (B.5)), we can write the reduced density matrix ρ_A as

$$\rho_A = \text{Tr}_B\, \rho = \cos^2(\Theta)\text{Tr}_B\, |\psi_{\text{odd}}\rangle\langle\psi_{\text{odd}}| + \sin^2(\Theta)\text{Tr}_B\, |\psi_{\text{even}}\rangle\langle\psi_{\text{even}}|, \tag{B.8}$$

where the trace of the mixed terms ($|\psi_{\text{odd}}\rangle\langle\psi_{\text{even}}|$, $|\psi_{\text{even}}\rangle\langle\psi_{\text{odd}}|$) vanishes due to the non-sharing of B basis states. Moreover, $\rho_A^{\text{odd}} = \text{Tr}_B\, |\psi_{\text{odd}}\rangle\langle\psi_{\text{odd}}|$ and $\rho_A^{\text{even}} = \text{Tr}_B\, |\psi_{\text{even}}\rangle\langle\psi_{\text{even}}|$ contribute separately to the spectrum of ρ_A due to the non-sharing of A basis states.

We now calculate the spectrum of ρ_A^{odd}. Note that the state $|\psi_{\text{odd}}\rangle$ represents a single ONC of the N particles and as a result the ONC i_A is uniquely determined by

i_B in the product states $|\psi_{i_A,j_A}^{n_A,\text{odd}}\rangle|\psi_{i_B,j_B}^{n_B,\text{odd}}\rangle$. Therefore, ρ_A^{odd} does not connect any pair of states, in the set $\{|\psi_{i_A,j_A}^{n_A,\text{odd}}\rangle\}$, with different ONC i_A. This result, combined with the formalism presented in Appendix A, allows us to identify that the sector of ρ_A^{odd} that connects states in $\{|\psi_{i_A,j_A}^{n_A,\text{odd}}\rangle\}$ with fixed PP j_A is diagonal with $\binom{N}{n}$ equal non-zero elements of value $\frac{1}{N!}$. $\binom{N}{n}$ is the number of possible ONCs in the partition A with $n_A = n$ and we only consider the contribution of a single PP j_B to $\text{Tr}_B |\psi_{\text{odd}}\rangle\langle\psi_{\text{odd}}|$. It then follows from Appendix A that the non-zero eigenvalues of ρ_A^{odd} can be obtained by rescaling the above eigenvalues by a factor of $n_A!n_B! = n!(N-n)!$. By an equivalent set of arguments ρ_A^{even} has the same eigenvalues. Combining all the above and using Eq. (B.8), we find that ρ_A has two sets of eigenvalues: $\binom{N}{n}$ eigenvalues of $\cos^2(\Theta)/\binom{N}{n}$ and $\binom{N}{n}$ eigenvalues of $\sin^2(\Theta)/\binom{N}{n}$. Therefore, the Rényi entanglement entropies are

$$S_\alpha(n) = \ln\binom{N}{n} + \frac{1}{1-\alpha}\ln\left[\cos^{2\alpha}(\Theta) + \sin^{2\alpha}(\Theta)\right], \tag{B.9}$$

and the von Neumann entropy ($\alpha = 1$) is

$$S_1(n) = \ln\binom{N}{n} - \cos^2(\Theta)\ln\left[\cos^2(\Theta)\right] - \sin^2(\Theta)\ln\left[\sin^2(\Theta)\right]. \tag{B.10}$$

According to Eqs. (B.9) and (B.10), the maximum entropy corresponds to $\Theta = \pi/4$ and $3\pi/4$ ($|\Psi\rangle = \frac{e^{i\delta}}{\sqrt{2}}|\psi_{\text{odd}}\rangle + \frac{1}{\sqrt{2}}|\psi_{\text{even}}\rangle$), where all the $2\binom{N}{n}$ eigenvalues of ρ_A are equal and thus all the Rényi entropies are equal to

$$S_\alpha(n) = \ln\binom{N}{n} + \ln 2. \tag{B.11}$$

For $\Theta = 0$ and $\pi/2$, $|\Psi\rangle = |\psi_{\text{odd}}\rangle$ or $|\psi_{\text{even}}\rangle$, only $\binom{N}{n}$ equal eigenvalues survive yielding a minimum entropy of

$$S_\alpha(n) = \ln\binom{N}{n}. \tag{B.12}$$

These limits can be seen in Fig. 6 for $V/t \gg 1$.

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