Operationally accessible entanglement of one dimensional spinless fermions

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For indistinguishable itinerant particles subject to a superselection rule fixing their total number, a portion of the entanglement entropy under a spatial bipartition of the ground state is due to particle fluctuations between subsystems and thus is inaccessible as a resource for quantum information processing. We quantify the remaining operationally accessible entanglement in a model of interacting spinless fermions on a one dimensional lattice via exact diagonalization and the density matrix re normalization group. We find that the accessible entanglement exactly vanishes at the first order phase transition between a Tomonaga-Luttinger liquid and phase separated solid for attractive interactions and is maximal at the transition to the charge density wave for repulsive interactions. Mention the physical importance of the flat state here.

I. INTRODUCTION

The entanglement of a quantum mechanical system can be exploited as a resource, allowing spatially separated parties to perform protocols (*e.g.* dense coding[1], teleportation[2] and quantum cryptography[3]) not feasible in a classical setting. The quantification of the exact amount of entanglement encoded in a given state is thus an important task that can be accomplished by studying the von Neumann entropy of a subsystem[4,5]. The situation can become more complicated in a condensed matter setting[6], especially when considering an eigenstate of some physical Hamiltonian governing a system of indistinguishable and itinerant interacting particles, whose total number is fixed. Unlike an optical system of photons, conservation of total particle number N for atoms or electrons may restrict the set of possible local operations, often referred to as a superselection rule (SSR)[7], and can potentially limit the amount of entanglement that can be physically accessed[8–12]. This can be understood as originating from the fundamental inability to create coherent superposition states with different particle number in a subsystem – entanglement due to particle fluctuations alone cannot be utilized without access to a global phase reference[13]. In a pioneering work, Wiseman and Vaccaro[14] demonstrated that by averaging the von Neumann entanglement entropy of spatial modes over sectors corresponding to all possible numbers of particles in the subsystem defining those modes, they could place an upper bound on the amount of entanglement that could be transferred to a quantum register using local operations and classical communication. This quantity, known as the *accessible entanglement entropy*, has been previously studied for few-particle[14–19] or non-interacting[20,21] systems. However, the interplay between interactions and a SSR fixing the total particle number has yet to be fully explored. This is especially acute as many of the proposed or currently implemented quantum simulators[22], including those employing ultracold atoms[23], trapped ions[24] and electrons[25,26], are subject to fixed total N.

To address this, we perform a systematic study of the accessible entanglement in an interacting model of spinless fermions, (the "$t-V$ model"), on a one dimensional lattice, which is known to exhibit a host of interesting behavior[27], including first and second order quantum phase transitions between both classically ordered and quantum disordered phases. We employ large scale exact diagonalization (ED) to study the ground state entanglement as a function of interaction strength for systems including up to 32 sites at different filling fractions. In order to study the finite size scaling of the accessible entanglement near the quantum phase transition to the localized charge density wave state, we perform density matrix renormalization group (DMRG) calculations using the ITensor library[28]. In the limits of infinitely strong repulsive and attractive interactions, as well as at a special interaction corresponding to a "flat" ground state where all possible occupations in the system contribute with equal weight, we derive analytical results for the accessible entanglement. We study both the originally defined von Neumann measure[14], as well as the its recently introduced Rényi generalization[21].

Validation and Applications:

- Confirmation of TLL result from Goldstein and Sela[29]
- comparison with OEE in Bose-Hubbard model? i.e. soft vs. hard-core bosons.
- applications: new form of Rényi generalized accessible entanglement entropy?
- can be measured in experiments via the Rényi entropy see e.g.: Refs. 30–33 item
- other definitions of accessible entanglement[34–36], etc. which do not include the physical SSR
- entanglement as a diagnostic of phase transitions, see e.g.[37]

Contributions:

- Confirmation that a real system of spin polarized electrons may act as a substantial entanglement resource for quantum information applications.

- Present evidence of scaling of the accessible entanglement entropy at a quantum phase transition.

In the remainder of this paper we begin with a careful definition of the accessible entanglement entropy and discuss some physical situations where its behavior is currently understood. We then move on to the definition of the model in question, the so-called $t-V$ model, and derive a number of new results in some analytically tractable limits. The full phase diagram is then explored via ED and DMRG, where we answer the question of the exact amount of entanglement that can be extracted from a finite size system of interacting one dimensional lattice fermions. We conclude with a brief discussion on the effects of filling fraction and what role the accessible entanglement might play in the study of quantum phase transitions.

II. ACCESSIBLE ENTANGLEMENT

A. The Rényi Entanglement Entropy

The amount of entanglement that exists between some partition A and its compliment $\bar{A}$ of a quantum many-body system in pure state $|\Psi\rangle$ can be quantified via the Rényi entanglement entropy which depends on an index α :

$$S_\alpha(\rho_A) = \frac{1}{1-\alpha} \ln \mathrm{Tr}\, \rho_A^\alpha \tag{1}$$

where ρ_A is the reduced density matrix of partition A obtained by tracing out all degrees of freedom in $\bar{A}$ from the full density matrix:

$$\rho_A = \mathrm{Tr}_{\bar{A}}\, \rho = \mathrm{Tr}_{\bar{A}} |\Psi\rangle\langle\Psi| \tag{2}$$

The Rényi entropy is a monotonically decreasing function of α for $\alpha > 1$ and is bounded from above by the von Neumann entropy, $S_1(\rho_A) = -\mathrm{Tr}\, \rho_A \ln \rho_A$.

For a quantum many-body system subject to physical laws conserving some quantity (particle number, charge, spin, etc.), the set of local operations on the state $|\Psi\rangle$ are limited to those that don't violate the corresponding global superselection rule. For the remainder of this paper, we will focus on our discussion on the case of fixed total N and thus we are restricted to only those operators which locally preserve the particle number in A. The effect this has on the amount of entanglement that can be transferred to a qubit register is apparent from the simple example (adapted from Ref. 15 of one particle confined to two spatial modes A and $\bar{A}$ corresponding to site occupations. Then, for the state $|\Psi\rangle = \left(|1\rangle_A \otimes |0\rangle_{\bar{A}} + |0\rangle_A \otimes |1\rangle_{\bar{A}}\right)/\sqrt{2}$, Eq. (1) gives that $S_1 = \ln 2$. However, this entanglement cannot be transferred to a register prepared in initial state $|0\rangle_R$ via a `SWAP` gate:

$$\begin{aligned}&\texttt{SWAP}\, |0\rangle_R \otimes \left(|1\rangle_A \otimes |0\rangle_{\bar{A}} + |0\rangle_A \otimes |1\rangle_{\bar{A}}\right)/\sqrt{2} \\ &= \frac{1}{\sqrt{2}}\left(|0\rangle_R \otimes |0\rangle_A \otimes |1\rangle_{\bar{A}} + |1\rangle_R \otimes |0\rangle_A \otimes |0\rangle_{\bar{A}}\right)\end{aligned}$$

where the last term is not physically allowed due to the restriction that the number of particles in the system is fixed to be 1. The post-swap result remains in a product state and the amount of transferable entanglement is identically zero.

B. von Neumann Accessible Entanglement: $\alpha = 1$

Thus, Eq. (1), which includes the effects of non-local number fluctuations between A and $\bar{A}$, overcounts the amount of entanglement that can be accessed from the system. To quantify the physical reduction, Wiseman and Vaccaro[14] suggested that for the case of $\alpha = 1$ a more appropriate measure should weight contributions to the entanglement coming from each superselection sector corresponding to the number of particles n in A:

$$S_1^{\mathrm{acc}}(\rho_A) = \sum_{n=0}^{N} P_n S_1(\rho_{A_n}). \tag{3}$$

Here ρ_{A_n} is defined to be the reduced density matrix of A, projected onto the subspace of fixed local particle number n

$$\rho_{A_n} = \frac{1}{P_n}\mathcal{P}_{A_n}\rho_A\mathcal{P}_{A_n} \tag{4}$$

accomplished via a projection operator $\mathcal{P}_{A_n}$ where $\mathcal{P}_{A_n}|\Psi\rangle = |n\rangle_A \otimes |N-n\rangle_{\bar{A}}$. P_n is the probability of measuring n particles in A:

$$P_n = \mathrm{Tr}\, \mathcal{P}_{A_n}\rho_A\mathcal{P}_{A_n} = \langle\Psi|\mathcal{P}_{A_n}|\Psi\rangle\,. \tag{5}$$

As the projection constitutes a local operation which can only decrease entanglement, it is clear that $S_1^{\mathrm{acc}}(\rho_A) \le S_1(\rho_A)$. Moreover, the difference

$$\Delta S_1(\rho_A) \equiv S_1(\rho_A) - S_1^{\mathrm{acc}}(\rho_A) \tag{6}$$

can be determined by noting that the superselection rule guarantees that $[\rho_A, \hat{n}] = 0$ where $\hat{n}$ is the number operator acting in partition A. Thus ρ_A is block-diagonal in n and it can be shown[20] that

$$\Delta S_1(\rho_A) = H_1(\{P_n\}) \tag{7}$$

where

$$H_1(\{P_n\}) = -\sum_{n=0}^{N} P_n \ln P_n. \tag{8}$$

is the Shannon entropy of the number probability distribution. It is instructive to consider Eq. (7) for the special case of a discrete Gaussian distribution, $P_n \propto e^{-(n-\langle n\rangle)^2/2\sigma^2}$ where $H_1 = \ln\left(2\pi e\sigma^2 + \frac{1}{12}\right)$ depends only on the variance of P_n

$$\sigma^2 \equiv \langle n^2\rangle - \langle n\rangle^2 = \sum_{n=0}^{N} n^2 P_n - \left(\sum_{n=0}^{N} n P_n\right)^2. \quad (9)$$

Thus, when the number fluctuations are Gaussian, the von Neumann accessible entanglement is completely determined by the variance.

C. Rényi Accessible Entanglement: $\alpha \neq 1$

Computing the accessible entanglement for a many-body system is a difficult task for $\alpha = 1$, as full state tomography is required to reconstruct the density matrix ρ. However, for integer values with $\alpha > 1$ a replica trick can be used to recast $\mathrm{Tr}\rho_A^\alpha$ as the expectation value of some local operator[38]. This advance has led to a boon of new entanglement results using both computational[18,39–42] and experimental[30–33,43,44] methods. Motivated by this progress, two of us recently generalized the accessible entanglement to the case of Rényi entropies with $\alpha \neq 1$ and found that[21]:

$$S_\alpha^{\rm acc}(\rho_A) = \frac{\alpha}{1-\alpha}\ln\left[\sum_n P_n \mathrm{e}^{\frac{1-\alpha}{\alpha}S_\alpha(\rho_{A_n})}\right] \quad (10)$$

which reproduces Eq. (3) in the limit $\alpha \to 1$. While not physically transparent in this form, the modification from the $\alpha = 1$ case results from replacing the geometric mean in Eq. (3) with a general power mean whose form is constrained by the physical requirement that

$$0 \le \Delta S_\alpha \le \ln(N+1) \quad (11)$$

where the upper bound is equal to the support of P_n. Eq. (10) can also be interpreted as the quantum generalization of the conditional classical Rényi entropy[45–49], subject to physical constraints[21]. The arguments leading to Eq. (7) can then be generalized (see the supplemental material of Ref. [21]) leading to

$$\Delta S_\alpha \equiv S_\alpha - S_\alpha^{\rm acc} = H_{1/\alpha}\left(\{P_{n,\alpha}\}\right) \quad (12)$$

where we introduce the classical Rényi entropy of P_n

$$H_\alpha\left(\{P_n\}\right) = \frac{1}{1-\alpha}\ln\sum_n P_n^\alpha \quad (13)$$

and

$$P_{n,\alpha} = \frac{\mathrm{Tr}\left[\mathcal{P}_{A_n}\rho_A^\alpha\mathcal{P}_{A_n}\right]}{\mathrm{Tr}\ \rho_A^\alpha} = \frac{P_n^\alpha\ \mathrm{Tr}\ \rho_{A_n}^\alpha}{\mathrm{Tr}\ \rho_A^\alpha} \quad (14)$$

can be interpreted as a normalization of partial traces of ρ_A^α, where the SSR fixing the total particle number leads to $\mathrm{Tr}\ \rho_A^\alpha = \sum_n \mathrm{Tr}\left[\mathcal{P}_{A_n}\rho_A^\alpha\mathcal{P}_{A_n}\right]$ and thus guarantees the normalization of $P_{n,\alpha}$. Note that we have defined $P_{n,1} \equiv P_n$ for notational consistency. For brevity, let $H_\alpha(\{P_n\}) \equiv H_\alpha$ from here onwards.

Writing the difference ΔS_α as the classical Rényi entropy of the fictitious probability distribution $P_{n,\alpha}$, simplifies the calculation of ΔS_α and clarifies its properties, e.g., the fact that H_α is positive and bounded from above by $H_0 = \ln(N+1)$ guarantees that ΔS_α satisfies the physical requirement in Eq. (11).[21] In addition, $P_{n,\alpha}$ is fully determined by P_n and the full and the projected traces of ρ_A^α, i.e. $\mathrm{Tr}\ \rho_A^\alpha$ and $\mathrm{Tr}\ \rho_{A_n}^\alpha$, which can be measured using the experimental and numerical methods mentioned above.

D. Previous Results

While the accessible entanglement entropy can be used to diagnose the feasibility of using a many-body state of quantum matter as an entanglement resource, exact results are mostly limited to non-interacting systems. For a condensate of free bosons, the projected reduced density matrix ρ_{A_n} is always pure for any n and thus the accessible entanglement is zero[18]. For free fermions, early calculations[17] found $S_1^{\rm acc} \neq 0$ in a thermal state under a non-contiguous spatial bipartition of two sites on a one-dimensional lattice. More recent work on non-interacting spinless fermions[20,21] found that the SSR fixing the total particle number reduces the accessible entanglement by an amount that is only subleading in $\ln\ell$, with ℓ the size of the spatial bipartition. This result hinges on the realization that the probability distribution $P_{n,\alpha}$ defined in Eq. (14) is Gaussian with an average that is independent of α and a variance σ_α^2 that scales as $\ell^{d-1}\ln\ell/\alpha$ in d spatial dimensions. As the spatial entanglement S_α scales as $\ell^{d-1}\ln\ell$,[50] $\Delta S_\alpha/S_\alpha \sim \ln\left(\ell^{d-1}\ln\ell\right)/\left(\ell^{d-1}\ln\ell\right)$ which vanishes as $\ell \to \infty$.

For critical systems in $1d$ described by Luttinger liquid theory, (or more generally any conformal field theory with a conserved U(1) current), the particle number probability distribution P_n is expected to be Gaussian with a variance $\sigma^2 = K\ln\ell/\pi^2$ in the limit $\ell \gg 1$[20,51,52], where K is the Luttinger parameter. A result by Goldstein and Sela[29] can be employed to investigate $P_{n,\alpha}$ for Luttinger liquids which turns out to be Gaussian with the same average as P_n but with modified variance: $\sigma_\alpha^2 = \sigma^2/\alpha \overset{\ell\gg 1}{\to} K/\alpha\pi^2\ln\ell$. As a result

$$\begin{aligned}\Delta S_\alpha|_{\rm LL} &= H_{1/\alpha}\left(\{P_{n,\alpha}\}\right) = H_\alpha \\ &= \frac{1}{2}\ln\sigma^2 + \frac{1}{2}\ln\left[2\pi\alpha^{1/(\alpha-1)}\right]. \end{aligned} \quad (15)$$

Eq. (15) can be combined with the known result for the spatial entanglement entropy of a critical $1d$ system[38,53,54]

$$S_\alpha|_{1d\,\rm CFT} = \frac{c}{6}\left(1+\frac{1}{\alpha}\right)\ln\frac{\ell}{a} + \mathrm{O}(1), \quad (16)$$

where c is the central charge and a is a short distance cutoff, to see that the fraction of non-accessible entanglement entropy $\Delta S_\alpha/S_\alpha$, vanishes asymptotically as $\ln(\ln \ell)/\ln \ell$ in the Luttinger liquid phase.

Studies of the interaction dependence of $S^{\rm acc}$ have been previously limited to bosonic systems in $1d$. Quantum Monte Carlo simulations of harmonically trapped and harmonically interacting bosons identified a maxima in the accessible entanglement as a function of interaction strength[18]. Exact diagonalization of the $1d$ Bose-Hubbard model at unit filling for systems of up to $N = 16$ demonstrated that $S_2^{\rm acc}$ vanishes in the limit of strong and weak interactions.[19] Interestingly, $S_2^{\rm acc}$ was maximal near the superfluid-insulator phase transition and appeared to obey phenomenological scaling for the limited system sizes that could be studied. For an extended Bose-Hubbard model of four modes that includes pair-correlated hopping, exact diagonalizaition and variational calculations identified an interesting regime with strong pair-correlations where a matter wave beam-splitter operation on the ground state results in all entanglement being accessible[55].

Missing from this list is any system of interacting fermions and we now present numerical results for spinless fermions in one spatial dimension.

III. THE $t-V$ MODEL OF INTERACTING SPINLESS FERMIONS

A. Description and Solution

To investigate the behavior of accessible entangelment in an interacting fermionic system, we consider the $t-V$ model defined by a one-dimensional lattice of L sites occupied by N spinless fermions and governed by the Hamiltonian

$$H = -t\sum_i \left(c_i^\dagger c_{i+1} + \text{h.c.}\right) + V\sum_i n_i n_{i+1} \tag{17}$$

where $c_i^\dagger$ and c_i denote the fermionic creation and annihilation operators at site i, $\{c_i, c_j^\dagger\} = \delta_{i,j}$, and $n_i = c_i^\dagger c_i$. Here, $t > 0$ and V represent the nearest-neighbor hopping amplitude and interaction strength, respectively. We consider a half-filled lattice ($L = 2N$), unless mentioned otherwise and we use periodic boundary conditions (PBC) for an odd N, while for even N we use antiperiodic boundary conditions (APBC) to avoid complications arising from the degenerate ground state.

Eq. (17) can be mapped onto the XXZ spin-1/2 chain (at fixed magnetization) which is exactly solvable via Bethe ansatz[27,56,57] (see e.g. [58] for a recent pedagogical review). For $-2 < V/t < 2$, at low energies and long wavelengths, the system can be understood as a Tomonaga-Luttinger liquid (TLL) where the TLL parameter K at half filling, is[59]

$$K = \frac{\pi}{2\cos^{-1}\left[-V/(2t)\right]}\,. \tag{18}$$

In this language, $0 < K < 1$ corresponds to repulsive ($V > 0$) interactions, $K > 1$ to attractive ($V < 0$) interactions, and non-interacting fermions ($V = 0$) have $K = 1$. By increasing the relative interaction strength $|V/t|$, the system undergoes two phase transitions, a first order phase transition to a single fermionic cluster phase at $V/t = -2$, ($K = \infty$) and a continuous one at $V/t = 2$, ($K = 1/2$) to charge-density wave (CDW) phase. A schematic phase diagram is shown in Fig. 1.

B. Exact Ground State Results For Accessible Entanglement

In this section we derive a number of exact and asymptotic results for the accessible entanglement entropy of the $t-V$ model using insights gained from the structure of the ground states depicted in Fig. 1. Results for the von Neumann accessible entanglement are summarized in Table I.

Interaction	$S_1^{\rm acc}(\rho_A)$	ΔS_1
$V/t \to \infty$	$\left[1+(-1)^\ell\right]\ln(2)/2^\dagger$	$\left[1-(-1)^\ell\right]\ln(2)/2^\dagger$
$V/t \to -\infty$	$\frac{L-2}{2}\ln(2)$	$\ln(L/2)^\natural$
$V/t = -2$	$0^{\dagger\ddagger}$	$\frac{1}{2}\ln(L)^\natural$

TABLE I. Analytical results for the accessible entanglement in the ground state of the $t-V$ model with N fermions on L sites under a spatial bipartition consisting of $\ell = L/2$ contiguous sites. Symbols indicate approximations or generalizations with $\natural$ marking that the expression is asymptotically valid in the limit $L \gg 1$, $\dagger$ means $\ell < L$ and $\ddagger$ that the result is true for any filling fraction $N < L$.

1. $V/t \to \infty$

In the limit $V/t \to \infty$ and at half filling, the system reduces its energy by separating every two fermions by at least one empty site and thus the ground state $|\Psi_{V/t\to\infty}\rangle = (|\psi_{\rm even}\rangle + |\psi_{\rm odd}\rangle)/\sqrt{2}$ is an equal superposition of two occupation states. In one state the fermions occupy sites with only even indices ($|\psi_{\rm even}\rangle = |0101\ldots0101\rangle$) and in the other, they occupy sites with only odd indices $|\psi_{\rm odd}\rangle = |1010\ldots1010\rangle$).

If we now consider spatial bipartition A consisting of ℓ consecutive sites, we can write

$$\begin{aligned}\left|\Psi_{V/t\to\infty}\right\rangle = \frac{1}{\sqrt{2}}\left|\psi_{\rm even}\right\rangle_A \otimes \left|\psi_{\rm even}\right\rangle_{\bar{A}} \\ + \frac{1}{\sqrt{2}}\left|\psi_{\rm odd}\right\rangle_A \otimes \left|\psi_{\rm odd}\right\rangle_{\bar{A}}\,,\end{aligned} \tag{19}$$

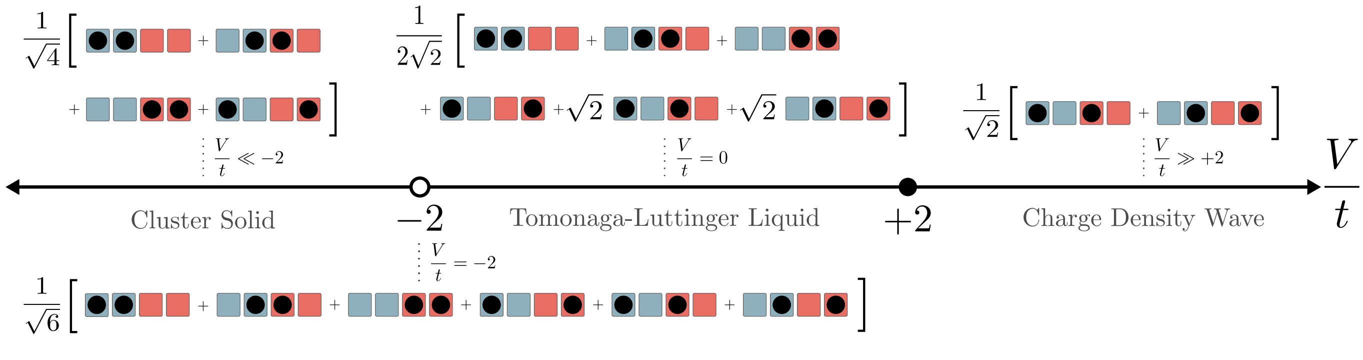

FIG. 1. Phase diagram of the $t-V$ model accompanied by pictures of candidate ground states for $N=2$ fermions on a $L=4$ site lattice. For the purposes of measuring accessible entanglement, the lattice has been bipartitioned into spatial subregions A (blue) and $\bar{A}$ (red), each of size $\ell=2$. We assume periodic boundary conditions. In the limit of strong attractive interactions where $V/t \ll -2$, the particles cluster together and there are L equally probable configurations corresponding to all translations of the cluster. At the first order phase transition where $V/t=-2$, all $\binom{L}{N}$ configurations are equally probable resulting in a flat state. In the TLL phase with $|V/t|<2$, particles are delocalized and we have included a characteristic state corresponding to free fermions ($V=0$). In the limit of strong repulsive interactions where $V/t \gg 2$, fermions maximize their distance from each other resulting in a charge density wave (CDW) phase. The open and closed circles on the V/t axis denote a first order and continuous phase transition, respectively.

resulting in the reduced density matrix

$$\rho_A = \frac{1}{2}\left|\psi_{\text{even}}\right\rangle_A \left\langle\psi_{\text{even}}\right| + \frac{1}{2}\left|\psi_{\text{odd}}\right\rangle_A \left\langle\psi_{\text{odd}}\right|.$$

For even ℓ, both of $|\psi_{\text{even}}\rangle_A$ and $|\psi_{\text{odd}}\rangle_A$ represent $\ell/2$ fermions as the number of sites with odd indices is equal to the number of sites with even indices. Therefore, the number of particles in partition A is fixed to $\ell/2$ and the entanglement entropy of the projected state $\mathcal{P}_{A_{n=\ell/2}}\left|\Psi_{V/t\to\infty}\right\rangle$ is $S_\alpha(\rho_{A_{n=\ell/2}}) = \ln 2$ with $P_{n=\ell/2}=1$ resulting in an overall accessible entanglement entropy $S_\alpha^{\text{acc}}(\rho_A) = \ln 2$. The picture is different for odd ℓ where the number of sites with odd indices differs from the number of sites with even indices by 1. In this case one of the states $|\psi_{\text{even}}\rangle_A$ and $|\psi_{\text{odd}}\rangle_A$ will represent $(\ell-1)/2$ fermions while the other represents $(\ell+1)/2$ fermions and therefore the projected state $\mathcal{P}_{A_{n=(\ell\pm1)/2}}\left|\Psi_{V/t\to\infty}\right\rangle$ is a separable state yielding zero entanglement entropy $S_\alpha^{\text{acc}}(\rho_A)=0$. For any partition size ℓ, regardless of its parity, the spectrum of ρ_A consists of two equal eigenvalues fixing the spatial entanglement entropy $S_\alpha(\rho_A)$ to $\ln 2$.

2. $V/t \to -\infty$

In the other extreme, $V/t\to-\infty$ and for any number of fermions $0<N<L$, the system minimizes its energy by forming a cluster of fermions that extends over any consecutive N sites. The ground state of the system, in this case, is an equal superposition of all L possible clusters. Once more, considering a partition A of ℓ consecutive sites, we can write the ground state as

$$\left|\Psi_{V/t\to-\infty}\right\rangle = \frac{1}{\sqrt{L}}\sum_n\sum_{i,j}|n,i\rangle_A\otimes|N-n,j\rangle_{\bar{A}}\ , \quad (20)$$

where $|n,i\rangle_A$ is the i^{th} configuration having n particles in partition A and $|N-n,j\rangle_{\bar{A}}$ is the j^{th} configuration with $N-n$ particles in its spatial compliment $\bar{A}$. Since the state is a superposition of L particle configuration states, ρ_A can have at most L non-zero eigenvalues. This defines an upper bound on $S_\alpha(\rho_A)\le\ln L$.

The simplicity of the state $\left|\Psi_{V/t\to-\infty}\right\rangle$ allows us to classify the projected state $\mathcal{P}_{A_n}\left|\Psi_{V/t\to-\infty}\right\rangle$ that corresponds to having n particles in partition A as follows. If the state $\mathcal{P}_{A_n}\left|\Psi_{V/t\to-\infty}\right\rangle$ has partition A or its complement $\bar{A}$ either empty or fully occupied then $\left|\Psi_{V/t\to-\infty}\right\rangle$ must be a separable state with $S_\alpha(\rho_{A_n})=0$. What remains are the projected states $\mathcal{P}_{A_n}\left|\Psi_{V/t\to-\infty}\right\rangle$ in which both of A and $\bar{A}$ have at least one empty and one occupied site. Due to the existence of the fermion cluster, knowing the configuration of the n particles in partition A fully determines the configuration of the $N-n$ particles in partition $\bar{A}$. Moreover, there can be only two such configurations that correspond to the fermionic cluster emerging into the partition A – either from its left or right end, such that $\mathcal{P}_{A_n}\left|\Psi_{V/t\to-\infty}\right\rangle = \frac{1}{\sqrt{L}}\sum_{i=1}^{2}|n,i\rangle_A\otimes|N-n,i\rangle_{\bar{A}}$, where $\langle n,1|n,2\rangle_A = \langle N-n,1|N-n,2\rangle_{\bar{A}} = 0$. This gives $S_\alpha(\rho_{A_n})=\ln 2$ and $P_n=2/L$. A simple counting then gives the number of projected states m that yield non zero entanglements as $\min\{\ell, L-\ell, N, L-N\}-1$. The resulting accessible entanglement is given by

$$S_\alpha^{\text{acc}}(\rho_A) = \frac{\alpha}{1-\alpha}\ln\left[\frac{2m}{L}2^{\frac{1-\alpha}{\alpha}}+1-\frac{2m}{L}\right], \quad (21)$$

which simplifies to

$$S_1^{\text{acc}}(\rho_A) = \frac{2m}{L}\ln 2, \quad (22)$$

in the von Neumann case $\alpha=1$. From Eq. (21) we see that $S_\alpha^{\rm acc}(\rho_A)$ is an increasing function of m. For a given L, the maximum value of m is $L/2-1$ which is achieved for $\ell = N = L/2$. In this case $S_1^{\rm acc}(\rho_A) = \frac{L-2}{L}\ln 2$ and for $L \gg 1$ we can write $S_\alpha^{\rm acc}(\rho_A) \approx \ln 2$.

To calculate the spatial entanglement entropy of this state, in general, we need the full spectrum of ρ_A. Based on the above there will be $2m$ eigenvalues of ρ_A that are equal to $1/L$. In addition, there are two more eigenvalues which correspond to one of the partitions being either empty or fully occupied. Counting the number of such occupation states gives the eigenvalues $(|\ell - N| + 1)/L$ and $(|\ell + N - L| + 1)/L$. Now if we consider the conditions for maximizing $S_\alpha^{\rm acc}(\rho_A)$, i.e., at half-filling and with half-partition, we find that ρ_A has a flat spectrum with L eigenvalues and thus $S_\alpha(\rho_A)$ is saturated at its upper bound, $S_\alpha(\rho_A) = \ln L$, and therefore $\Delta S_\alpha \approx \ln(L/2)$, for $L \gg 1$.

3. $V/t = -2$

Now we turn our attention to the very interesting case of the first order phase transition at $V/t = -2$, where the ground state $|\Psi_{V/t=-2}\rangle$ is an equal superposition of all $\binom{L}{N}$ possible configurations of N fermions on L sites. (see Appendix A for proof). In the language of the XXZ model this corresponds to the isotropic ferromagnetic point[60]. If we project $|\Psi_{V/t=-2}\rangle$ into a state with n particles in partition A and in one of its $\binom{\ell}{n}$ possible configurations, we get an equal superposition of $\binom{L-\ell}{N-n}$ occupation states which differ only by the configuration of the $N-n$ particles in $\bar{A}$. Therefore, we can immediately construct the desired Schmidt decomposition by inspection:

$$|\Psi_{V/t=-2}\rangle = \frac{1}{\sqrt{\binom{L}{N}}} \sum_n \sqrt{\binom{\ell}{n}\binom{L-\ell}{N-n}}\, |n\rangle_A \otimes |N-n\rangle_{\bar{A}}. \tag{23}$$

Here, each of the normalized states $|n\rangle_A$ and $|N-n\rangle_{\bar{A}}$ is an equal superposition of all of the possible configurations of n and $N-n$ particles in partitions A and $\bar{A}$, respectively.

For the state above, the projected reduced density matrix $\rho_{A_n} = |n\rangle_A\langle n|_A$ is a pure state and thus, for any n, $S_\alpha(\rho_{A_n}) = 0$. As a result, for any partition size ℓ, the accessible entanglement $S_\alpha^{\rm acc}(\rho_A) = 0$. Moreover, the spectrum of ρ_A is given by the particle number probability distribution $P_n = \binom{\ell}{n}\binom{L-\ell}{N-n}/\binom{L}{N}$ where we have used the fact that the block-diagonal structure of ρ_A in n allows us to write $\rho_A = \sum_n P_n \rho_{A_n}$. Furthermore, for this state, $S_\alpha(\rho_A) = H_{1/\alpha}(\{P_{n,\alpha}\}) = H_\alpha(\{P_n\})$

Let us consider the behavior of $S_\alpha(\rho_A)$ in the limit $L \gg 1$ and, for clarity, we focus on an equal bipartition at half-filling: $\ell = N = L/2$. Here, $P_n = \binom{\ell}{n}^2/\binom{2\ell}{\ell}$ and asymptotically it is a Gaussian distribution in n with variance $\sigma^2 = L/16$ and thus $S_\alpha(\rho_A) = \Delta S_\alpha = \frac{1}{2}\ln\left(2\pi\sigma^2\alpha^{(\alpha-1)^{-1}}\right) \approx \frac{1}{2}\ln L$.

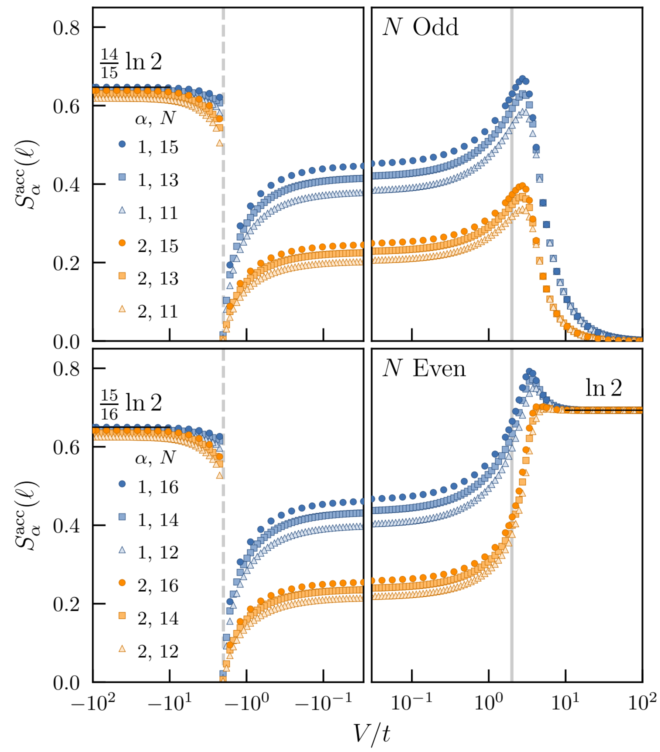

FIG. 2. Accessible entanglement entropy $S_\alpha^{\rm acc}(\ell)$ for $\alpha = 1, 2$ in the ground state of the $t-V$ model as a function of interaction strength V/t at half-filling, $N = L/2$. The top panel shows the results for an odd number of total particles: $N = 11, 13, 15$ and the bottom, for even: $N = 12, 14, 16$. The solid and dashed gray vertical lines indicate the locations of the known phase transitions for the model, $V/t = \pm 2$. For $N = 15, 16$ the asymptotic results computed in Section III in the limits $V/t \to \pm\infty$ for $S_1^{\rm acc}$ are shown as solid black lines.

IV. NUMERICAL RESULTS

To test the validity of the predictions in the previous section, we calculate the accessible entanglement in the ground state of the $t-V$ model, defined in section III, via numerical exact diagonalization for small systems (up to 32 sites) and using DMRG for larger systems (up to 98 sites), where the calculations are performed using the ITensor C++ library[28]. We focus on half-filling ($N = L/2$) and with a spatial partition size of $\ell = L/2$ contiguous sites, unless otherwise noted.

Fig. 2 shows the von Neumann and second Rényi accessible entanglement entropies, $S_1^{\rm acc}$ and $S_2^{\rm acc}$, as a function of the dimensionless interaction strength $-100 \le V/t \le 100$ for the six largest system studied by ED. To illustrate the effects that the parity of N has on $S_\alpha^{\rm acc}$, the top and bottom panels of Fig. 2 correspond to odd and even N, respectively.

A. Phase transitions and limiting cases of V/t

Starting from the regime of strong attractive interactions, $V/t = -100$, in Fig. 2, we see that $S_1^{\mathrm{acc}}(\rho_A)$ is rapidly converging to the expected value $(1 - 1/N)\ln 2$ in the limit $V/t \to -\infty$ (Eqs. (21) and (22)). This asymptotic result persists down to nearly $V/t = -10$ for large system sizes. Increasing V/t further, $S_\alpha^{\mathrm{acc}}(\rho_A)$ decreases slowly until we get closer to the first order phase transition at $V/t = -2$, (see section III B 3.), where $S_\alpha^{\mathrm{acc}}(\rho_A)$ decreases rapidly until it vanishes exactly at the transition point. This result holds for all N. As we increase V/t beyond -2, $S_\alpha^{\mathrm{acc}}(\rho_A)$ grows in the TLL regime as interaction driven liquid correlations build up until it eventually peaks in the vicinity of the infinite system critical point ($V/t = 2$) and eventually saturates to its limiting $V/t \to \infty$ value by $V/t \simeq 100$ which depends on the particle number parity: $S_\alpha^{\mathrm{acc}} \to 0$ for N odd and $S_\alpha^{\mathrm{acc}} \to \ln 2$ for N even. Exact diagonalization results up to $L = 32$ sites indicate that finite size effects are most visible in the Tomonaga-Luttinger liquid phase and this is especially true as we approach the continuous phase transition at $V/t = 2$ where a maxima begins to develop in the accessible entanglement entropy.

Quantum information measures have been known for some time to show signatures at continuous and discrete phase transitions, both at $T = 0$ and finite temperature[37,61–70] including the case of spinless fermions under consideration here[63,71–74]. A commonality amongst these studies is that the information quantity in question (entanglement entropy, negativity, concurrence, purity, etc.) develops some feature akin to an order parameter. Here, an analysis of the exact diagonalization data shows that the accessible entanglement develops a maximum at a coupling strength $\frac{V}{t}|_{\max} \sim \mathrm{O}(1)$. Making the empirical observation that the accessible entanglement appears to behave like a susceptibility, we perform an analysis of how the distance of the maxima from the infinite system size critical point ($\delta = \frac{V}{t}|_{\max} - 2$) depends on the system size L to search for power law scaling.

In order to investigate the existence of such scaling using larger system sizes than are possible with ED we employ DMRG where the total number of particles N is fixed and the resulting entanglement spectrum can be sorted according to the corresponding numbers of particles n and $N - n$ in the two partitions of the system[28]. This allows for the analysis of up to $L = 98$ sites at half-filling with the results shown in Figure 3 where the DMRG is benchmarked against ED for $N = 15$ (periodic boundary conditions). Performing a 2-parameter fit of the DMRG data to $\frac{V}{t}|_{\max} = 2 + \mathcal{A}N^{-1/\nu}$ supports a finite-size scaling form $\delta \sim L^{-1/\nu}$, with exponent $1/\nu \simeq 0.3$.

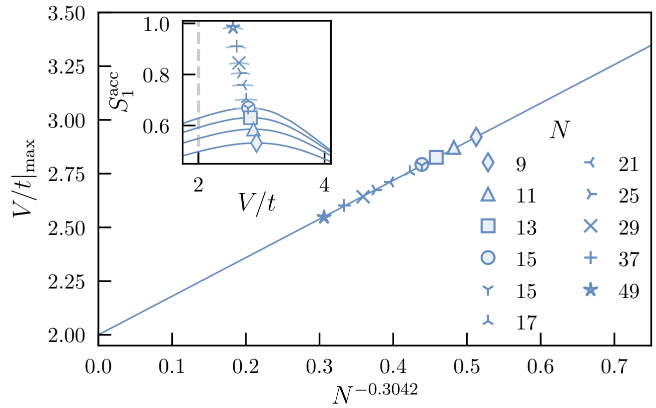

FIG. 3. Interaction strength at which the maximum S_1^{acc} occurs as a function of the total number of particles N. Finite size corrections were explored by a 2-parameter fit of $\ln N$ vs. $\ln(V/t - 2)$ and support scaling toward the infinite size phase transition at $V/t = 2$. Inset: The interaction dependence of S_1^{acc} for various N in the neighborhood of $\frac{V}{t}|_{\max}$ shows an evolving peak.

B. Reduction of entanglement due to particle fluctuations between subsystems

The difference between the full and accessible von Neumann entanglement entropies, $S_1 - S_1^{\mathrm{acc}} \equiv \Delta S_1 = H_1$, is equal to the Shannon entropy $H_1 = -\sum_n P_n \ln P_n$ of the particle number distribution[20]. From the asymptotic results in Table I we expect ΔS_1 to be maximal in the limit of strong attractive interactions where it behaves like $\ln L$ as extensive particle fluctuations between spatial subsystems contribute to the entanglement. In the opposite limit $V/t \to \infty$, we expect the difference to converge to a constant (N odd) or zero (N even) where repulsion strongly suppresses number fluctuations. This behavior is confirmed in Fig. 4 where we show the interaction dependence of ΔS_1 computed via exact diagonalization for $N = 15, 16$ (large circles). Fig. 4 also includes the entanglement reduction computed from the numerically determined variance of P_n (small circles) under the assumption that P_n is a continuous Gaussian distribution with mean $\langle n \rangle$ described by:

$$P_n \approx \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{-(n - \langle n \rangle)^2}{2\sigma^2}\right] \tag{24}$$

with Shannon entropy (see Eq. (15)):

$$H_1 = \Delta S_1 \approx \frac{1}{2}\ln\left(2\pi e \sigma^2\right) .$$

The resulting agreement the exact ΔS_1 with the asymptotic large-N result is surprisingly good over the entire range of $|V/t| \lesssim 2$ where P_n might still be expected to retain strong signatures of discreteness at these finite values of N. Moreover, we can quantitatively capture the

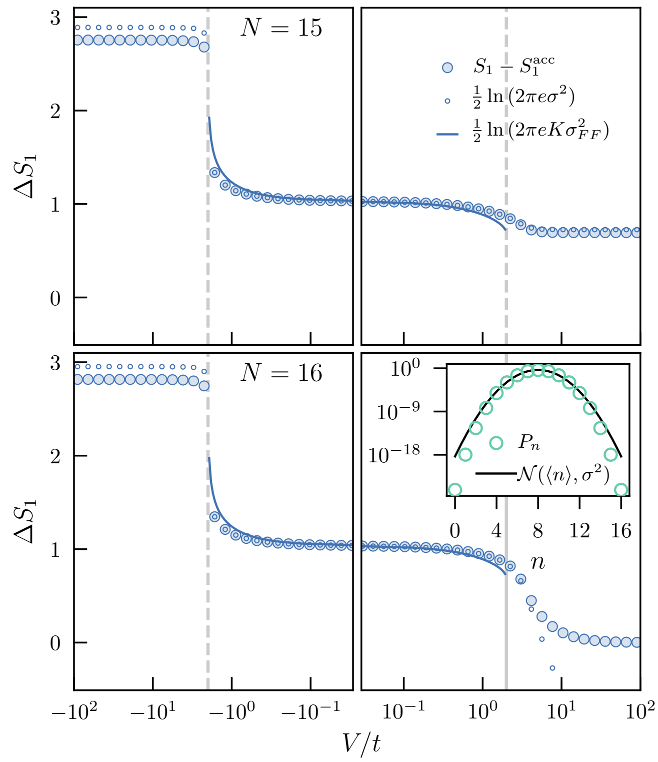

FIG. 4. Difference between the von Neumann and accessible entanglement entropies $S_1 - S_1^{\rm acc}$ (large circles) and the Shannon entropy of a Gaussian distribution, $\frac{1}{2}\ln 2\pi e\sigma^2$ (small circles) as functions of interaction strength V/t. Results were determined via exact diagonalization for the ground state of Eq. (17) with $N = 15, 16$. Agreement between the large and small symbols demonstrates the rapid convergence of P_n to a Gaussian. Solid lines are computed from the theoretical variance of the number of fermions in region A inside the Tomonaga-Luttinger liquid phase $\sigma^2 = K\sigma_{FF}^2$, where K is the Luttinger parameter computed via Eq.(18) and σ_{FF}^2 is the exact variance for free-fermions ($V/t = 0$).

interaction dependence of ΔS_1 (solid line) using the predicted Gaussian form and variance of the number distribution at low energies within the TLL regime (in the thermodynamic limit) using $\sigma^2 = K\sigma_{FF}^2$[20,51,52] where the Luttinger parameter K is computed using Eq. (18) and σ_{FF} is the variance of P_n for free fermions.

The exact finite size probabilities P_n are compared with a Gaussian distribution $\mathcal{N}(\langle n\rangle, \sigma^2)$ having the same mean $\langle n\rangle$ and variance σ^2 in the inset of Fig. **??** for $N = 15, 16$ and $V/t = -1.5$. On a logarithmic scale, the agreement looks excellent. However, to quantify the limitations of the asymptotic approximation we restrict to the case of even N, where the symmetry of the distribution P_n at half-filling guaranties that $\langle n\rangle = N/2$ is an integer such that $\delta n = n - \langle n\rangle$ is also an integer. Using the Poisson summation formula for a Gaussian function we find:

$$\sum_{\delta n=-\infty}^{\infty} e^{-\frac{(\delta n)^2}{2\sigma^2}} = \sqrt{2\pi\sigma^2}\left[1 + 2\sum_{\delta n=1}^{\infty} e^{-2\pi^2\sigma^2(\delta n)^2}\right], \tag{25}$$

where the summation on the right-hand side represents the error in the normalization of P_n which decreases with increasing variance σ^2 (see[75] for the odd N case). For the data presented in Figs. 4 and **??**, the value of σ^2 is 0.772 ($N = 16$) and 0.772 ($N = 15$) leading to a corresponding error of $\sim 10^{-6}$. Taking the derivative of both sides of Eq. (25) with respect to σ^2 shows that the variance of P_n calculated using its expression in Eq. (24) is well approximated by σ^2 in the same limits.

We can extend this analysis to

Also, replacing σ^2 by σ^2/α in Eq. (25), explains the deviation of the classical Rényi entropy H_α of P_n for higher Rényi indices $\alpha > 1$ from the continuous Gaussian distribution result (Eq. (15)) as we increase α as shown in Fig. **??**.

The expectation that, in the TLL phase, the distribution $P_{n,\alpha}$ is asymptotically Gaussian with variance $\sigma_\alpha^2 = \sigma^2/\alpha$, implies that the proportionality $P_{n,\alpha} \sim P_n^\alpha$ should hold. In general, having the previous proportionality dictates that $H_{1/\alpha}(\{P_{n,\alpha}\}) = H_\alpha$ and thus the difference $\Delta S_\alpha = H_\alpha$. Fig. 5 confirms this result even for $\alpha = 10$ where the continuous Gaussian distribution result fails (Fig. **??**). To confirm that this surprising agreement ($\Delta S_\alpha = H_\alpha$) is a consequence of the the proportionality $P_{n,\alpha} \sim P_n^\alpha$, in Fig. 6, we compare P_n with $A_\alpha P_{n,\alpha}^{1/\alpha}$ for different values of α, where A_α is a normalization factor. The figure shows an excellent data collapse of $A_\alpha P_{n,\alpha}^{1/\alpha}$ on P_n in the TLL regime.

Driven by the excellent agreement, we test another asymptotic result. In TLL phase the variance σ_α^2 is expected to approachthe value of $K\sigma_{FF}^2/\alpha$. This means that asymptotically and for a fixed α, we expect that distribution $P_{n,\alpha}(K)$ for a given interaction strength K to be proportional to $\sim P_{n,\alpha}(K = 1)^{1/K}$. In the inset of Fig. 7 we see that our results does not show the, asymptotically, expected data collapse as in the previous case. This could be due to strong a sub-leading correction to the expected linear scaling of the variance with the TLL prametr K.

HB: Why? This needs to be further explained, i.e. talk about the scale, the inset, and the lack of collapse.

V. DISCUSSION

In this paper we have presented a systematic study of how interactions affect the amount of operationally accessible entanglement that could be extracted from the ground state of a system of one-dimensional spinless lattice fermions where the total number of particles is fixed. The existence of this superselection rule (fixed N) limits the set of physical operations that can be performed with the result that the entanglement entropy under a spatial mode bipartition provides an absolute upper bound

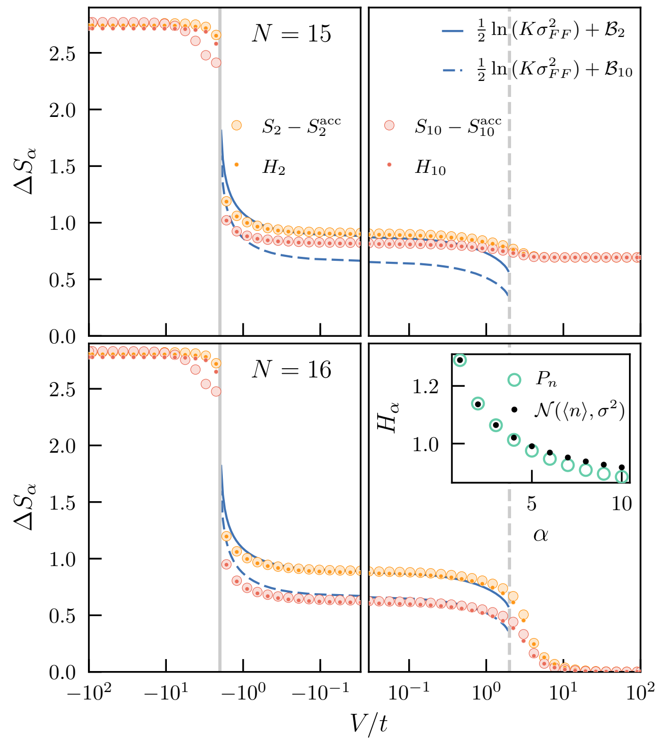

FIG. 5. Difference between the Rényi and accessible entanglement entropy $S_\alpha - S_\alpha^{\mathrm{acc}}$ and H_α as functions of interaction strength V/t for $\alpha = 2, 10$. In general, H_α should provide a lower bound for ΔS_α (i.e, $H_\alpha \leq S_\alpha$). Also, S_α^{acc} should be non-increasing in α. It can be seen that both relations hold in all phases of the $t-V$ model.

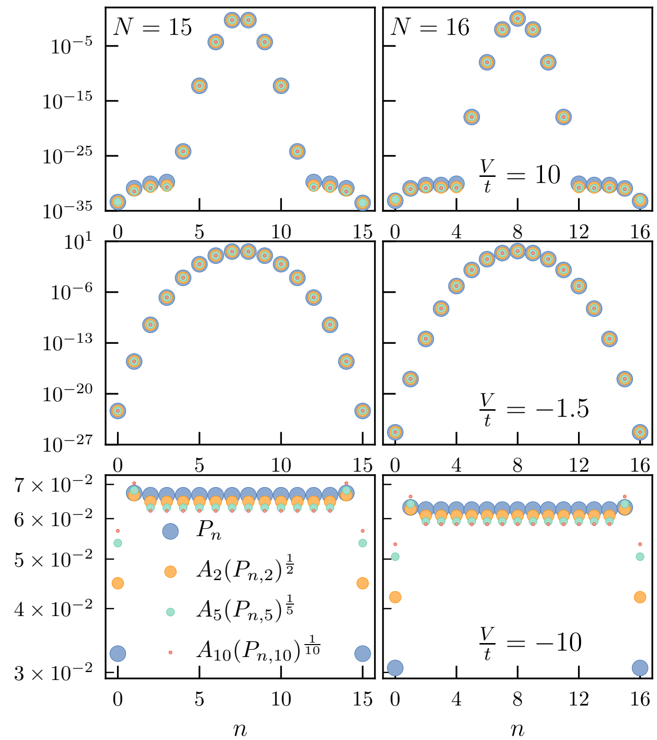

FIG. 6. Probabilities of measuring a state with n particles in subregion A, as a function of n. The probabilities in the TLL regime are known to be Gaussian, as seen from Eq.6. Here, they have been raised to $1/\alpha$ in order to cancel out the α dependence of the exponential part. For the middle plot, the interaction strength lies in the TLL regime and, consequently, the probabilities collapse to the same values in all the range after the α dependence has been cancelled. The top and bottom plots show results outside of the TLL regime, where the probabilities are not Gaussian.

on the accessible entanglement. We have derived analytic results for the von Neumann ($\alpha = 1$) and generalized Rényi ($\alpha \neq 1$) accessible entanglement in a few special cases (see Table I). In the limit of strong attractive interactions, the ground state is a superposition of all translations of a single cluster of N fermions and the accessible entanglement is reduced by $\ln N$ while still obeying a volume law. For strong repulsive interactions at half filling, the ground state is a superposition of possible density waves commensurate with the number of sites and the accessible entanglement is equal to the spatial entanglement for even N (no reduction), while it is reduced by a constant term to zero for odd N. Finally, exactly at the first order phase transition at $V/t = -2$, the ground state is an equal weight superposition of all possible fermion occupation states and the accessible entanglement is identically zero for all filling fractions and system sizes. This constitutes the maximal possible reduction where all of the spatial entanglement entropy in the critical phase which scales as the logarithm of the subsystem size is due to particle fluctuations. This result highlights the importance of understanding the role of classical number fluctuations in itinerant many-body systems when using entanglement entropy as a phase diagnostic. The drastic reduction in entanglement after projection into fixed particle number subsectors is reminiscent of Yang's η-paired state[76] under the quantum disentangled liquid diagnostic[77–79] which involves a partial projection onto spin degrees of freedom.

DMRG and phase transition (temp) – Investigating the scaling of the accessible entanglement with the system size require us to consider larger systems than what we have so far which is behold our numerical capabilities. The difficulties arise from the fact that DMRG is more suitable for finding states with a small amount of spatial entanglement and works better with open boundary conditions while the states we are targeting contains a large amount of entanglement that increases with the system size even faster near the critical point and we consider periodic boundary conditions in our study.

- scaling theory? Is anything special about the equal partition?
- speculation about area law violating states (Motzkin walks?)

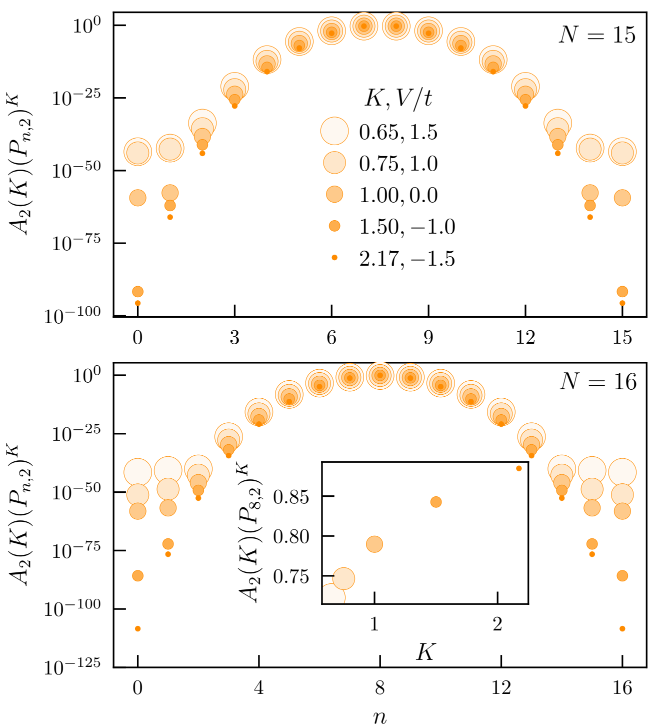

FIG. 7. Probabilities of measuring a state with n particles in subregion A, as a function of n. This time, the probabilities have been raised to the Luttinger Parameter K, after calculating for several K values. The probabilities seem to collapse nearly to the same value near the middle of the distribution. The inset plot shows the K dependence of the probability for fixed particle number in A, $n = 8$. This helps illustrate that the probabilities are proportional to K near the middle, as opposed to inversely proportional at the ends.

- other methods (beyond accessible) to deal with entanglement in indistinguishable itinerant particles, i.e. Refs. [80].

In general, ΔS_α with $\alpha \neq 1$ is not equal to the classical Rényi entropy H_α of the particle number distribution P_n as one might expect as a Rényi generalization of the measurement entropy considering Eq. (7). However, this true if the distribution $P_{n,\alpha}$ is proportional to P_n^α. In addition, if we consider P_n to be Gaussian with viarance σ^2 then

$$\Delta S_\alpha = H_\alpha = \frac{1}{2}\ln\left(\sigma^2\right) + \frac{1}{2}\ln\left(2\pi\alpha^{1/(\alpha-1)}\right) \tag{26}$$

VI. ACKNOWLEDGMENTS

We benefited from discussion with C. M. Herdman and I. Klich. This research was supported in part by the National Science Foundation (NSF) under award No. DMR-1553991 (A.D.). All computations were performed on the Vermont Advanced Computing Core supported in part by NSF award No. OAC-1827314.

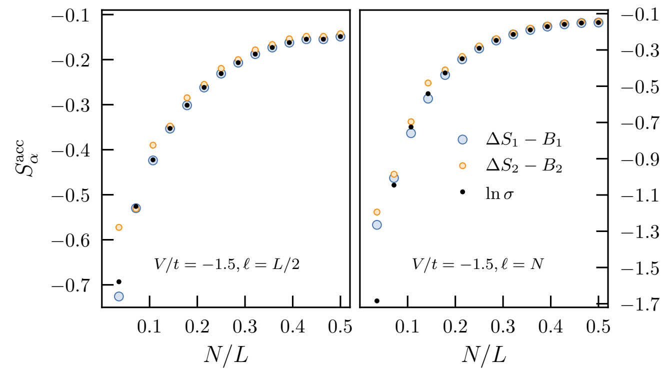

FIG. 8. Accessible entanglement entropies $S_\alpha^{\rm acc}(\ell)$ for $\alpha = 1, 2$ as a function of filling fraction N/L. The lattice size was kept fixed at $L = 28$ sites and the total number of particles were $N = 1, 2, 3 \ldots 14$. For the left column, the spatial partition ℓ was kept fixed at half the lattice size, $\ell = L/2$. For the right column, it was set to equal the total number of particles N. The interaction strengths V/t are indicated in each of the plots and correspond to values from each of the three phases of the $t - V$ model.

Appendix A: Ground state of the $t - V$ model for $V/t = -2$

Consider the Hamiltonian of the $t - V$ model given in Eq. (17) at the special interaction strength $V = -2t$ corresponding to the first order phase transition:

$$H = -t\sum_{i=1}^{L}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) - 2t\sum_{i=1}^{L} n_i n_{i+1} \tag{A1}$$

where we assume periodic boundary conditions for N even and anti-periodic boundary conditions for N odd.

1. Fermion occupation basis

We study the effect of H in the N fermion occupation basis $\{|\psi_a\rangle\}$, where the index a runs over all of the $\binom{L}{N}$ possible configurations. For example, for $N = 2$ and $L = 4$ there are six such states: $|\psi_a\rangle \in \{|1100\rangle, |1010\rangle, |1001\rangle, |0110\rangle, |0101\rangle, |0011\rangle\}$.

Starting with the potential operator $\mathcal{V} \equiv -2t\sum_{i=1}^{L} n_i n_{i+1}$ which is diagonal in this basis, we have

$$\mathcal{V}|\psi_a\rangle = -2t\, n_a^{(11)}|\psi_a\rangle\,, \tag{A2}$$

where $n_a^{(11)}$ counts the number of bonds connecting two occupied sites in the state $|\psi_a\rangle$. The hopping operator

$\mathcal{T} \equiv -t\sum_{i=1}^{L}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)$ turns $|\psi_a\rangle$ into a superposition of all the states $|\psi_b\rangle$ connected to $|\psi_a\rangle$ by moving one particle to a neighboring empty site. We can write:

$$\mathcal{T}\,|\psi_a\rangle = -t\sum_{b\in \mathsf{S}_a}|\psi_b\rangle\ , \tag{A3}$$

where S_a is the resulting index set of occupation states $|\psi_b\rangle$, i.e. $b \in \mathsf{S}_a \iff \langle\psi_b|\mathcal{T}|\psi_a\rangle \neq 0$. The cardinality of S_a is

$$\begin{aligned}\mathrm{card}(\mathsf{S}_a) &\equiv \sum_{b\in\mathsf{S}_a} 1\\ &= n_a^{(10)} + n_a^{(01)}\\ &= 2N - 2n_a^{(11)},\end{aligned} \tag{A4}$$

where $n_a^{(10)}$ ($n_a^{(01)}$) counts the number of occupied-empty (empty-occupied) bonds in $|\psi_a\rangle$ and in the last line we have used the fact that the total number of particles on a ring is (independent of the index a)

$$N = n_a^{(11)} + (n_a^{(10)} + n_a^{(01)})/2. \tag{A5}$$

A general matrix element in the fermion occupation basis is given by:

$$\langle\psi_c|\mathcal{T}|\psi_a\rangle = -t\begin{cases}1 & c\in\mathsf{S}_a\\ 0 & \text{otherwise}\end{cases} \tag{A6}$$

which is guaranteed to be real, thus

$$\langle\psi_c|\mathcal{T}|\psi_a\rangle = \langle\psi_a|\mathcal{T}|\psi_c\rangle \Rightarrow c\in\mathsf{S}_a \iff a\in\mathsf{S}_c. \tag{A7}$$

This is a useful result that can be used to swap the order of restricted and un-restricted summations.

Let us know consider the action of $\mathcal{T}$ on a general state $|\Psi\rangle = \sum_a \mathcal{C}_a|\psi_a\rangle$ where $\mathcal{C}_a \in \mathbb{C}$:

$$\begin{aligned}\mathcal{T}\,|\Psi\rangle &= -t\sum_a \mathcal{C}_a \sum_{b\in\mathsf{S}_a}|\psi_b\rangle\\ &= -t\sum_c |\psi_c\rangle \sum_a \mathcal{C}_a \sum_{b\in\mathsf{S}_a}\langle\psi_c|\psi_b\rangle\\ &= -t\sum_c|\psi_c\rangle\left[\sum_a \mathcal{C}_a\sum_{b\in\mathsf{S}_a}\delta_{c,b}\right]\end{aligned} \tag{A8}$$

where we have inserted a resolution of the identity operator $\sum_c |\psi_c\rangle\langle\psi_c| = \mathbb{1}$ into the second line. Now, $\sum_{b\in\mathsf{S}_a}\delta_{c,b} \neq 0 \iff c\in\mathsf{S}_a$ and using Eq. (A7) we can write

$$\sum_a \mathcal{C}_a \sum_{b\in\mathsf{S}_a}\delta_{c,b} = \sum_{a\in S_c}\mathcal{C}_a\,. \tag{A9}$$

Substituting into Eq. (A8) above and relabelling $a \leftrightarrow c$ leads to the general result:

$$\mathcal{T}\,|\Psi\rangle = -t\sum_a\sum_{c\in\mathsf{S}_a}\mathcal{C}_c\,|\psi_a\rangle\,. \tag{A10}$$

Written in this form, we can combine Eq. (A10) with Eqs. (A2) and (A4) to compute the action of the full Hamiltonian at $V = -2t$ on $|\Psi\rangle$:

$$\begin{aligned}H\,|\Psi\rangle &= -t\sum_a\left[\sum_{c\in\mathsf{S}_a}\mathcal{C}_c + 2n_a^{(11)}\mathcal{C}_a\right]|\psi_a\rangle\\ &= -2tN\,|\Psi\rangle - t\sum_a\sum_{c\in\mathsf{S}_a}(\mathcal{C}_c - \mathcal{C}_a)\,|\psi_a\rangle\ .\end{aligned} \tag{A11}$$

2. The Flat State

From Eq. (A11) it is immediately apparent that the flat state

$$|\Psi_0\rangle = \frac{1}{\sqrt{\binom{L}{N}}}\sum_a|\psi_a\rangle \tag{A12}$$

is an eigenstate of H with energy $-2tN$. To prove that $|\Psi_0\rangle$ is indeed the ground state, we consider matrix elements of the shifted operator $H' = H + 2tN$ for a general state $|\Psi\rangle$ expanded in the fermion occupation basis:

$$\begin{aligned}\langle\Psi|H'|\Psi\rangle &= -t\sum_{a,b}\sum_{c\in\mathsf{S}_a}(\mathcal{C}_c - \mathcal{C}_a)\,\langle\psi_b|\psi_a\rangle\,\mathcal{C}_b^*\\ &= t\sum_a\sum_{c\in\mathsf{S}_a}\left(|\mathcal{C}_a|^2 - \mathcal{C}_a^*\mathcal{C}_c\right)\\ &= t\sum_a\sum_{c\in\mathsf{S}_a}\left(|\mathcal{C}_c|^2 - \mathcal{C}_c^*\mathcal{C}_a\right)\end{aligned} \tag{A13}$$

where we have swapped the summations (and relabelled) in the last line making use of Eq. (A7). Now, we can rewrite the matrix element as:

$$\begin{aligned}\langle\Psi|H'|\Psi\rangle &= \frac{t}{2}\sum_a\sum_{c\in\mathsf{S}_a}\left(|\mathcal{C}_a|^2 - \mathcal{C}_a^*\mathcal{C}_c + |\mathcal{C}_c|^2 - \mathcal{C}_c^*\mathcal{C}_a\right)\\ &= \frac{t}{2}\sum_a\sum_{c\in\mathsf{S}_a}|\mathcal{C}_a - \mathcal{C}_c|^2 \geq 0.\end{aligned} \tag{A14}$$

Thus H' is a positive operator and the flat state $|\Psi_0\rangle$ is the ground state of H at $V = -2t$ for fixed N.

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