Rényi Generalization of the Accessible Entanglement Entropy

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Operationally accessible entanglement in bipartite systems of indistinguishable particles could be reduced due to restrictions on the allowed local operations as a result of particle number conservation. In order to quantify this effect, Wiseman and Vaccaro [Phys. Rev. Lett. **91**, 097902 (2003)] introduced an operational measure of the von Neumann entanglement entropy. Motivated by advances in measuring Rényi entropies in quantum many-body systems subject to conservation laws, we derive a generalization of the operationally accessible entanglement that is both computationally and experimentally measurable. Using the Widom theorem, we investigate its scaling with the size of a spatial subregion for free fermions and find a logarithmically violated area law scaling, similar to the spatial entanglement entropy, with at most a double-log leading-order correction. A modification of the correlation matrix method confirms our findings in systems of up to 10^5 particles.

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Entanglement encodes the amount of nonclassical information shared between complementary parts of an extended quantum state. For a pure state described by density matrix ρ, it can be quantified via the Rényi entanglement entropies: $S_\alpha(\rho_A) = (1-\alpha)^{-1}\ln \mathrm{Tr}\rho_A^\alpha$, where ρ_A is the reduced density matrix of subsystem A and S_α is a nonincreasing function of α. While the evaluation of the $\alpha = 1$ (von Neumann) entanglement entropy requires a complete reconstruction of ρ [1,2], integer values with $\alpha > 1$ can be represented as the expectation value of a local operator [3]. This has enabled entanglement measurements in a wide variety of many-body states, via both quantum Monte Carlo [4–8] and experimental quantum simulators employing ultracold atoms [9–14]. In these systems, the conservation of total particle number N may restrict the set of possible local operations (a superselection rule) and can potentially limit the amount of entanglement that can be physically accessed [15–22]. For example, while a superfluid of N bosonic ^{87}Rb atoms in a one-dimensional optical lattice is highly entangled under a bipartition into spatial subregions [10], much of the entanglement is generated by particle fluctuations that cannot be transferred to a quantum register without access to a global phase reference [23]. Wiseman and Vaccaro introduced an *operational* measure of entropy to quantify these effects [17], but it is limited to the special case of $\alpha = 1$ and thus cannot be used in tandem with current simulation and experimental studies of entanglement.

In this Letter, we study how the operationally accessible entanglement can be generalized to the Rényi entropies with $\alpha \neq 1$. Recalling its definition for $\alpha = 1$, it is constructed by averaging the contributions to S_1 coming from each physical number of particles in the subsystem:

$$S_1^{\mathrm{acc}}(\rho_A) = \sum_{n=0}^{N} P_n S_1(\rho_{A_n}), \tag{1}$$

where $\rho_{A_n} = \mathcal{P}_{A_n}\rho_A\mathcal{P}_{A_n}/P_n$ is the projection into the sector of n particles in A, A_n, via $\mathcal{P}_{A_n}$ which occurs with probability $P_n = \mathrm{Tr}\mathcal{P}_{A_n}\rho_A\mathcal{P}_{A_n}$. This projection constitutes a local operation which can only decrease entanglement by an amount bounded by the maximum entropy of the classical number fluctuation probability distribution P_n. Thus, a conservation law on the total number of particles imposes that any Rényi generalization of Eq. (1) to S_α^{acc} must satisfy $0 \le S_\alpha - S_\alpha^{\mathrm{acc}} \le \ln D$, where D is the support of P_n. Under this physical constraint, we show that a direct extension of Eq. (1) to $\alpha \neq 1$ is not generally appropriate.

Instead, we reconsider the problem in terms of the mathematical relationship between the von Neumann and $\alpha \neq 1$ Rényi entropies—that of a geometric to power mean—and identify a unique measure:

$$S_\alpha^{\mathrm{acc}}(\rho_A) = \frac{\alpha}{1-\alpha}\ln \sum_n P_n e^{[(1-\alpha)/\alpha]S_\alpha(\rho_{A_n})}, \tag{2}$$

which not only provides a lower bound on the amount of accessible entanglement entropy in a pure state but is measurable with current technologies for integer $\alpha > 1$.

We validate that Eq. (2) reproduces Eq. (1) as $\alpha \to 1$ and prove that it is a nonincreasing function of Rényi index α in analogy with S_α. We show that $S_\alpha^{\mathrm{acc}} = 0$ when all particles have condensed into a single mode, e.g., a Bose-Einstein condensate, and demonstrate that, in the limit of large subsystem size, it agrees with the known behavior of S_1^{acc}

for free fermions in d spatial dimensions [24]—that the fixed total particle number reduces the accessible entanglement only by a subleading logarithm, $S_\alpha^{\mathrm{acc}} \approx S_\alpha - \frac{1}{2}\ln S_\alpha$. Such asymptotic scaling is expected for $1d$ critical systems with fixed N that can be described by a conformal field theory, where the particle number distribution is Gaussian [25,26].

The main contributions of this work are (i) the introduction of the Rényi generalization of the accessible entanglement entropy, (ii) an investigation of its asymptotic scaling properties for free fermions via the Widom theorem supported by exact calculations for noninteracting $1d$ lattice fermions, and (iii) a discussion of how the accessible entanglement could be measured in ultracold atomic lattice gases using current technology.

We begin with the observation that the Rényi entanglement entropy with $\alpha \neq 1$ is a generalization of the $\alpha = 1$ von Neumann entanglement entropy obtained by replacing a geometric mean with respect to the reduced density matrix ρ_A with a power mean. Extending this idea to $S_1^{\mathrm{acc}}(\rho_A)$ in Eq. (1), there are now two geometric means to be replaced: one over ρ_A and one over the number probability distribution P_n. The resulting generalization is given by (see the derivation in Supplemental Material [27])

$$S_\alpha^{\mathrm{acc}}(\rho_A;\gamma) = -\ln\left(\sum_n P_n (\mathrm{Tr}\rho_A \rho_A^{\alpha-1})^{\gamma/(\alpha-1)}\right)^{1/\gamma}, \quad (3)$$

where we have introduced an as of yet undetermined power mean exponent $\gamma = \gamma(\alpha)$. In the limit $\gamma \to 0$, one recovers the direct extension of Eq. (1): $S_\alpha^{\mathrm{acc}}(\rho_A;0) = \sum_{n=0}^{N} P_n S_\alpha(\rho_{A_n})$, which was previously proposed to study a system of bosons in one dimension [29].

Defining $\Delta S_\alpha(\gamma) \equiv S_\alpha(\gamma) - S_\alpha^{\mathrm{acc}}(\gamma)$ as the important quantity which captures the reduction of the entanglement due to a superselection rule, we now explore what restrictions are imposed on the exponent γ by the physical constraint that $0 \le \Delta S_\alpha(\gamma) \le \ln D$. To this end, we consider the example of a reduced density matrix of a spatial partition of ℓ sites, obtained from a pure state of $N \gg 1$ particles, where the number fluctuations are described by the normalized distribution: $P_n = A_N \exp[-(N-n)/\sqrt{N}]$. The corresponding eigenvalues of ρ_A are equal for each n: $\lambda_{n,i} = \ell^{-n} A_N \exp[-(N-n)/\sqrt{N}]$, where $i = 1, \ldots, \ell^n$. In this case, $D = N+1$, and the asymptotic dependence of $\Delta S_{\alpha>1}(\gamma)$, to leading order, on N for $\gamma \neq 1 - \alpha^{-1}$ is given by $\Delta S_{\alpha>1}(\gamma) \approx [(\alpha/(\alpha-1)) - (1/\gamma)]\sqrt{N}$ for $\gamma > 0$ and $\Delta S_{\alpha>1}(\gamma) \approx -N\ln\ell$ for $\gamma \le 0$, which violates the condition $0 \le \Delta S_\alpha(\gamma) \le \ln D$ for any $\gamma \neq 1-\alpha^{-1}$. If we modify the above example by rearranging the probabilities in the reverse order, i.e., replacing P_n with P_{N-n}, we arrive at the same conclusion for $\alpha < 1$ (see Supplemental Material [27] for a complete proof).

For $\gamma = 1 - \alpha^{-1}$, it can be proven that the inequality $0 \le \Delta S_\alpha(\gamma) \le \ln D$ is satisfied in general [27]. Moreover, for this case, S_α^{acc} represents a lower bound for S_1^{acc} for $\alpha > 1$ (upper bound for $\alpha < 1$); i.e., S_α^{acc} is a nonincreasing function of α, and, by construction, $\lim_{\alpha\to 1} S_\alpha^{\mathrm{acc}} = S_1^{\mathrm{acc}}$ [27]. Substituting $\gamma = 1 - \alpha^{-1}$ in Eq. (3), we obtain Eq. (2), which we propose as the unique Rényi generalization of the accessible entanglement entropy.

For more physical insight into the form of this measure, we appeal to a previously noticed connection between the von Neumann accessible entanglement and the Shannon conditional entropy [24,30]. If the spectrum of the reduced density matrix ρ_A is treated as a joint probability distribution of two random variables, one of which is the number of particles n in partition A, then Eq. (1) is equivalent to the conditional entropy of the probability distribution, where the condition is information of n in the subregion. Many different candidate measures for the classical conditional Rényi entropy have been proposed [31–35], but if one requires that they satisfy both monotonicity and the weak chain rule, then the classical limit of Eq. (2) is recovered.

Having understood the origin of the Rényi generalized accessible entanglement entropy, in order to actually perform computations, we exploit the fact that, for pure states of N particles, ρ_A is block diagonal in n, and thus Eq. (2) can be conveniently rewritten as

$$S_\alpha^{\mathrm{acc}} = S_\alpha - H_{1/\alpha}(\{P_{n,\alpha}\}), \quad (4)$$

where $H_\alpha(\{P_n\}) = (1-\alpha)^{-1}\ln\sum_n P_n^\alpha$ is the Rényi generalization of the Shannon entropy of P_n,

$$P_{n,\alpha} = \frac{\mathrm{Tr}[\mathcal{P}_{A_n}\rho_A^\alpha \mathcal{P}_{A_n}]}{\mathrm{Tr}\rho_A^\alpha} \quad (5)$$

is a normalization of partial traces of ρ_A^α, and $P_{n,1} = P_n$. From Eq. (4), one immediately recovers the previously known result for $\alpha = 1$ that $\Delta S_1 = H_1$ [24], where we write $H_\alpha \equiv H_\alpha(\{P_n\})$ for simplicity.

In the remainder of this Letter, we use Eqs. (4) and (5) to calculate the Rényi generalized accessible entanglement for two simple models of noninteracting particles. First, we consider the case of N noninteracting bosons on a d-dimensional hypercubic lattice of L^d sites with unit lattice spacing. The ground state consists of all particles condensed into one single-particle mode $|\Psi\rangle = (N!)^{-1/2}(\Phi_0^\dagger)^N|0\rangle$, where $\Phi_0^\dagger = \sum_j B_j b_j^\dagger$ and $b_j^\dagger$ creates a boson on site j with $\sum_j |B_j|^2 = 1$. We take a spatial bipartition A that contains a set of ℓ^d contiguous sites and decompose $\Phi_0^\dagger = \sqrt{p_A}\Phi_A^\dagger + \sqrt{p_{\bar{A}}}\Phi_{\bar{A}}^\dagger$ with $p_A = |\langle 0|\Phi_A\Phi_0^\dagger|0\rangle|^2$, $p_{\bar{A}} = 1 - p_A$, and $\Phi_A^\dagger$ acts in A, and similarly for the complement $\bar{A}$. Then, the ground state can be directly written as the Schmidt decomposition

$$|\Psi\rangle = \sum_{n=0}^{N} \lambda_n^{1/2}|n\rangle_A \otimes |N-n\rangle_{\bar{A}},$$

where $\lambda_n = \binom{N}{n} p_A^n p_{\bar{A}}^{N-n}$, $|n\rangle_A = (n!)^{-1/2}(\Phi_A^\dagger)^n|0\rangle_A$, and $|N-n\rangle_{\bar{A}} = [(N-n)!]^{-1/2}(\Phi_{\bar{A}}^\dagger)^{N-n}|0\rangle_{\bar{A}}$. For free bosons, $p_A = (\ell/L)^d$ [7,36]. The reduced density matrix ρ_A obtained by tracing out $\bar{A}$ is thus pure for each n: $\rho_{A_n} = |n\rangle\langle n|$ resulting in $S_\alpha = H_\alpha$ and $P_{n,\alpha} = P_n^\alpha / \sum_n P_n^\alpha \Rightarrow S_\alpha^{\rm acc} = 0$. This is expected for the Bose-Einstein condensate where, for $N \gg 1$ with p_A fixed, $P_n = \lambda_n$ approaches a Gaussian distribution and $S_\alpha = H_\alpha \approx \frac{1}{2}\ln N$ [36,37] is generated from particle fluctuations between subregions.

To understand the behavior of $S_\alpha^{\rm acc}$ for fermionic statistics, we focus on a microscopic model of noninteracting fermions on a d-dimensional lattice where the correlation matrix method [38–42] is applicable. This provides an exponential simplification of the calculation of $S_\alpha(\rho_A)$ and allows for the investigation of its asymptotic behavior. In this case, A corresponds to some collection of ℓ^d lattice sites, and the eigenvalues of ρ_A that correspond to having n particles in partition A are $\lambda_{n,a} = \prod_{j=1}^{\ell^d}[\nu_j^{n_{j,a}}\bar{\nu}_j^{(1-n_{j,a})}]$, where the index a runs over all possible configurations of the occupation numbers $n_{j,a} \in \{0,1\}$ with $n = \sum_j n_{j,a}$ $\forall$ a and $\bar{\nu}_j = 1 - \nu_j$. Here, ν_j are the eigenvalues of the correlation matrix $(\mathsf{C}_A)_{ij} = \langle c_i^\dagger c_j\rangle = \mathrm{Tr}\rho_A c_i^\dagger c_j$, where i and j are restricted to the spatial partition A and $c_i^\dagger$ (c_i) creates (annihilates) a spinless fermion at lattice site i $(c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij})$ [38].

This approach can be generalized to calculate the particle number projected Rényi entanglement $S_\alpha(\rho_{A_n}) = S_\alpha + (1-\alpha)^{-1}\ln(P_{n,\alpha}/P_n^\alpha)$ and thus $S_\alpha^{\rm acc}(\rho_A)$. However, as we are interested in the reduction of entanglement due to the presence of superselection rules, we focus on the difference $\Delta S_\alpha = S_\alpha - S_\alpha^{\rm acc}$, which depends only on

$$P_{n,\alpha} = \sum_a \prod_{j=1}^{\ell^d}[\nu_{j,\alpha}^{n_{j,a}}\bar{\nu}_{j,\alpha}^{(1-n_{j,a})}], \tag{6}$$

where $\nu_{j,\alpha} = \nu_j^\alpha/(\nu_j^\alpha + \bar{\nu}_j^\alpha)$. An important first step is the observation that $P_{n,\alpha}$ has the form of a Poisson-binomial distribution [43] with ℓ^d different success probabilities $\nu_{j,\alpha}$ [44]. In order to investigate the asymptotic scaling of ΔS_α with linear subsystem size ℓ, we need to consider the behavior of $P_{n,\alpha}$ or, alternatively, its characteristic function (Fourier transform) $\chi_\alpha(\lambda) = \prod_{i=1}^{\ell^d}[1 - \nu_{j,\alpha} + \nu_{j,\alpha}e^{i\lambda}]$, which can be expressed in terms of the matrix C_A as

$$\ln\chi_\alpha(\lambda) = \mathrm{Tr}\ln[1 - \mathsf{C}_{A,\alpha} + \mathsf{C}_{A,\alpha}e^{i\lambda}], \tag{7}$$

where $\mathsf{C}_{A,\alpha} \equiv \mathsf{C}_A^\alpha/[\mathsf{C}_A^\alpha + (1-\mathsf{C}_A)^\alpha]$. This form is convenient, as the $\alpha = 1$ case, providing access to the scaling of $P_{n,1} = P_n$, has already been obtained for the d-dimensional free Fermi gas by means of the Widom theorem [24,45–51]. Motivated by these results, we calculate the characteristic function $\chi_\alpha(\lambda)$ for a d-dimensional spatial subregion with dimensionless linear size ℓ in the limit $\ell \gg 1$, where ℓ is now treated as a continuous variable. We find that $P_{n,\alpha}$ is a normal distribution with the same average as P_n and variance $\sigma_\alpha^2 = \sigma^2/\alpha \sim \ell^{d-1}\ln\ell/\alpha$, where σ^2 is the variance of P_n [27]. In this case, $P_{n,\alpha} \sim P_n^\alpha \Rightarrow H_{1/\alpha}(\{P_{n,\alpha}\}) = H_\alpha(\{P_n\})$, leading to

$$\Delta S_\alpha \approx H_\alpha \approx \ln\sqrt{2\pi\sigma^2\alpha^{1/(\alpha-1)}} \sim \frac{1}{2}\ln(\ell^{d-1}\ln\ell), \tag{8}$$

which, if compared to the asymptotic scaling of $S_\alpha \sim \ell^{d-1}\ln\ell$ [49], implies that $\Delta S_\alpha \approx \frac{1}{2}\ln S_\alpha$. We thus conclude that fixed N reduces the Rényi generalized accessible entanglement of the free Fermi gas only by a subleading double logarithm of ℓ for $\ell \gg 1$.

To confirm the asymptotic predictions of Eq. (8), we now apply the extended correlation matrix method introduced above to a model of N free spinless lattice fermions on a ring of $2N$ sites (half filling) governed by the Hamiltonian $\mathcal{H} = -\sum_i(c_i^\dagger c_{i+1} + \mathrm{H.c.})$ [52]. The correlation matrix for the ground state Fermi sea is $(\mathsf{C}_A)_{ij} = [\sin(\pi(i-j)/2)]/[2N\sin(\pi(i-j)/2N)]$. We studied systems with up to $N = 10^5$ fermions and partition size $\ell = 10^5$ sites, where we calculate ΔS_α and H_α using $P_{n,\alpha}$ which we obtain via a recursion relation for the Poisson-binomial distribution [53]:

$$P_{n,\alpha}(j) = \nu_{j,\alpha}P_{n-1,\alpha}(j-1) + \bar{\nu}_{j,\alpha}P_{n,\alpha}(j-1). \tag{9}$$

The desired distribution is reached after ℓ recursive steps; i.e., $P_{n,\alpha} = P_{n,\alpha}(\ell)$, and Eq. (9) drastically reduces the complexity to an $O(\ell^2)$ algorithm [53].

The results in Fig. 1 demonstrate the predicted logarithmic scaling of ΔS_2 with $\sigma^2 = 2\sigma_2^2$ as well as the fact that asymptotically, $\Delta S_2 \approx H_2$, i.e., that $P_{n,2}$ appears to behave as a continuous normal distribution. For this particular case of free fermions, we find that $S_\alpha - S_\alpha^{\rm acc} > H_\alpha$, but this may not be generically true in interacting models. Additionally, as seen in Fig. 2, P_n is very narrow, with $\sigma^2 < 1.4$, and thus the main contribution comes from only a few points around its peak. This suggests that, to truly reach the asymptotic regime, we need to further increase σ^2 by several orders of magnitude beyond our current numerical capability.

As an alternative, we generalize the known asymptotic behavior of ν_j [54–56] to $\nu_{j,\alpha}$ as

$$\nu_{j,\alpha} = \left[1 + \exp\left(\frac{-\alpha\pi^2(\ell - 2j + 1)}{2[\ln(8\ell) + \gamma_{\rm em}]}\right)\right]^{-1}, \tag{10}$$

where $\gamma_{\rm em} \approx 0.6$ is the Euler-Mascheroni constant, and calculate the characteristic function $\chi_\alpha(\lambda)$ of $P_{n,\alpha}$. We find that $P_{n,\alpha}$ is asymptotically a normal distribution with variance $\sigma_\alpha^2 = \ln\ell/(\alpha\pi^2)$ for any $\alpha > 0$ [27] extending the results of the Widom theorem for $d = 1$ to real-valued

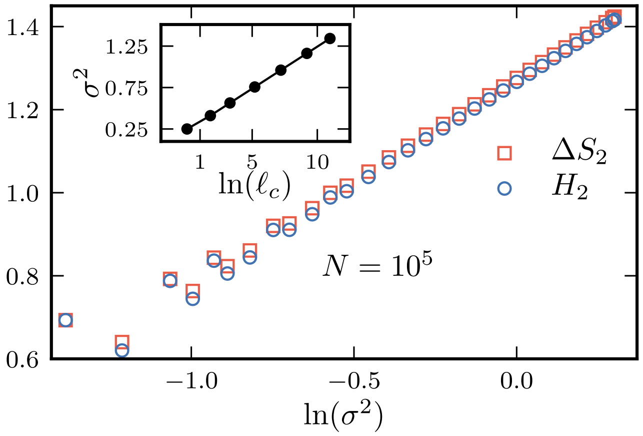

FIG. 1. Scaling of the difference between the Rényi and accessible entanglement entropy, ΔS_2 and H_2, with the log of the variance of P_n, $\ln(\sigma^2)$, for subregions up to $\ell = 10^5$ connected sites. The results were calculated using the correlation matrix method for free fermions in the ground state of $\mathcal{H}$. Inset: Scaling of σ^2 with $\ln(\ell_c)$, where $\ell_c = (2N/\pi)\sin(\pi\ell/(2N))$ is the chord length, highlighting the double logarithmic growth of the width of the distribution P_n.

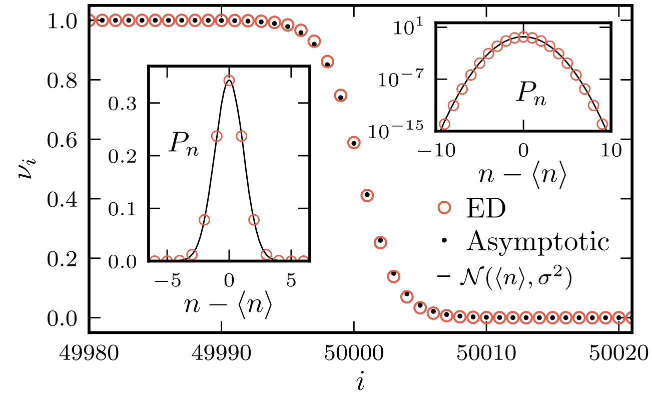

FIG. 2. The spectrum of the correlation matrix C_A of free fermions calculated via exact diagonalization (empty circles) and from the asymptotic relation in Eq. (10) (filled circles) for $N = 10^5$ at half filling with partition size $\ell = 10^5$. Insets: The corresponding number probability distribution P_n vs $n - \langle n \rangle$ on a linear (left) and log (right) scale. The solid line shows a normal distribution $\mathcal{N}$ with the average $\langle n \rangle$ and variance σ^2 of P_n demonstrating its convergence but narrow width.

α. This is further validated using Eq. (10) with $\ell \approx e^{3000}$ as shown in Fig. 3.

Thus, for free fermions, superselection rules fixing the total number of particles only marginally reduce the accessible entanglement that can be transferred from a many-body state to a quantum register. This is also true for interacting $1d$ fermions in the Luttinger liquid regime [24,57]. The free fermion result is robust even when extending to noncontiguous subregions, e.g., a partition of size $\ell = N$ corresponding to even (odd) sites where the correlation matrix is diagonal and $\nu_{j,\alpha} = \nu_j = \frac{1}{2}$. Here, $S_\alpha = \ell \ln 2$ and $P_{n,\alpha} = P_n \ \forall \ \alpha$ are described by a simple binomial distribution (normal distribution, asymptotically) with ℓ equal success probabilities $\nu = \frac{1}{2}$. Thus, $\sigma^2 = \ell/4$ and $\Delta S_\alpha \sim \ln \sigma^2$, yielding $\Delta S_\alpha \sim \frac{1}{2} \ln S_\alpha$.

This picture can be drastically altered by strong interactions [58] or in bosonic systems [29], where the contribution of particle fluctuations to entanglement are large and the accessible entanglement is suppressed to zero.

In summary, by exploiting a general relation between geometric and power means, we derive a unique measure S_α^{acc} in Eq. (2) which generalizes the accessible entanglement in the presence of a superselection rule, previously defined only for von Neumann entropies, to the more readily measurable Rényi entanglement entropies S_α.

This definition preserves the limit $\alpha \to 1$, provides a lower bound on S_1^{acc} for $\alpha > 1$, and is smaller than S_α while not exceeding the maximum information lost to particle fluctuations. $S_\alpha^{\mathrm{acc}} = 0$ for a Bose-Einstein condensate of fixed total particle number, while, for free fermions, we find that the corresponding superselection rule reduces the amount of accessible entanglement from its unconstrained value by a subleading correction that asymptotically scales as the logarithm of the width of the probability distribution describing particle fluctuations in the subregion. We confirm this prediction numerically using the correlation matrix method on a lattice model of free fermions, where we have simplified the calculation by relating the required partial traces ρ_A^α to the Poisson-binomial distribution which can be calculated using a simple recursion relation. This method can be extended to other models of noninteracting fermions, including those with long-range or correlated

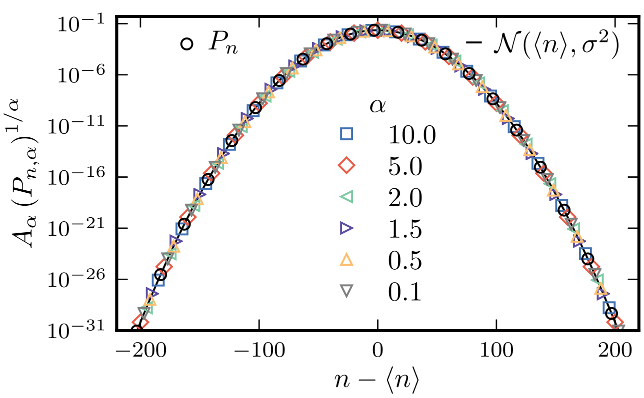

FIG. 3. Collapse of the rescaled probability distribution $A_\alpha(P_{n,\alpha})^{1/\alpha}$ to P_n for different values of α, where A_α is a normalization factor. The solid line shows a normal distribution $\mathcal{N}$ with the average $\langle n \rangle$ and variance σ^2 of P_n. The data were obtained using the correlation matrix method with the asymptotic eigenvalues ν_j [Eq. (10)] and $\ln \ell = 3000$. We find a perfect collapse for both integer (supported by the Widom theorem) and noninteger values of α.

hopping, as well as disordered systems, where contributions to the entanglement entropy from particle fluctuations will be further suppressed. It is interesting to speculate on how the ideas discussed here could be further generalized to understand the effects of superselection rules on entanglement without resorting to a particular mode bipartition [59–62].

The functional form of the Rényi generalized accessible entanglement depends only on the full and particle number projected reduced density matrices that can be directly computed by creating copies of a physical system. It is thus accessible using current simulation [4–8] and experimental [10,13,14] techniques for both bosons and fermions for integer $\alpha \geq 2$ by histogramming ρ_A^α into bins corresponding to the number of particles n observed in the subregion with appropriate postselection [29]. The experimental measurement of the Rényi generalized accessible entanglement entropy and confirmation of its robust scaling in fermionic systems would, in combination with a protocol for its extraction and transfer to a register, support such many-body phases as a potential resource for quantum information processing.

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