

Evidence for Unbounded Growth of the Number Entropy in Many-Body Localized Phases

Maximilian Kiefer-Emmanouilidis,^{1,2} Razmik Unanyan,¹ Michael Fleischhauer,¹ and Jesko Sirker²
¹*Department of Physics and Research Center OPTIMAS, University Kaiserslautern, 67663 Kaiserslautern, Germany*
²*Department of Physics and Astronomy, University of Manitoba, Winnipeg R3T 2N2, Canada*

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We investigate the number entropy S_N —which characterizes particle-number fluctuations between subsystems—following a quench in one-dimensional interacting many-body systems with potential disorder. We find evidence that in the regime which is expected to show many-body localization and where the entanglement entropy grows as $S \sim \ln t$ as function of time t , the number entropy grows as $S_N \sim \ln \ln t$, indicating continuing subdiffusive particle transport at a very slow rate. We demonstrate that this growth is consistent with a relation between entanglement and number entropy recently established for non-interacting systems.

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Introduction.—The time dependence of the entanglement entropy $S(t)$ after a quantum quench offers insights into the dynamics of quasiparticles and the influence of conservation laws. Well studied are quenches starting from a product state in clean lattice models with short-range hoppings and interactions. In this case, the generic picture is one of quasiparticles propagating through the system with a velocity bounded by the Lieb-Robinson velocity v_{LR} [1–3]. The entanglement entropy is then proportional to the entangled region created by the quasiparticle excitations. For a subsystem with volume ℓ^d in d dimensions, this leads to $S \sim \ell^{d-1}t$ for times $v_{LR}t \ll \ell$ and a volume-law saturation, $S \sim \ell^d$, at times $v_{LR}t \gg \ell$. This picture has been confirmed in free scalar field theories [4] and in one-dimensional systems which are conformally invariant [5]. An obvious exception from a linear increase of the entanglement entropy after a quench and from a volume-law scaling at long times are disordered noninteracting systems in an Anderson localized (AL) phase [6]. In this case, the spreading of excitations is limited to the localization length ξ_{loc} leading to an area law, $S \sim \ell^{d-1}\xi_{loc}$, instead of a volume law at long times. The increase of the entanglement entropy after the quench is therefore bounded [7].

In recent years, the question of localization in the presence of interactions—termed *many-body localization* (MBL)—has attracted renewed interest [8–13]. For the spin-1/2 Heisenberg chain with local magnetic fields drawn from a box distribution, numerical data appear consistent with a transition from an ergodic phase at small disorder to a nonergodic MBL phase at strong disorder [10,14,15]. One of the hallmarks of MBL as compared to AL is the unbounded logarithmic growth of S after a quench [9,16,17]. Recently, evidence for $S \sim \ln t$ has also been obtained in an experiment on cold atomic gases [18]. Here a quench in a one-dimensional Aubry-André model of interacting bosons was studied with single atom resolution.

In such systems where the total particle number (or similarly the total magnetization) is conserved, the von Neumann entropy can be split into two parts, $S = S_N + S_c$ [18–21]. Here

$$S_N = -\sum_n p(n) \ln p(n) \quad (1)$$

is the number entropy with $p(n)$ the probability of finding n atoms in the considered subsystem (also referred to as charge [20] or fluctuation entropy [21]). The configurational entropy S_c then contains the contributions to entanglement due to configurational correlations. This splitting of S is not only useful from an experimental perspective because $p(n)$ can be determined by single-site resolution atomic imaging [18] but also offers further insights into questions of localization and ergodicity. Very recently, we have shown that in any noninteracting fermionic system $S^{(2)} \propto \exp(S_N^{(2)})$ where $S^{(2)}$ is the second Rényi entropy and $S_N^{(2)}$ the corresponding number entropy. In other words, a growth in the entanglement entropy is always accompanied by a logarithmically slower growth in the number entropy [22].

An exception to this picture of correlated dynamics of entanglement and number entropies is expected to occur in many-body localized phases. Here S_N is believed to saturate after a quantum quench, indicating localization, while S continues to grow in time. It has been argued that MBL systems are described at long times by effective Hamiltonians [23,24]

$$H = \sum_l \varepsilon_l \eta_l + \sum_{l,l'} J_{ll'} \eta_l \eta_{l'} + \dots, \quad (2)$$

with exponentially many local conserved charges $[H, \eta_l] = 0$, random energies ε_l , and amplitudes $J_{ll'}$ which

decay exponentially with distance between these charges. As a consequence of the coupling terms $\sim J_{ll'}$, a region of length ℓ will become entangled over time $t \sim e^\ell$. Since the entanglement entropy is extensive, one then expects $S \sim \ell \sim \ln t$ [25] consistent with the numerical and experimental observations. Note that in the Anderson case $J_{ll'} \equiv 0$ and η_l are the occupation number operators of the single-particle localized eigenstates. If Eq. (2) is a valid effective description of MBL phases of matter, then the increase in entanglement at long times is entirely due to the continuing buildup of configurational entanglement S_c . Since the conserved charges η_l are local, the number entropy S_N has to be bounded, reflecting the expected localized and nonergodic character of this phase. On the other hand, the experimental data for the number entropy in Ref. [18] appear to show a slow increase, although a detailed analysis of the number entropy as a function of system size and disorder strength has not yet been performed. Furthermore, it has recently been suggested that paradigmatic models expected to show MBL phases might ultimately be ergodic at very long times [26,27].

These recent results motivate us to investigate the number entropy in systems believed to show MBL. In this Letter, we provide evidence that the picture of MBL phases based on effective Hamiltonians (2) might be incomplete. For all system sizes and times we can access numerically, we find that the number entropy grows as $S_N \sim \ln \ln t$ even at strong disorder and does not show any signs of saturating. We, furthermore, present evidence that the relation $S^{(2)} \propto \exp(S_N^{(2)})$, proven for free fermionic systems in [22], also appears to hold in the interacting case, both in the ergodic and in the MBL phase, with proportionality factors renormalized by interactions and disorder.

Number entropies.—If we split a one-dimensional system S into two parts, A and B , then the Rényi entanglement entropies are given by

$$S^{(\alpha)} = (1 - \alpha)^{-1} \ln \text{tr} \rho_A^\alpha, \quad (3)$$

where ρ_A is the reduced density matrix of the considered subsystem. The von-Neumann entanglement entropy is given by $S \equiv S^{(1)} = \lim_{\alpha \rightarrow 1} S^{(\alpha)}$. If the total particle number is conserved, then we can write $S^{(\alpha)} = (1 - \alpha)^{-1} \ln[\sum_n p^\alpha(n) \text{tr} \rho_A^\alpha(n)]$ where $\rho_A(n)$ is the block of the reduced density matrix with particle number n normalized such that $\text{tr} \rho_A(n) = 1$. If there is only a single configuration for each n then $\text{tr} \rho_A^\alpha(n) = \text{tr} \rho_A(n) = 1$. We thus call $S_N^{(\alpha)} = (1 - \alpha)^{-1} \ln \sum_n p^\alpha(n)$ the Rényi number entropy, generalizing Eq. (1). Any additional entanglement is due to different configurations in each particle sector having finite probability and is thus part of what we call the Rényi configurational entropy.

System.—To be concrete, let us consider a half-filled fermionic model

$$H = -J \sum_j (c_j^\dagger c_{j+1} + \text{H.c.}) + \sum_j D_j n_j + V \sum_j n_j n_{j+1}, \quad (4)$$

with nearest-neighbor hopping amplitude J , interaction V , and on site disorder $D_j \in [-D/2, D/2]$. Here $n_j = c_j^\dagger c_j$ is the particle number at site j . Using a Jordan-Wigner transformation, this model can be mapped onto a spin-1/2 XXZ chain with magnetic field disorder. For $V = 2J$, in particular, one obtains the isotropic Heisenberg model which is the most studied system to investigate MBL physics. We set $J = 1$ and $\hbar = 1$ in the following.

Thermalization.—If such a system after a quantum quench thermalizes to a high temperature state, then a region of size 2ℓ will contain ℓ particles on average and every arrangement of particles will approximately have equal probability. If we now cut the thermalized region in half, then the probability to find n particles in one half is $p(n) = \binom{\ell}{n} \binom{\ell}{\ell-n} / \binom{2\ell}{\ell}$. For large n, ℓ this distribution can be approximated by a continuous distribution and one finds for all Rényi number entropies (including $\alpha \rightarrow 1$) in the ergodic case $S_N^{(\alpha)} = \text{const.} + \frac{1}{2} \ln \ell$ with $S_N^{(\alpha)} > S_N^{(\alpha+1)}$ [22]. If the excitations in the system spread as t^ν after the quench then the thermalized regions have size $\ell \sim t^\nu$ and we obtain

$$S_N^{(\alpha)}(t) = \text{const} + \frac{\nu}{2} \ln t. \quad (5)$$

Localization.—The presence of disorder (i.e., $D \neq 0$) can prevent thermalization and lead to localized states. The simple scaling argument why free particles ($V = 0$) on a lattice with short-range hoppings become localized for strong potential disorder works as follows [6,28,29]. A real hopping process requires a resonance, i.e., an energy matching between the two sites involved in the hopping process. Assuming a random, homogeneous distribution of the corresponding energies, the smallest energy difference between two states in a subsystem of volume ℓ^d decreases as ℓ^{-2d} in d dimensions on average. The transport between quasidegenerate states needs on the order of $n \sim \ell$ hopping processes and the amplitude for such a virtual n -site hopping process falls off exponentially with distance. Therefore distant resonances have a vanishingly small probability to proliferate and to delocalize the system. A noninteracting system at sufficiently strong disorder will therefore be in an AL phase and both S and S_N will saturate. In one dimension, even arbitrarily weak disorder is sufficient to localize all states. The crucial question then is what influence interactions have on the probability of distant resonances.

If the model (4) is in an AL phase for $V = 0$, a localized basis $\{|\psi_l\rangle\}$ exists such that the noninteracting Hamiltonian becomes diagonal, $H_0 = \sum_l \epsilon_l \eta_l = \sum_l \epsilon_l d_l^\dagger d_l$. We can transform (4) to this localized basis using $c_j^\dagger = \sum_l \langle \psi_l | \phi_j \rangle d_l^\dagger$, where $|\phi_j\rangle$ is the original Wannier basis.

Here l can be understood as the index of the site around which the localized single-particle wave function is centered, i.e., $|\langle \psi_l | \phi_j \rangle|^2 \sim \exp(-|l - j|/\xi_{\text{loc}})$ where ξ_{loc} is the localization length. If we transform the interaction part to the new basis, we find contributions describing density-density interactions between localized orbitals as well as hopping processes between these orbitals. The density-density part is given by $H_{\text{int}}^{(1)} = \sum_{l,l'} J_{ll'} \eta_l \eta_{l'}$ with an amplitude which decays exponentially with distance between the orbitals, $J_{ll'} \sim V \exp(-|l - l'|/\xi_{\text{loc}})$. If this would be the only relevant correction due to interactions, then particles would remain localized with $H_{\text{int}}^{(1)}$ causing a logarithmic buildup of configurational entanglement, see Eq. (2). However, the interaction also leads to a correlated hopping between the single-particle orbitals $|\psi_l\rangle$

$$H_{\text{int}}^{(2)} = \sum_{l,l',k,k'} K_{ll'kk'} d_l^\dagger d_{l'} d_k^\dagger d_{k'}, \quad (6)$$

with unequal lattice sites and exponentially decaying amplitude $K_{ll'kk'}$. Similar to the AL case, one then has to consider the possibility of resonances destroying localization. In contrast, hopping processes are now long ranged so that both direct and virtual transitions to distant sites are possible. The smallest expected average mismatch in energy, $\Delta\varepsilon = \varepsilon_l - \varepsilon_{l'} + \varepsilon_k - \varepsilon_{k'}$, on a subsystem of length ℓ now decreases as ℓ^{-4} . Without taking the renormalization of the bare energies ε_l into account, one would thus still conclude that distant resonances do not proliferate. On the other hand, numerical and experimental data [30] indicate that for small disorder interactions do destroy the localized phase. In other words, in this case energy renormalizations do seem to lead to a proliferation of resonant hopping processes. For strong disorder, on the other hand, it has been argued that the processes (6) are irrelevant, particles are localized, and Eq. (2) is the proper effective model [31,32]. However, these results are based on approximations. The proof of MBL for weak interactions in Ref. [32], in particular, is based on an assumption about limited level attraction in the statistics of energy eigenvalues.

Numerical results.—Since the question about the relevance of resonances ultimately cannot be decided analytically, we investigate the number entropy for the model (4) by exact diagonalization (ED). We concentrate on $V/J = 2$ corresponding to the isotropic Heisenberg model. In our notation the critical coupling, where all eigenstates are expected to become localized, is $D_c/J \approx 14$ [10,14]. We study quenches starting from half-filled random product states, averaging over both disorder realizations and initial states. If not stated otherwise the data shown for $L \leq 18$ are obtained by standard full diagonalizations of the Hamiltonian, averaged over 10 000 disorder realizations for $L \leq 14$ and 3000 realizations for $L > 14$, while a second order Trotter-Suzuki decomposition of the time evolution

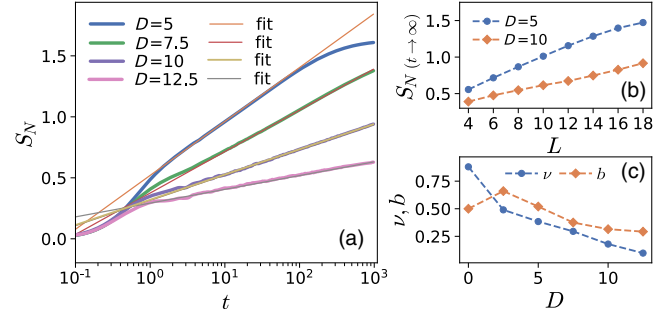


FIG. 1. S_N for $D < D_c \approx 14$: (a) $S_N(t)$ for $L = 24$, with 500 disorder realizations and logarithmic fits, $S_N = (\nu/2) \ln t + b$. (b) $S_N(t \rightarrow \infty)$ for different system sizes L . (c) Prefactors ν and constants b of the logarithmic fits as a function of D for $L = 24$.

operator is used for $L = 24$, see [33] for details. The entropies are always calculated for systems with open boundary conditions and blocks of length $\ell = L/2$.

Let us first consider the regime $D < D_c$ where there is consensus that the system is ergodic. ED [39,40], large-scale density-matrix renormalization group (DMRG) calculations [41,42], and phenomenological numerical renormalization groups [43,44] furthermore find subdiffusive transport either all the way down to zero disorder or up to a second critical disorder below which transport becomes diffusive. In contrast to the linear-in-time spreading of excitations in the clean case, it now takes time $t \sim \ell^{1/\nu}$ for excitations to spread across a region of length ℓ with $\nu = 1/2$ corresponding to diffusion. We therefore expect $S \sim \ell \sim t^\nu$ while S_N is given by Eq. (5). This scaling of $S(t)$ in the ergodic regime is consistent with DMRG calculations for infinite chains with binary disorder [42] and with ED [40] for box disorder. In Fig. 1, results for the number entropy of model (4) at various disorder strengths $D < D_c$ are shown. We find that $S_N(t)$ grows logarithmically consistent with Eq. (5) and thus ergodic behavior. This

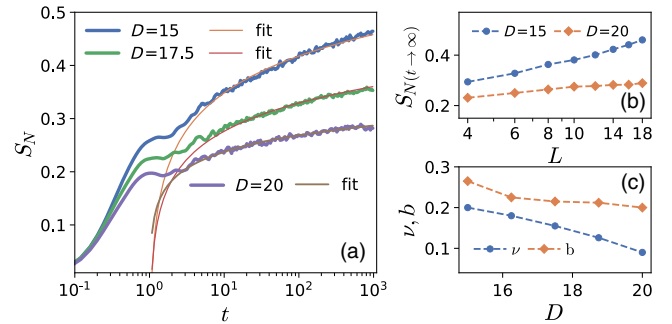


FIG. 2. S_N for $D > D_c$: (a) $S_N(t)$ for $L = 24$ and double logarithmic fits, $S_N = (\nu/2) \ln \ln t + b$. (b) $S_N(t \rightarrow \infty)$ for different system sizes L . (c) Prefactor ν and constant b of the double logarithmic fits as a function of D for $L = 24$, see also [33].

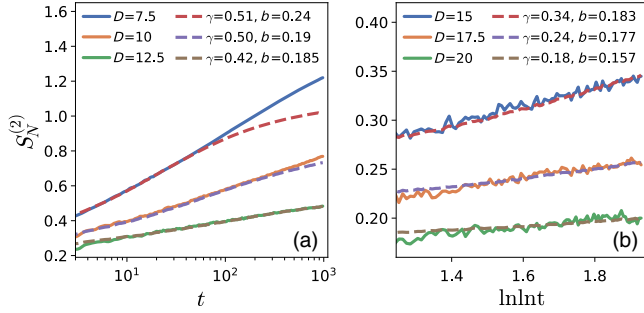


FIG. 3. $S_N^{(2)}$ and bound (7) for (a) $D < D_c$, and (b) $D > D_c$. The renormalization parameter γ appears to decrease monotonically with increasing D .

is also supported by the close to linear scaling of the saturation value $S_N(t \rightarrow \infty)$ with system size. Finally, we note that the prefactor ν decreases continuously as a function of disorder D and appears to approach zero for $D \rightarrow D_c$. The precise behavior close to the transition point is very difficult to extract from our numerics and outside the scope of our work. The results for the number entropy are qualitatively consistent with previous results for the scaling of the current [41] and of the bipartite particle number fluctuations Δn [16,45].

Turning to the case $D > D_c$, it is expected that it then takes time $t \sim e^\ell$ to entangle regions over a distance ℓ . The resulting scaling of the von-Neumann entropy $S \sim \ln t$ has been demonstrated already by various methods and for a number of different models and our results are consistent with such a scaling as well. Our main new result are the data for the number entropy presented in Fig. 2. We find that the number entropy continues to increase as $S_N \sim \ln \ln t$ and that the saturation value continues to grow as a function of length as in the ergodic case $D < D_c$, however, now only approximately logarithmically. For the numerically accessible times and lengths we find no indications for a saturation of the number entropy as would be expected if the system is localized. Note that $S_N \sim \ln \ln t$ is exactly the scaling which is anticipated if the system is ultimately ergodic and $t \sim e^\ell$ is not only the relevant scaling for the buildup of configurational entanglement but also for the spreading of particles [see derivation of Eq. (5)]. As a function of disorder strength D we find that the prefactor ν of the double logarithmic growth is decreasing continuously. There are no indications for a sharp transition. Let us also comment on the bipartite particle fluctuations Δn investigated previously [16,45]. Our results (not shown) are consistent with $\Delta n(t)$ growing without bounds and $\Delta n(t \rightarrow \infty, L)$ increasing with increasing system size L .

To provide further support for an unbounded growth of the number entropy, we now show that the numerical results are consistent with a relation recently proven in the noninteracting case [22]. There we found that

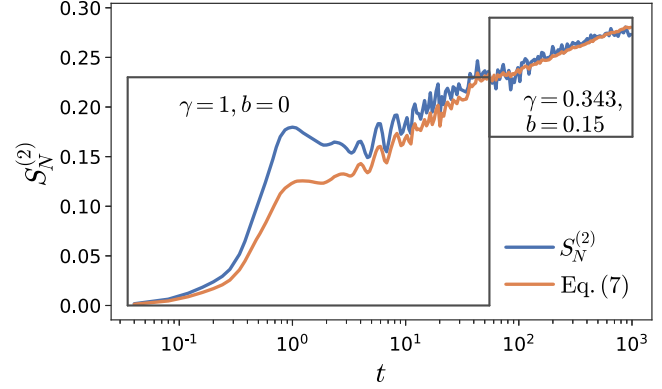


FIG. 4. $S_N^{(2)}$ for model (4) with binary disorder $D = 20$ and segments with equal D limited to four sites (1000 disorder realizations). For $t < t_{\text{Th}}$ an unrenormalized bound ($\gamma = 1$) holds while γ is renormalized for $t > t_{\text{Th}}$, see text.

$$S_N^{(2)} \geq \gamma \left\{ \frac{S^{(2)}}{2 \ln 2} - \ln \left[I_0 \left(\frac{S^{(2)}}{2 \ln 2} \right) \right] \right\} + b \quad (7)$$

provides a tight bound with $\gamma = 1$, $b = 0$, and I_0 being the modified Bessel function. In other words, a growth of the second Rényi entropy $S^{(2)}$ is always accompanied by a growth, albeit logarithmically slower, of the corresponding number entropy $S_N^{(2)}$. In Fig. 3 we show that this bound with a renormalized γ (and curves shifted by $b > 0$ for ease of presentation) appears to remain valid in the interacting case both for $D < D_c$ and $D > D_c$. Note that in the interacting case, i.e., $V \neq 0$, γ appears to decrease continuously with increasing D but does not show indications of a sharp transition.

Finally, we want to consider a system with very strong disorder to check whether the increase of the number entropy is transient. To this end, we consider the model (4) with binary disorder $D_j \in \{-D/2, D/2\}$. For $D \rightarrow \infty$ this will result in finite segments which are coupled by the interaction term but not by hopping processes. We, furthermore, limit the size of segments with equal potential $\pm D/2$ to four lattice sites. In this case, the disorder is no longer uncorrelated but this should only help in reducing the timescale where $S_N^{(2)}$ potentially saturates. Numerically, we find that the bound (7) also holds in this case, see Fig. 4. For $t \lesssim t_{\text{Th}}$, where $t_{\text{Th}} \sim \exp(D/\Omega)L^2$ [26,33] is the Thouless time with Ω being a constant, the original bound in the noninteracting case ($\gamma = 1$) holds, while a renormalized bound holds for longer times. In the thermodynamic limit, $S_N^{(2)}$ thus appears to grow without bounds in this model as well.

Conclusions.—The slow increase of the number entropy $S_N \sim \ln \ln t$ and the increase of the saturation value as a function of system size, found in our numerical simulations, are not expected in an MBL phase. There are at least two different possible interpretations of these data. First, it

cannot be excluded that the observed behavior after all is transient and that S_N in the thermodynamic limit does saturate at very long times. While this interpretation would not challenge the established phenomenology of MBL phases, it is then an open question to understand the origin of such a long-time transient behavior as well as the time and length scales where particle fluctuations ultimately cease to grow. While finite-size effects have been suggested to strongly affect numerical studies of MBL [46], we note that in contrast to Ref. [26] our data—which also challenge the established MBL phenomenology—are obtained at strong disorder. Second, it is possible that hopping processes introduced by the interaction term (6) are relevant and resonances do exist. A possible scenario would be that for $D > D_c$ the dynamic scaling $t \sim e^\ell$ does hold, leading to a logarithmic growth of the entanglement entropy but that the same dynamical scaling also holds for the spreading of particles resulting in an unbounded growth $S_N \sim \ln \ln t$. While this implies that the system is ultimately ergodic at very long timescales, it will not drastically alter the behavior on experimentally accessible timescales: MBL systems would still be good quantum memories and the Hamiltonian (2) an effective description.

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