Editors' Suggestion

Sub-ballistic Growth of Rényi Entropies due to Diffusion

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We investigate the dynamics of quantum entanglement after a global quench and uncover a qualitative difference between the behavior of the von Neumann entropy and higher Rényi entropies. We argue that the latter generically grow sub-ballistically, as $\propto \sqrt{t}$, in systems with diffusive transport. We provide strong evidence for this in both a U(1) symmetric random circuit model and in a paradigmatic nonintegrable spin chain, where energy is the sole conserved quantity. We interpret our results as a consequence of local quantum fluctuations in conserved densities, whose behavior is controlled by diffusion, and use the random circuit model to derive an effective description. We also discuss the late-time behavior of the second Rényi entropy and show that it exhibits hydrodynamic tails with three distinct power laws occurring for different classes of initial states.

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Introduction.—The far-from-equilibrium dynamics of closed quantum many-body systems has been at the center of much recent attention, both theoretically and experimentally [1–5]. In systems where the eigenstate thermalization hypothesis [3,6,7] holds, the density matrix of a finite subsystem ρ_A relaxes to a Gibbs state with an extensive entropy that stems from the entanglement with the rest of the system, making the dynamics of entanglement integral to the understanding of equilibration. This question has recently become amenable to experimental probes in systems of cold atoms, through the measurement of Rényi entropies, $S_\alpha \equiv [1/(1-\alpha)] \log \mathrm{tr}(\rho_A^\alpha)$. The theoretically most relevant of these is the von Neumann entropy, $S_{\alpha\to 1} \equiv -\mathrm{tr}(\rho_A \log \rho_A)$. Experimentally, however, for large subsystems only entropies with integer $\alpha \geq 2$ are currently accessible [5,8–11]. It is therefore important to understand how their behavior might differ from that of S_1.

In generic clean systems, the von Neumann entropy is expected to grow linearly in time for approximately homogeneous initial states ("global quenches"). This is understood for integrable systems from a quasiparticle description [12–15], but it also holds for thermalizing models [16], where it has recently been described using a "minimal cut" picture [17–19]. A generic linear growth of S_2 has also been proposed in Refs. [20,21], based on the ballistic spreading of operators—this is consistent with existing results both in integrable systems [22–24] and in models with no conservation laws [25–28]. Here we argue that this picture changes drastically in systems exhibiting diffusive transport of some conserved quantity (spin, charge, energy, etc.) [29–31]: we find that $S_{\alpha>1}$ grows diffusively, as $\sqrt{t}$. This arises because entropies with $\alpha > 1$ are sensitive to the presence of a few anomalously large eigenvalues of the reduced density matrix, while S_1 is dominated by the many exponentially small eigenvalues. The possibility of such qualitative differences was discussed for global cat states in Ref. [18]; here we propose that it arises much more generally, without the need to fine-tune the initial state.

Numerical results.—We consider a local random unitary circuit with a conserved U(1) charge as a minimal model of

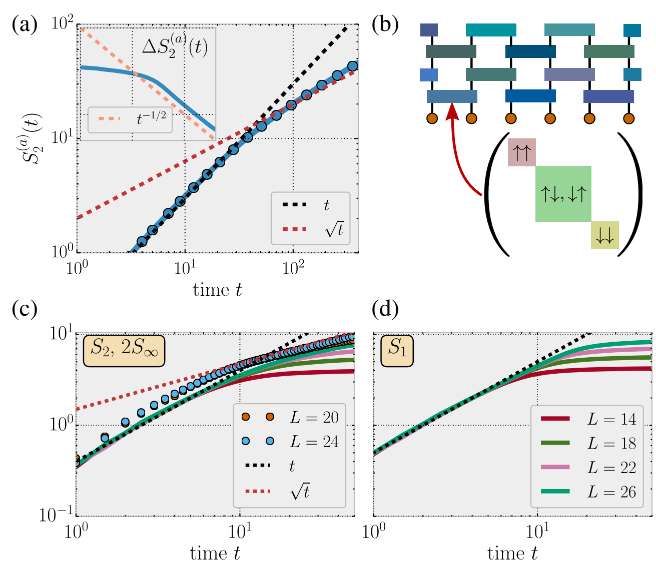

FIG. 1. (a) Growth of (annealed average) second Rényi entropy in a spin-1/2, U(1) symmetric random circuit, averaged over all product states. At long times the growth is diffusive ($\propto \sqrt{t}$). Inset: The discrete time derivative $\Delta S_2^{(a)}(t) \equiv S_2^{(a)}(t+1) - S_2^{(a)}(t)$ decays as $t^{-1/2}$. (b) Geometry of the random circuit and block structure of the gates. (c) Rényi entropies of the tilted field Ising model Eq. (1), S_2 (solid lines) and $2S_\infty$ (dots) show a similar crossover to sub-ballistic growth, while (d) the von Neumann entropy grows mostly linearly.

local quantum dynamics with diffusive transport [32,33]. We take a spin-$1/2$ chain and evolve it with two-site unitary gates that are block diagonal in the total z spin [Fig. 1(b)]. Each unitary consists of three independent Haar random blocks, corresponding to the states $\{\uparrow\uparrow\}$, $\{\uparrow\downarrow,\downarrow\uparrow\}$, $\{\downarrow\downarrow\}$. In every time step we apply such two-site gates first on all even, then on all odd bonds of the chain, and the different gates in the circuit are all independently chosen. Clearly, this circuit conserves the total Pauli z component, $\sum_x Z_x$.

We examine the circuit-averaged purity $\bar{\mathcal{P}}$, where the purity is $\mathcal{P} \equiv e^{-S_2} = \mathrm{tr}(\rho_A^2)$. This defines the annealed average Rényi entropy, $S_2^{(a)} \equiv -\log \bar{\mathcal{P}}$, which lower bounds the average, $\overline{S_2} \geq S_2^{(a)}$. $\bar{\mathcal{P}}$ is represented as a classical partition function, using the mapping derived in Ref. [33], which we evaluate using standard tensor network methods [34,35], making sure that the results are converged in both system size and bond dimension. Moreover, we average over all initial product states exactly. As shown in Fig. 1(a), we find that at long times the entanglement grows as $S_2^{(a)} \propto \sqrt{t}$. Note that the same quantity would grow linearly if we removed the conservation law [25,26]; thus we attribute its slow growth to diffusive transport.

Next, we consider the spin-$1/2$ Hamiltonian,

$$H = J\sum_{r=1}^{L-1} Z_r Z_{r+1} + \sum_{r=1}^{L}(h_z Z_r + h_x X_r) - J(Z_1 + Z_L), \quad (1)$$

known as the tilted field Ising model. The last term is included to decrease boundary effects. We choose $J = 1$, $h_x = (5+\sqrt{5})/8$, and $h_z = (1+\sqrt{5})/4$, as the same model was previously shown to have diffusive energy transport and linear von Neumann entropy growth [16]. Figures 1(c) and 1(d) show the growth of different entropies, averaged over $N = 50$ ($N = 20$) random product states for system sizes $L = 12$–24 ($L = 26$). Here we average the entropies, not their exponentials, unlike the random circuit case. We observe a mostly linear growth of S_1, as in Ref. [16]. S_2, however, has a crossover to sublinear growth at long times. Although the times we can reach are limited by finite system size, the long-time behavior is consistent with $S_2 \propto \sqrt{t}$. The results become clearer when considering the min-entropy, $S_{\alpha\to\infty}$, which provides an upper bound on $S_{\alpha>1} \leq [\alpha/(\alpha-1)]S_\infty$. We find that S_∞ is less sensitive to finite size effects, and exhibits a more pronounced crossover towards $\sqrt{t}$ growth [dots in Fig. 1(c)]. Similar results hold also for particular initial states, without averaging [36]. The behavior of the random circuit and Hamiltonian models leads us to conjecture that diffusive growth of $S_{\alpha>1}$ is a generic consequence of diffusive hydrodynamic transport. In the following, we provide further justification of this conjecture.

Heuristic argument.—We interpret our results in terms of the following nonrigorous argument. Let us focus on a Z-conserving discrete local time evolution, $U(t) = \prod_{\tau<t} U(\tau, \tau+1)$, on an infinite chain, and consider the bipartite entanglement at a cut between sites x and $x+1$. We write the time evolved state as a "sum over histories", $|\psi(t)\rangle = \sum_{\{\sigma(\tau)\}} A(\{\sigma(\tau)\})|\sigma\rangle$, where $A(\{\sigma(\tau)\})$ is the probability amplitude of a world history $\{\sigma(\tau)\}|_{0\leq\tau\leq t}$ in the Z basis. We split this sum into two parts: (i) histories for which the sites x, $x+1$ have both spins up at all times $\tau > t_{\mathrm{loc}}$ for some local equilibration time $t_{\mathrm{loc}} \sim \mathcal{O}(1)$ and (ii) all remaining paths. Let $|\phi_0(t)\rangle$ and $|\phi_1(t)\rangle$ denote the normalized states corresponding to (i) and (ii) respectively. Then $|\psi(t)\rangle = c_0|\phi_0(t)\rangle + c_1|\phi_1(t)\rangle$. By construction, $|\phi_0\rangle$ has an $\mathcal{O}(1)$ Schmidt rank for a bipartition across the bond x, $x+1$, accumulated before t_{loc}. Denoting this Schmidt rank by χ, one can then use the Eckart-Young theorem [37,38] to lower bound the largest Schmidt value of $|\psi\rangle$ as

$$\chi(\Lambda_{\max}^{\psi})^2 \geq |\langle\phi_0|\psi\rangle|^2 = |c_0 + c_1\langle\phi_0|\phi_1\rangle|^2. \quad (2)$$

We will now argue that if transport is diffusive, the rhs is expected to decay slower than exponentially with time.

We first need to estimate the probability that the sites x, $x+1$ remain in the state $\uparrow\uparrow$ at all times $t > t_{\mathrm{loc}}$. The simplest approximation is to treat every $\downarrow$ in the system as an independently diffusing particle. In this case, the probability that all particles that are to the left of x at t_{loc} remain on the same side is a product of the probabilities for particles starting at different positions. The relevant contribution comes from particles that are initially within some region of size $\mathcal{O}(\sqrt{Dt})$ near the entanglement cut, where D is the diffusion constant. Therefore, we expect the probability to decay at long times as $|c_0|^2 \propto e^{-\gamma\sqrt{Dt}}$ for some constant γ [39].

To bound the overlap $\langle\phi_0|\phi_1\rangle$, we can apply the Eckart-Young theorem again, this time for $|\phi_1\rangle$, which gives $|\langle\phi_0|\phi_1\rangle|^2 \leq \chi(\Lambda_{\max}^{\phi_1})^2$. Consequently, if $|\phi_1\rangle$, which corresponds to typical histories, has Rényi entropies $S_{\alpha>1}$ that grow faster than $\sqrt{t}$, then the second term on the rhs of Eq. (2) will be negligible at long times compared to c_0, resulting in $\chi(\Lambda_{\max}^{\psi})^2 \gtrsim e^{-\gamma\sqrt{Dt}}$. If $\Lambda_{\max}^{\phi_1} \sim e^{-\sqrt{t}}$, then there is, in principle, a possibility of cancellation between the two terms, such that the rhs of Eq. (2) decays faster then $\sim e^{-\sqrt{t}}$; however, this would be highly fine-tuned and we see no sign of such cancellation when computing the rhs in the random circuit model.

This argument implies that at long times there should be a growing distance between the largest Schmidt value, $\Lambda_{\max} \equiv e^{-S_\infty/2} \sim e^{-\gamma\sqrt{Dt}}$, and typical ones which we still expect to be exponentially small, $\sim e^{-vt}$, in accordance with the linear growth of S_1 [16]. As mentioned previously, the former upper bounds Rényi entropies, $S_{\alpha>1} \leq [\alpha/(\alpha-1)]S_\infty$. This shows that at long times, $t \gg v^2/D$, all $\alpha > 1$ entropies are controlled by the largest Schmidt value, making their growth diffusive, provided that all degrees of freedom couple to some conserved quantity. The time for this sub-ballistic growth to set in depends also on the Rényi index, diverging in the limit $\alpha \to 1$. The von Neumann entropy itself is unconstrained by S_∞, dominated instead by the many exponentially small Schmidt values, leading to its linear growth.

While the above argument is presented in the language of spin conservation, we expect it to generalize to energy conserving systems in the form of rare events where the time evolved state locally resembles the ground state [40]. This is in agreement with our numerical results in Fig. 1(c).

Effective model.—To get a further analytical handle on this problem, we return to our random circuit model and modify it along the lines of Ref. [32], adding an extra, nonconserved q-state system to each site. This makes the size of each Haar random unitary larger by a factor of q^2, allowing us to derive an effective model that governs the evolution of $S_2^{(a)}$ in the large q limit. As we shall see, the result decomposes into the sum of two contributions: a $\propto t$ part from the nonconserved degrees of freedom, and a $\propto \sqrt{t}$ part associated to the conserved spins.

To begin, note that the purity can be written as the expectation value of an operator on two identical copies of the original system [8,26,41,42]. Imagine two copies of a single site, with Hilbert space $\mathcal{H} \otimes \mathcal{H}$, and define the one-site SWAP operator $\mathcal{F}$, such that $\mathcal{F}(|i\rangle \otimes |j\rangle) \equiv |j\rangle \otimes |i\rangle$, where $\{|i\rangle\}$ is a basis in $\mathcal{H}$. Then the half-chain purity is $\mathcal{P}(x) = \mathrm{tr}(\mathcal{F}(x)[\rho \otimes \rho]) \equiv \langle \mathcal{F}(x) \rangle$, where $\mathcal{F}(x) \equiv \prod_{\leq x} \mathcal{F}$ is a string of SWAP operators, acting on one half of the entanglement cut [Figs. 2(a) and 2(b)]. Instead of evolving the state, we can therefore evolve the operator $\mathcal{F}(x)$ in time. Averaging over a random gate on sites x, $x+1$, to leading order in $1/q$ it evolves as [36]

$$\mathcal{F}(x) \to (2q)^{-1} \sum_{y=x\pm 1} \mathcal{F}(y) + \tilde{\mathcal{F}}_x(y), \qquad (3)$$

where we have introduced new "two-copy" operators,

$$\tilde{\mathcal{F}}_x(y) \equiv (Z_{x,x+1} \otimes Z_{x,x+1}) \mathcal{F}(y), \qquad (4)$$

with $Z_{x,x+1} \equiv (Z_x + Z_{x+1})/2$, and the tensor product referring to the two copies of the system. These are similar to $\mathcal{F}(x)$, but multiplied by the Z operators that measure the conserved spin on sites near the entanglement cut.

To see how the entanglement evolves, one also needs equations of motion for $\tilde{\mathcal{F}}_x(y)$. This can be done analogously, by averaging over two-site gates, resulting in the following effective model. The operators in Eq. (4), and their subsequent circuit-averaged evolution, may be expressed as a sum of dressed SWAP operators of the form $\prod_y (Z_y^{n_y^{(r)}} \otimes Z_y^{n_y^{(b)}}) \mathcal{F}(x')$, where $\{n_y^{(r,b)} = 0, 1\}$. We refer to $\{n_y^{(r,b)}\}$ as configurations of "red" and "blue" particles, while x' (the end point of the SWAP string) is called the "cut position". Apart from an overall suppression factor of $2/q$ in each step, the circuit-averaged dynamics gives a Markov process on configurations defined by these variables. This effective Markov dynamics has the following properties: away from the cut, the particles independently obey diffusion with hard-core interactions, conserving the number of each species. The cut itself also diffuses, moving one site either to the left or the right, while emitting and absorbing an even number of particles at each step [Fig. 2(d)]. One can show that the probability of emission versus absorption decreases with the number of particles on the two sites directly at the cut, changing sign at half filling [36].

The SWAP string and both types of particles evolve as unbiased random walks; therefore, by time t we expect them to occupy a region of width $l(t) \propto \sqrt{t}$. Monte Carlo simulations of the stochastic dynamics show [Fig. 2(e)] that the particle densities are Gaussian around x. We therefore take a mean field approximation and write the probability of a string ending at x and a distribution of particles $\{n_y^{(r,b)} = 0, 1\}$ as

$$p(x, n^{(r)}, n^{(b)}) \propto e^{-x^2/2l(t)^2} e^{-[1/2l(t)^2] \sum_y (n_y^{(r)} + n_y^{(b)}) y^2}, \qquad (5)$$

if $\sum_y (n_y^{(r)} + n_y^{(b)})$ is even, and zero otherwise. With this ansatz, one can evaluate the half-chain purity at time t. For translation invariant product states, the result reads

$$\mathcal{P}(t) \propto \left(\frac{2}{q}\right)^t \prod_y \left(1 - \frac{1 - |\langle Z_y \rangle|}{1 + e^{y^2/2l(t)^2}}\right)^2. \qquad (6)$$

This product has relevant contributions only from a window of $|y| \lesssim \sqrt{t}$; hence, it decays as $e^{-\gamma\sqrt{t}}$. Note that γ is larger when $|\langle Z_y \rangle|$ is smaller. By expanding each term in

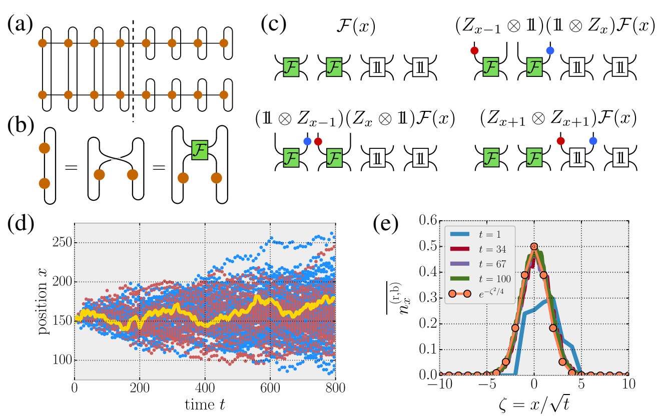

FIG. 2. Effective model at $q \to \infty$. (a) The purity $\mathcal{P}$, written in terms of the state ρ as a matrix product operator. (b) This can be rewritten by introducing the SWAP operator $\mathcal{F}$. (c) Half-chain "SWAP string" $\mathcal{F}(x)$, along with a few of the terms on the rhs of Eq. (3), with red and blue particles representing local Z_x operators. (d) These particles obey a random walk with hard-core interactions, spreading out diffusively, which (e) leads to a Gaussian density profile.

$e^{-y^2/2l(t)^2}$, we can approximate the product as $\approx e^{-\sqrt{2\pi}(1-|\langle Z\rangle|)l(t)}$, which is in good agreement with Monte Carlo results, at least away from $\langle Z\rangle \approx 0$. Note that Eq. (6) looks very similar to the probability of rare events from our heuristic argument in the simplest approximation of independently diffusing particles.

Using Eq. (6), at large q we get $S_2^{(a)} = \log(q/2)t + a\sqrt{t}$, with $a \sim \mathcal{O}(1)$. Here, $\log(q/2)$ is exactly the large q limit of $v_E(q) = \log[(q+1/q)/2]$, the entanglement velocity of a nonsymmetric random circuit with q states per site [25,26]. Moreover, the linear in t term is independent of the initial state. This suggests the following interpretation: there is an entanglement $v_E(q)t$ coming entirely from nonconserved degrees of freedom, while the conserved spins are responsible for the $\propto \sqrt{t}$ term. This is supported by numerical results [36], which show that $S_2^{(a)}(t) - v_E(q)t$ has only weak q dependence and grows as $\sqrt{t}$ for any q, including the original model with $q = 1$, where $S_2^{(a)}$ is purely diffusive [Fig. 1(a)]. This is true despite the ballistic spread of local operators [32,33], showing that recent arguments [20,21,25] for exponential decay of $\mathcal{P}$ fail in the present context, and subtle correlations between the spreading of different operators cannot be neglected. Our results also suggest that the minimal cut picture of entanglement growth [18] does not accurately capture the behavior of $S_{\alpha>1}$ [43].

Long-time tails.—Diffusive modes also have a strong influence on the long-time behavior of finite subsystems, which we turn to next. The entanglement eventually saturates to an equilibrium value predicted by the appropriate Gibbs ensemble, provided the eigenstate thermalization hypothesis holds and the initial state clusters [1,3,6,7]. We now show that the approach of S_2 to this thermodynamic value is also affected by diffusion and shows long-time hydrodynamic tails. Interestingly, we find that the nature of these tails depends strongly on the initial conditions, leading to the appearance of three different power laws, $t^{-1/2}$, t^{-1}, and $t^{-3/2}$. In particular, we uncover a difference between states at zero and finite chemical potential.

We take a spin-1/2 chain and rewrite the reduced density matrix of a small subsystem of l sites by inserting a complete basis of operators σ^μ, given by products of local Pauli operators acting on the subsystem [20]. This yields $S_2 = l\log 2 - \log(1 + \sum_\mu \langle\sigma^{\mu 2}\rangle)$, where the identity is excluded from the sum. Let $\langle\delta\sigma^\mu\rangle \equiv \langle\sigma^\mu\rangle - \langle\sigma^\mu\rangle_{\text{eq}}$ denote the deviation from equilibrium. Then at long times

$$|S_2 - S_{2,\text{eq}}| \propto \sum_\mu (2\langle\sigma^\mu\rangle_{\text{eq}}\langle\delta\sigma^\mu\rangle + \langle\delta\sigma^\mu\rangle^2). \qquad (7)$$

Thus the long-time tails that describe how expectation values equilibrate appear directly in the Rényi entropy.

One immediate consequence of Eq. (7) is that the hydrodynamic tails can differ between states at half filling and away from half filling. At precisely half filling, the leading order term is $\langle\delta\sigma^\mu\rangle^2$, while away from half filling $\langle\sigma^\mu\rangle_{\text{eq}}\langle\delta\sigma^\mu\rangle$ is expected to dominate. Generically, hydrodynamic observables in d dimension should decay as $t^{-d/2}$ [29–31,44], with subleading corrections $\mathcal{O}(t^{-3d/4})$. Therefore, we generically expect a saturation as $\propto t^{-d}$ for states at half filling (infinite temperature) and $\propto t^{-d/2}$ otherwise. However, this expectation can change for certain initial states, where all hydrodynamic variables have $\langle\delta\sigma^\mu\rangle = 0$ initially. In this case one expects the leading diffusive tail to vanish and subleading corrections to take over. In particular, in the 1D random circuit model one can argue [36] that the leading contribution for translation invariant product states should be of order $t^{-3/2}$.

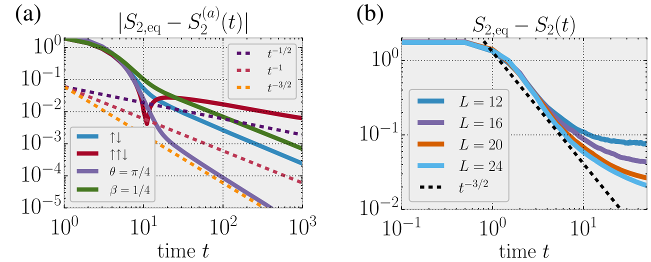

FIG. 3. (a) Saturation of $S_2^{(a)}$ for a four-site subsystem in the spin-1/2 random circuit for different initial states. States away or at half filling generically saturate as $t^{-1/2}$, t^{-1}, respectively. States with hydrodynamic variables in equilibrium at all times saturate with subleading exponent $t^{-3/2}$. (b) The same $t^{-3/2}$ saturation is present for random product states in the tilted field Ising model Eq. (1) (three-site subsystem, averaged over 50 initial states).

We observe these three distinct power laws in $S_2^{(a)}$ for the spin-1/2 random circuit, as shown in Fig. 3(a). We find that Néel-like states ($|\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\ldots\rangle$) with less then half filling exhibit an overshooting effect, approaching their equilibrium value from above, as $t^{-1/2}$. Finitely correlated states at half filling $[(|\beta\rangle \propto e^{\beta\sum_{r=0}^{L-1} Z_r Z_{r+1}}(|\uparrow\rangle + |\downarrow\rangle)^{\otimes L}]$ saturate as t^{-1}, and tilted ferromagnetic states ($|\theta\rangle \equiv e^{i\theta\sum_{r=1}^{L} Y_r}|\uparrow\rangle$) as $t^{-3/2}$. We also provide evidence of the $t^{-3/2}$ tail for random product states in the tilted field Ising Hamiltonian Eq. (1), shown in Fig. 3(b).

Discussion.—Our results reveal a previously overlooked qualitative difference between the von Neumann and $\alpha > 1$ Rényi entropies. We gave a heuristic argument, indicating that the latter are strongly influenced by local quantum fluctuations which can lead to diffusive growth for the entropy in systems with diffusive transport. We presented evidence for this in two cases: a random circuit model and a thermalizing Hamiltonian. Our results indicate that diffusion leads to a separation of scales, where the half-chain density matrix contains a few largest eigenvalues that decay slowly and become well separated from the bulk of the spectrum made up by exponentially small eigenvalues: S_2 is dominated by the former, while S_1 by the latter, such that they provide insight into different aspects of thermalization. In particular, S_1 and $S_{\alpha>1}$ reveal distinct timescales of thermalization, scaling, respectively, as $\propto l$ and $\propto l^2$ with subsystem size l.

We expect our results to generalize to higher dimensions. In that case, the SWAP string becomes a "membrane" [17–19]. One can generate a 2D time evolution using a random circuit of two-site gates [26], in which case our Eq. (3) remains valid, with the membrane emitting Z_x operators that diffuse on the 2D lattice. A generalization of our heuristic argument would also suggest a similarly sub-ballistic growth for the Rényi entropy. It would be interesting to see if effects like this could show up in holographic calculations, by extending the results of Refs. [19,45] to Rényi entropies, or by refining the upper bound derived for Sachdev-Ye-Kitaev chains in Ref. [46].

It is an open question whether diffusion also affects the early-time growth of S_1, e.g., the form of subleading corrections. While slow relaxation of S_1 due to diffusion has been observed numerically [47], whether the rich variety of initial state-dependent power laws appear there also warrants further study. Another avenue for future investigation is in the field of disordered systems, where even the von Neumann entropy is expected to grow sub-ballistically, while transport becomes subdiffusive [48–50], eventually leading to many-body localization at strong disorder. Comparison of von Neumann and Rényi entropies could give further insight into the dynamics in these different regimes.

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Note added.—Recently, a follow-up work [38] appeared, which provided a proof of sub-ballistic growth of $S_{\alpha>1}$ for charge-conserving unitary circuits, under slightly different assumptions, and for a specific set of initial states. This work made us aware of the Eckart-Young theorem, which allowed us to tighten our heuristic argument, replacing one of its underlying assumptions with a milder condition.

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