

Renyi entropy of chaotic eigenstates

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Using arguments built on ergodicity, we derive an analytical expression for the Renyi entanglement entropies which, we conjecture, applies to the finite-energy density eigenstates of chaotic many-body Hamiltonians. The expression is a universal function of the density of states and is valid even when the subsystem is a finite fraction of the total system—a regime in which the reduced density matrix is not thermal. We find that in the thermodynamic limit, only the von Neumann entropy density is independent of the subsystem to the total system ratio V_A/V , while the Renyi entropy densities depend nonlinearly on V_A/V . Surprisingly, Renyi entropies S_n for $n > 1$ are convex functions of the subsystem size, with a volume law coefficient that depends on V_A/V , and exceeds that of a thermal mixed state at the same energy density. We provide two different arguments to support our results: the first one relies on a many-body version of Berry's formula for chaotic quantum-mechanical systems, and is closely related to the eigenstate thermalization hypothesis. The second argument relies on the assumption that for a fixed energy in a subsystem, all states in its complement allowed by the energy conservation are equally likely. We perform an exact diagonalization study on quantum spin-chain Hamiltonians to test our analytical predictions.

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I. INTRODUCTION

The observation that the quantum evolution of a closed quantum system can lead to thermalization of local observables puts the foundations of equilibrium statistical mechanics on a firmer footing [1–7]. In strong contrast to classical mechanics, where one often refers to an ensemble of identically prepared systems, quantum mechanics allows for the possibility that a single quantum state can encode the full equilibrium probability distribution function, and in fact, the full quantum Hamiltonian [8]. Specifically, consider a system of size V described by Hamiltonian H . The eigenstate thermalization hypothesis (ETH) [2–4] posits that the reduced density matrix for a finite energy density eigenstate $|E_n\rangle$ on subsystem A with $V_A \ll V$ is thermal: $\text{tr}_A |E_n\rangle\langle E_n| = \text{tr}_A (e^{-\beta H}) / \text{tr} (e^{-\beta H}) \stackrel{\text{def}}{=} \rho_{\text{th}}^A(\beta)$ where β^{-1} is the temperature corresponding to the eigenstate $|E_n\rangle$ and equals $dS/dE|_{E_n}$ where $S(E)$ is the microcanonical entropy (= logarithm of the density of states). In this work, we will employ the term “chaotic eigenstate” for the eigenstate $|E_n\rangle$ which obeys the ETH.

One basic question is whether there exist observables O whose support V_O scales with the total system size V while their expectation value $\langle E_n | O | E_n \rangle$ continues to satisfy some version of eigenstate thermalization. Standard analyses in statistical mechanics [9] do not provide an answer to such global aspects of thermalization. As pointed out in Ref. [8], at any fixed, nonzero V_A/V , one can always find operators with operator norm of order unity, for whom the difference $|\langle E_n | O | E_n \rangle - \text{tr}(\rho_{\text{th}}^A(\beta) O)|$ does not vanish and is of order unity. This implies that the trace norm distance $\frac{1}{2} |\text{tr}_A |E_n\rangle\langle E_n| - \rho_{\text{th}}^A(\beta)|_1$ does not vanish and is of order unity when V_A/V is held fixed while taking thermodynamic limit. Clearly, the expectation value of operators which are constrained by global conservation laws cannot behave thermally.

As an example, consider the operator $(H_A^2 - \langle H_A^2 \rangle) / V_A$, where H_A is the Hamiltonian restricted to region A . Its expectation value in an eigenstate tends towards zero when V_A approaches V , while it is nonzero and proportional to the specific heat in a thermal state. This raises the question of whether conserved quantities exhaust the set of operators that distinguish a pure state from a corresponding thermal state at the same energy.

One set of quantities that are particularly relevant to probe the global aspects of chaotic eigenstates are Renyi entropies: $S_n^A = \frac{1}{1-n} \ln(\text{tr} \rho_A^n)$. In fact $\text{tr}(\rho^2)$ is one of the simplest measures of how close to a pure state a potentially mixed quantum state is. For integer values of n , S_n^A has the interpretation of the expectation value of a cyclic permutation operator acting on the n copies of the system. Due to this, S_n^A can in principle be measured in experiments, and remarkably, an implementation for $n = 2$ was recently demonstrated in cold atomic systems [10].

The ground states of quantum many-body systems typically follow an area law for Renyi entropies (up to multiplicative logarithmic corrections): $S_n^A \sim L_A^{d-1}$ where d is the spatial dimension [11,12]. In strong contrast, finite energy density eigenstates of chaotic systems, owing to eigenstate thermalization, follow a volume law scaling: $S_n^A \sim L_A^d$ (see, e.g., [13]). Since we will often employ the term “volume law coefficient,” it is important to define it precisely. We define the volume law coefficient of an eigenstate as $\lim_{V \rightarrow \infty} S_n^A / V_A$ while keeping the ratio V_A/V fixed and less than 1/2. Note that in principle this coefficient can depend on the ratio V_A/V itself. For a thermal density matrix, $\rho = e^{-\beta H} / \text{tr} e^{-\beta H}$, the volume law coefficient is given by $n\beta(\mathfrak{f}(n\beta) - \mathfrak{f}(\beta)) / (n-1)$ where $\mathfrak{f}(\beta)$ is the free energy density at temperature β^{-1} . Therefore, in this example, the volume law coefficient is independent of V_A/V . Owing to eigenstate thermalization, the volume law coefficient of the Renyi entropy corresponding

to chaotic eigenstates is also given by exactly the same expression, at least in the limit $V_A/V \rightarrow 0$. One of the basic questions that we will address in this paper is what is the volume law coefficient corresponding to chaotic eigenstates when $V_A/V = O(1)$?

Reference [8] provided numerical evidence that the volume law coefficient for the von Neumann entropy S_1^A corresponding to chaotic eigenstates equals its thermal counterpart even when the ratio V_A/V ($< 1/2$) is of order unity. Furthermore, under the assumption that for a fixed set of quantum numbers in subsystem A , all allowed states in its complement \bar{A} are equally likely, Ref. [8] provided an analytical expression for the n th Renyi entropy S_n for infinite temperature eigenstates of a system with particle number conservation. This expression curiously leads to the result that when $n \neq 1$, the Renyi entropies S_n^A do not equal their thermal counterpart for any fixed nonzero V_A/V in the thermodynamic limit.

In a related development, Ref. [14] also studied reduced density matrix corresponding to chaotic eigenstates of a system with only energy conservation. They found that the eigenvalues are proportional to the number of eigenstates of the rest of the system consistent with energy conservation. This result is very similar to the aforementioned result in Ref. [8] for the infinite temperature eigenstates with particle number conservation—in that case the eigenvalues of the reduced density matrix were proportional to the number of eigenstates of the rest of the subsystem consistent with particle number conservation. Given this correspondence, one might expect that for chaotic systems with only energy conservation, only the von Neumann entropies equal their thermal counterpart, similar to the aforementioned example in Ref. [8]. This was already mentioned in Ref. [14] although Renyi entropies were not calculated.

In another development, Ref. [15] studied “canonical thermal pure quantum” (CTPQ) states which were introduced in Ref. [16]. These states reproduce several features of a thermal ensemble while being a pure state [16]. However, in contrast to the aforementioned result for infinite temperature eigenstates in Ref. [8], the volume law coefficient of the Renyi entropies for CTPQ states is independent of V_A/V and equals the thermal Renyi entropy density. Reference [15] compared the Renyi entropy of eigenstates of nonintegrable Hamiltonians with a fitting function based on CTPQ states.

In this paper, using a combination of arguments based on ergodicity and eigenstate thermalization, we derive an analytical expression for Renyi entropy of chaotic eigenstates. We follow two different arguments to arrive at the same result. First, we consider a translationally invariant “classical” Hamiltonian H_0 (which we define as a Hamiltonian all of whose eigenstates are product states) perturbed by an integrability breaking perturbation H_1 so that energy is the only conserved quantity for the full Hamiltonian $H = H_0 + \varepsilon H_1$. Physical arguments and numerical results strongly suggest that if one first takes the thermodynamic limit, and only then takes $\varepsilon \rightarrow 0$, the eigenstates of H are fully chaotic [17–24]. Following arguments inspired by Ref. [3], where eigenstates of a many-body chaotic system consisting of hard-sphere balls were studied, we argue that for ETH to hold for the eigenstates of H , they may be approximated by random superposition of the eigenstates of H_0 in an energy window of order $\varepsilon \ll$

V . This can be thought of as a many-body version of the Berry’s conjecture for a chaotic billiard ball system where the eigenstates are given by random superposition of plane waves [3,25]. We will use the moniker “Berry states” for these states. Related ideas have already been discussed in the context of one-dimensional integrable systems perturbed by a small integrability breaking term [20–22,26].

In the second approach, we consider states of the form $|\psi\rangle = \sum_{E_i^A + E_j^{\bar{A}} \in (E - (1/2)\Delta, E + (1/2)\Delta)} C_{ij} |E_i^A\rangle \otimes |E_j^{\bar{A}}\rangle$, with C_{ij} a random complex number, $|E_i^A\rangle$ an eigenstate of H_A , and $|E_j^{\bar{A}}\rangle$ that of $H_{\bar{A}}$. These states are exactly of the form suggested by “canonical typicality” arguments [27,28] and in the thermodynamic limit, reproduce the results of Ref. [14] for the matrix elements of the reduced density matrix. Given the results in Ref. [14], it is very natural to conjecture that eigenstates of local Hamiltonians mimic states drawn from such an ensemble. We will call this the “ergodic bipartition” conjecture. The advantage of working with wave functions, in contrast to the average matrix elements of the reduced density matrix, is that it allows us to calculate the average of the Renyi entropy itself, which is a much more physical quantity compared to the Renyi entropy of the averaged reduced density matrix. This distinction is particularly crucial in finite sized systems. We will compare our analytical predictions with the exact diagonalization, as well as directly with the CTPQ states.

Our main results are as follows:

(i) Renyi entropies are a universal function of the density of states of the system.

(ii) Renyi entropy density S_n^A/V_A depends on V_A/V when $n \neq 1$ as the thermodynamic limit is taken. For $n > 1$ ($n < 1$), S_n^A is always a convex (concave) function of V_A/V . $n = 1$ corresponds to a transition point between concavity and convexity, and correspondingly the von Neumann entropy is linear in V_A (see Fig. 1). Consequently, in the thermodynamic limit for any nonzero V_A/V , the volume law coefficient of the Renyi entropy S_n^A differs from the one derived from the thermal density matrix $\rho_{th}^A(\beta)$ or equivalently the canonical thermal pure quantum (CTPQ) states. For $n > 1$, it exceeds that of a thermal and CTPQ state, and for $n < 1$, it is less than that of a thermal and CTPQ state.

(iii) The Renyi entropy for a given V_A/V depends on the density of states at an energy density that is itself a function of V_A/V . This allows one to obtain information about the full spectrum of the Hamiltonian by keeping the Renyi index n fixed and only varying the ratio V_A/V . This is in strong contrast to the limit $V_A/V \rightarrow 0$ where S_n^A only encodes thermodynamical information at temperature β^{-1} and $(n\beta)^{-1}$.

The paper is organized as follows: In Sec. II we state the aforementioned Berry conjecture and the ergodic bipartition conjecture and demonstrate their relation to eigenstate thermalization. Section III contains our main results—here we provide analytical results on the Renyi entropies for the states introduced in Sec. II, and also compare them to aforementioned CTPQ states. In particular, we discuss the curvature dependence of the Renyi entropies, as well as provide simple examples where one can obtain closed form expressions. In Sec. IV, we numerically study Renyi entropies corresponding to spin-chain Hamiltonians and compare with our analytical

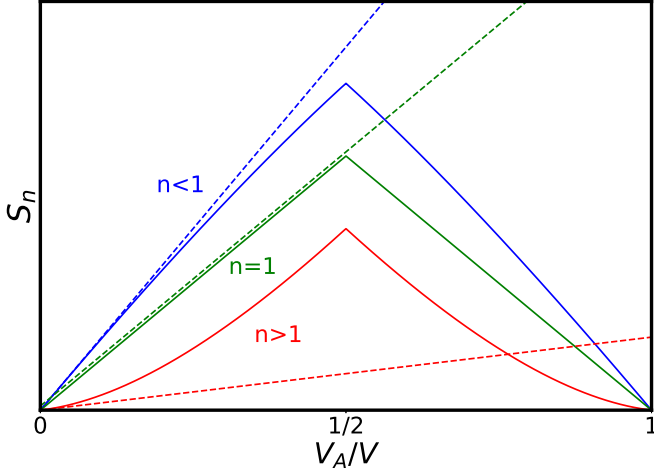


FIG. 1. The curvature dependence of the Renyi entropy S_n derived in the main text (solid lines) using arguments built on ergodicity: in the thermodynamic limit, S_n is a convex (concave) function of V_A/V for $n > 1$ ($n < 1$) with a cusp singularity at $V_A/V = 1/2$. The dashed lines correspond to the Renyi entropies of the thermal density matrix $\rho_{th}^A(\beta) = \exp(-\beta H_A)/Z$. S_n derived built on ergodicity equals the thermal counterpart for $V_A/V < 1/2$ at $n = 1$, while for $n \neq 1$ it equals the thermal counterpart only as $V_A/V \rightarrow 0$. For each line style, the lines shown in descending order from the top correspond to $n < 1$, $n = 1$, and $n > 1$ respectively.

predictions. In Sec. V, we discuss the implications of our results, and future directions.

II. NATURE OF CHAOTIC EIGENSTATES

Consider a many-body Hamiltonian H which we write as

$$H = H_A + H_{\bar{A}} + H_{A\bar{A}}, \quad (1)$$

where H_A , $H_{\bar{A}}$ denote the part of H with support only in real-space regions A and \bar{A} respectively, and $H_{A\bar{A}}$ denotes the interaction between A and \bar{A} . ‘‘Canonical typicality’’ arguments [27,28] imply that a typical state in the Hilbert space with energy E with respect to H has a reduced density matrix ρ_A on region A with matrix elements:

$$\langle E_i^A | \rho_A | E_i^A \rangle = \frac{1}{N} e^{S_{\bar{A}}(E - E_i^A)}, \quad (2)$$

where $|E_i^A\rangle$ is an eigenstate of H_A with energy E_i^A , $e^{S_{\bar{A}}(E - E_i^A)}$ is the number of eigenstates of $H_{\bar{A}}$ with energy $E_{\bar{A}}$ such that $E_A + E_{\bar{A}} \in (E - \frac{1}{2}\Delta, E + \frac{1}{2}\Delta)$ with $\Delta \ll E$, and N is the total number of states in the energy window:

$$N = \sum_i e^{S_{\bar{A}}(E - E_i^A)} = \sum_{E_A} e^{S_A(E_A) + S_{\bar{A}}(E - E_A)}. \quad (3)$$

One can obtain this result from two conceptually different viewpoints. On the one hand, one can consider the following mixed state Ω that defines a microcanonical ensemble at energy E :

$$\Omega = \frac{1}{N} \sum_{E_i^A + E_j^{\bar{A}} \in (E - (1/2)\Delta, E + (1/2)\Delta)} |E_i^A\rangle \otimes |E_j^{\bar{A}}\rangle \langle E_i^A| \otimes \langle E_j^{\bar{A}}|, \quad (4)$$

and then trace out the Hilbert space in region \bar{A} , thus obtaining Eq. (2). Alternatively, one can consider the following *pure state* introduced in Refs. [27,28]:

$$|E\rangle = \sum_{E_i^A + E_j^{\bar{A}} \in (E - (1/2)\Delta, E + (1/2)\Delta)} C_{ij} |E_i^A\rangle \otimes |E_j^{\bar{A}}\rangle, \quad (5)$$

where C_{ij} is a complex random variable. After averaging, one again obtains Eq. (2) when $V_A/V < 1/2$. The state in Eq. (5) is the random superposition of tensor product of eigenstates of H_A and $H_{\bar{A}}$ with the constraint of energy conservation, and we call it an ‘‘ergodic bipartition’’ (EB) state.

Recently, evidence was provided in Ref. [14] that the reduced density matrix corresponding to an *eigenstate* of translationally invariant nonintegrable Hamiltonians resembles the reduced density matrix of a pure state based on canonical typicality, and therefore also satisfy Eq. (2). Therefore it is worthwhile to explore whether the state in Eq. (5), which leads to Eq. (2), is a good representative of the eigenstate of a chaotic Hamiltonian.

To explore this question, we first note that the state in Eq. (5) recovers the correct energy fluctuation in an eigenstate [8], namely, $\Delta E_A^2 = cT^2 \frac{V_A V_{\bar{A}}}{V_A + V_{\bar{A}}}$ (see Appendix A) where c is the specific heat. Further, one readily verifies that the diagonal entropy for a subsystem A corresponding to this state equals the thermodynamic entropy $V_A s(E/V)$ where $s(x)$ denotes the entropy density at energy density x , as also expected from general, thermodynamical considerations [29].

Next, let’s first see whether the ergodic bipartition states in Eq. (5) satisfy ETH assuming that the eigenstates of H_A and $H_{\bar{A}}$ are chaotic. Clearly if an operator is localized only in A or \bar{A} , then its expectation value with respect to $|E\rangle$ trivially satisfies ETH by the very assumption that H_A and $H_{\bar{A}}$ are chaotic. Therefore, consider instead an operator $O = O_A O_{\bar{A}}$ where $O_A \in A$ and $O_{\bar{A}} \in \bar{A}$. Recall that the ETH implies that $\langle E_n | O | E_m \rangle = \overline{O(E/V)} \delta_{n,m} + \sqrt{\overline{O^2(E/V)}} e^{-S(\bar{E})/2} z_{n,m}$ where $\overline{O(E/V)}$ is the microcanonical expectation value of O at energy density E/V and therefore is a smooth function of E , $S(\bar{E})$ is the microcanonical entropy at energy $\bar{E} = (E_n + E_m)/2$, and $z_{n,m}$ is a complex random number with zero mean and unit variance.

The diagonal matrix element of O with respect to the state $|E\rangle$ in Eq. (5) is given by

$$\begin{aligned} \langle E | O | E \rangle &= \sum_{ij} |C_{ij}|^2 \langle E_i^A | O_A | E_i^A \rangle \langle E_j^{\bar{A}} | O_{\bar{A}} | E_j^{\bar{A}} \rangle \delta(E_i^A + E_j^{\bar{A}} - E) \\ &= \sum_{E_A} \frac{e^{V_A s(E_A/V_A) + V_{\bar{A}} s((E - E_A)/V_{\bar{A}})}}{e^{V s(E/V)}} \overline{O_A(E_A/V_A)} \overline{O_{\bar{A}}((E - E_A)/V_{\bar{A}})} \\ &= \overline{O_A(E/V)} \overline{O_{\bar{A}}(E/V)}, \end{aligned} \quad (6)$$

where the last equation in the sequence is derived by taking the saddle point from the one above. Clearly if O_A and $O_{\bar{A}}$ are located close to the boundary between A and \bar{A} (in units of thermal correlation length), then there is no reason to expect that $\overline{O_A(E/V)} \overline{O_{\bar{A}}(E/V)}$ is the correct answer for the expectation of O with respect to an actual eigenstate of the system. However, if O_A and $O_{\bar{A}}$ are located far from the boundary, then

the cluster decomposition of correlation functions implies that the above answer is indeed correct to a good approximation. Note that it is a smooth function of the energy, as required by ETH. A similar calculation shows that the off-diagonal matrix element $\langle E_n | O | E_m \rangle$ is proportional to $e^{-S(\bar{E})/2} z$ where $\bar{E} = (E_n + E_m)/2$ and z is a random complex number with zero mean and unit variance.

The above considerations indicate that the state $|E\rangle$ is a good representative of an eigenstate of H , *except* for the correlation functions of operators close to the boundary. Therefore, we expect that it correctly captures the bulk quantities, such as the volume law coefficient of Renyi entropies. As already noted, it correctly reproduces the energy fluctuations, as well as the diagonal entropy for an eigenstate. Conversely, we do not expect it to necessarily reproduce the subleading area-law corrections to the Renyi entropies, which may be sensitive to the precise way the eigenstates of H_A and $H_{\bar{A}}$ are “glued.”

In passing we note that Ref. [13] considered a perturbative treatment of the Hamiltonian $H = H_A + H_{\bar{A}} + \varepsilon H_{A\bar{A}}$ to the first order in ε . The wave functions thus argued to be obtained have some resemblance with the EB state [Eq. (5)]. However, to really obtain an EB state via this procedure, one would instead need to carry out the perturbation theory to an order that scales with the system size! This is because when V_A/V is nonzero, the EB state has extensive fluctuations of energy in subregion A , unlike the states considered in Ref. [13] which essentially have no fluctuations since they mix eigenstates of H_A in a small energy window.

A different starting point to obtain states that mimic chaotic eigenstates is provided by considering Hamiltonians H of the form

$$H = H_0 + \varepsilon H_1. \tag{7}$$

Here H_0 denotes a translationally invariant many-body local Hamiltonian whose eigenstates can be chosen as unentangled product states $\{|s_\alpha\rangle = |s_1^\alpha\rangle \otimes |s_2^\alpha\rangle \otimes \dots \otimes |s_L^\alpha\rangle\}$, and therefore corresponds to an integrable system with an infinite number of conserved quantities. The H_1 term breaks the integrability. Physical arguments as well as numerics strongly suggest that when H_1 is local, the system will show a crossover behavior from an integrable regime to a chaotic regime for $\varepsilon \sim 1/L^\beta$ [17–20,23,24]. In fact, following arguments similar to Ref. [3], where eigenstates of a hard sphere system were written as a random superposition of many-body plane waves so as to be consistent with ETH, in our case an eigenstate $|E\rangle$ of H in the limit $\varepsilon \rightarrow 0$ takes the form

$$\lim_{\varepsilon \rightarrow 0} \lim_{V \rightarrow \infty} |E\rangle = \sum_{\alpha} C_{\alpha} |s_{\alpha}\rangle \tag{8}$$

with

$$P(\{C_{\alpha}\}) \propto \delta\left(1 - \sum_{\alpha} |C_{\alpha}|^2\right) \delta(E_{\alpha} - E), \tag{9}$$

where the first and second delta function constraints impose the normalization and energy conservation respectively. This form of eigenstates closely resembles the Berry’s conjecture for the eigenstates of chaotic billiard ball systems [25], and therefore we will call such states “Berry states.” Again, sim-

ilar to the case of ergodic bipartition conjecture discussed above [Eq. (5)], one can readily verify that ETH holds true for the state in Eq. (8). Specifically, the diagonal matrix elements of an operator O match the canonical expectation value of O with respect to H_0 , while the off-diagonal matrix elements are proportional to $e^{-S(E)/2} z$ where z is a random complex number with zero mean. Note that we take H_0 to be translationally invariant to avoid the possibility of many-body localization [30].

Relation between ergodic bipartition states and berry states

The aforementioned Berry states can be thought of as a special case of ergodic bipartition states: if in Eq. (5) one substitutes for $|E_i^A\rangle$ and $|E_j^{\bar{A}}\rangle$ the eigenstates of $H_{0,A}$ and $H_{0,\bar{A}}$ respectively, where $H_{0,A}$ and $H_{0,\bar{A}}$ are restrictions of the integrable Hamiltonian H_0 in Eq. (7) to region A and \bar{A} , then the resulting state essentially corresponds to the Berry state [Eq. (8)]. However, there is a subtle distinction: the Berry state does not suffer from any boundary effects due to the $H_{A\bar{A}}$ term: the states $|s_{\alpha}\rangle$ that enter the definition of Berry state in Eq. (8) are eigenstates of the Hamiltonian H_0 defined on the entire system. In contrast, the ergodic bipartition states involve tensor products of the eigenstates of H_A and $H_{\bar{A}}$, and therefore do not reproduce the correlations near the boundary between A and \bar{A} correctly, as discussed above.

Due to this relation between the ergodic bipartition states and the Berry states, it turns out that from a technical standpoint, the calculations of their Renyi entropies—the central topic of our paper—are identical. This is the subject of our next section.

III. RENYI ENTROPY OF CHAOTIC EIGENSTATES

In this section we calculate Renyi entropy corresponding to the pure states in Eqs. (5) and (8). We will not write separate equations for these two set of states, because as already mentioned, the calculation as well as all the results derived in this section apply to either of them. We will be particularly interested in the functional dependence of Renyi entropies on the ratio V_A/V .

A. Universal dependence of Renyi entropy on many-body density of states

In principle, one can define three different kinds of averages to obtain Renyi entropies: (a) $S_n^A(\bar{\rho}_A) = \frac{1}{1-n} \ln\{\text{tr}[(\bar{\rho}_A)^n]\}$ (b) $S_n^A(\overline{\text{tr } \rho_A^n}) = \frac{1}{1-n} \ln(\overline{\text{tr } \rho_A^n})$ (c) $S_n^A(\overline{\text{tr } \rho_A^n}) = \frac{1}{1-n} \ln[\overline{\text{tr}(\rho_A^n)}]$. The physically most relevant measure is $S_{n,\text{avg}}$, however, it is also the hardest one to calculate due to averaging over the logarithm. As shown in Appendix B, the difference $|S_{n,\text{avg}} - S_n^A(\overline{\text{tr } \rho_A^n})|$ is exponentially small in the volume of the total system. Due to this result and the fact that $S_n^A(\overline{\text{tr } \rho_A^n})$ is calculable using standard tools, in this paper we will focus mainly on it, and with a slight abuse of notation, denote it as \bar{S}_n .

One may still wonder how good is the measure (a), i.e., $S_n^A(\bar{\rho}_A)$, since it’s the simplest one to calculate. Following Ref. [28], Levy’s lemma implies that the trace norm distance

between the average density matrix $\overline{\rho_A}$ and a typical density matrix of the ensemble vanishes exponentially in the total volume of the system. Combining this result with Fannes' inequality [31], $|S_1(\rho) - S_1(\sigma)| < |\rho - \sigma|_1 \ln(\mathcal{H})$ where \mathcal{H} is the size of the Hilbert space, one finds that in the thermodynamic limit, at least the von Neumann entropy for $\overline{\rho_A}$ should match with the other two measures up to exponentially small terms. This result doesn't however constrain the Renyi entropies for a general Renyi index. As we will discuss below, it turns out that the volume law coefficient corresponding to Renyi entropies is same for all three measures. At the same time, as discussed in detail in Sec. IV, for finite sized systems, $S_n^A(\text{tr } \rho_A^n)$ is always a better measure of $S_{n,\text{avg}}$ compared to $S_n^A(\overline{\rho_A})$ due to the aforementioned result that their difference is exponentially small in the volume (see Fig. 3).

To begin with, let us briefly consider $S_n^A(\overline{\rho_A}) = \frac{1}{1-n} \ln\{\text{tr}[(\overline{\rho_A})^n]\}$,

$$S_n^A(\overline{\rho_A}) = \frac{1}{1-n} \ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + n S_A^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)} \right]^n} \right], \quad (10)$$

where $S_A^M(E_A)$ denotes the logarithm of the density of states of H_A at energy E_A . Similarly, $S_A^M(E-E_A)$ denotes the logarithm of the density of states of $H_{\bar{A}}$ at energy $E-E_A$. Below, we will show that this expression matches that for $\overline{S_n^A}$ at the leading order in the thermodynamic limit when V_A/V is held fixed.

For brevity, from now on we will drop the superscript "A" on the Renyi entropies S_n^A for the rest of the paper. To analyze $\overline{S_n}$, our main focus, let us first consider the second Renyi

entropy $\overline{S_2}$. One finds (see Appendix C)

$$\overline{S_2} = -\ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + 2S_A^M(E-E_A)} + e^{2S_A^M(E_A) + S_A^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)} \right]^2} \right]. \quad (11)$$

Unlike $S_n^A(\overline{\rho_A})$, this expression is manifestly symmetric between A and \bar{A} . Most importantly, $\overline{S_2}$ is a *universal* function of the microcanonical entropy (= logarithm of density of states) for the system. Furthermore, when $V_A/V < 1/2$ is held fixed, in the thermodynamic limit (i.e., $V \rightarrow \infty$), $\overline{S_2}$ can be simplified as

$$\overline{S_2} = -\ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + 2S_A^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)} \right]^2} \right]. \quad (12)$$

Let's consider the limit $V_A/V \rightarrow 0$. Taylor expanding $S_A^M(E-E_A)$ as $S_A^M(E-E_A) = S_A^M(E) - \beta E_A$, one finds

$$\begin{aligned} \overline{S_2} &= -\ln \left[\frac{\text{tr } e^{-2\beta H_A}}{(\text{tr } e^{-\beta H_A})^2} \right] = -\ln \left[\frac{Z_A(2\beta)}{Z_A^2(\beta)} \right] \\ &= 2\beta [F_A(2\beta) - F_A(\beta)], \end{aligned} \quad (13)$$

where $F_A(\beta)$ is the free energy of H_A at temperature β^{-1} . This is exactly what one expects when the reduced density matrix is canonically thermal i.e., $\rho_A = e^{-\beta H_A} / \text{tr } e^{-\beta H_A}$. Evidently, this result is true only when $V_A/V \rightarrow 0$ and does not hold true for general values of V_A/V and we will explore this and related aspects in much detail below.

Following the same procedure as above, one can also derive the universal formula for the Renyi entropy at an arbitrary Renyi index n . For example, the explicit expression for the third Renyi entropy is (Appendix D)

$$\overline{S_3} = -\frac{1}{2} \ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + 3S_A^M(E-E_A)} + 3e^{2S_A^M(E_A) + 2S_A^M(E-E_A)} + e^{S_A^M(E_A) + S_A^M(E-E_A)} + e^{3S_A^M(E_A) + S_A^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)} \right]^3} \right]. \quad (14)$$

The explicit expression of n th Renyi entropy can be expressed as a logarithm of the sum of $n!$ terms. In the thermodynamic limit, however, only one of these terms is dominant, and the expression becomes (for $V_A/V < 1/2$)

$$\overline{S_n} = \frac{1}{1-n} \ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + n S_A^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)} \right]^n} \right]. \quad (15)$$

Note that this is identical to the Renyi entropy $S_n^A(\overline{\rho_A})$, Eq. (10). See Appendix D for details of the calculation.

B. Curvature of Renyi entropies and the failure of Page curve

Let us evaluate Eq. (15), in thermodynamic limit $V \rightarrow \infty$ with $f = V_A/V (< 1/2)$ held fixed. The thermodynamic limit allows one to use the saddle point approximation technique. The numerator can be written as

$$\sum_{E_A} e^{S_A^M(E_A) + n S_A^M(E-E_A)} = \sum_{u_A} e^{V_A s(u_A) + n V_{\bar{A}} s(u_{\bar{A}})}, \quad (16)$$

where u_A denotes the energy density in A while $u_{\bar{A}}$ denotes the energy density in \bar{A} consistent with energy conservation, and $s(u)$ is the entropy density at energy density u . Thus,

$$u_{\bar{A}} = \frac{u}{1-f} - \frac{f}{1-f} u_A. \quad (17)$$

where $u = E/V$ is the energy density corresponding to the eigenstate under consideration. At the saddle point, the sum over u_A is dominated by the solution to the equation:

$$\left. \frac{\partial s(u)}{\partial u} \right|_{u=u_A^*} = n \left. \frac{\partial s(u)}{\partial u} \right|_{u=u_{\bar{A}}^*} \quad (18)$$

and therefore the numerator equals $e^{V[f s(u_A^*) + n(1-f)s(u_{\bar{A}}^*)]}$ in thermodynamic limit.

On the other hand, the denominator is

$$\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)} = \sum_{u_A} e^{V_A s(u_A) + V_{\bar{A}} s(u_{\bar{A}})} = e^{V s(u)}, \quad (19)$$

where we have used the fact that the saddle point for the denominator is $u_A^* = u_A^* = u$, i.e., it is unchanged from the energy density of the eigenstate under consideration.

Combining the above results, \overline{S}_n is therefore given by

$$\overline{S}_n = \frac{V}{1-n} [fs(u_A^*) + n(1-f)s(u_A^*) - ns(u)], \quad (20)$$

where u_A^* and u_A^* are obtained by solving the saddle point condition Eq. (18). This is the central result of our paper. Several observations can be made immediately:

(1) When $n = 1$, $u_A^* = u$, i.e., the von Neumann entanglement entropy S_1 depends only on the density of states at the energy density corresponding to the eigenstate for all values of $f = V_A/V$. Furthermore, the volume law coefficient of S_1 is strictly linear with V_A , i.e., $S_1 = s(u)V_A$ for $f < 1/2$. We will call such linear dependence the ‘‘Page curve’’ [32,33], as is conventional. As discussed in the Introduction, this result was also argued for in Refs. [8,14].

(2) When $n \neq 1$, the Renyi entropy density S_n/V_A as $V \rightarrow \infty$ for fixed $f = V_A/V$ depends on f , and thus the Renyi entropies have a nontrivial curvature dependence when plotted as a function of V_A/V . Perhaps most interestingly, as shown in Appendix E, the curvature $\frac{d^2 S_n}{df^2}$ depends only on the sign of $n - 1$:

$$\begin{aligned} \overline{S}_n(f) & \text{ is convex for } n > 1, \\ \overline{S}_n(f) & \text{ is concave for } n < 1. \end{aligned} \quad (21)$$

(3) The saddle point equation [Eq. (18)] implies that for a fixed Renyi index n , the energy density u_A^* that determines the volume law coefficient of \overline{S}_n depends on f . Therefore, different values of f encode thermodynamical information at different temperatures. Recall that in contrast, as $f \rightarrow 0$, the n th Renyi entropy depends only on the free energy densities at temperature β^{-1} and $(n\beta)^{-1}$.

We recall that the Renyi entanglement entropies S_n corresponding to a typical state in the Hilbert space [32–36] equal $\ln(\mathcal{H}_A)$ where \mathcal{H}_A is the size of the Hilbert space in region A (assuming $\mathcal{H}_A < \mathcal{H}_{\bar{A}}$). For a system with a local Hilbert space dimension $\mathcal{H}_{\text{local}}$, this translates as a volume law for Renyi entropies, i.e., $S_n^n = V_A \ln(\mathcal{H}_{\text{local}})$ as long as $f < 1/2$ [e.g., in a spin-1/2 system, $S_n^n = V_A \ln(2)$]. This result matches the entropy corresponding to a thermal ensemble at infinite temperature. Based on this, one might have expected that for an eigenstate of a physical Hamiltonian at temperature β^{-1} , the Renyi entropies are perhaps given by their canonical counterparts, i.e., $S_n = V_A n \beta [\mathfrak{f}(n\beta) - \mathfrak{f}(\beta)] / (n - 1)$ for all $f < 1/2$, a finite temperature version of the Page curve [$\mathfrak{f}(\beta)$ is the free energy density]. *Our result indicates that this is not the case, and Renyi entropies for $n \neq 1$ do not follow such a Page curve.*

An example: Renyi entropy for system with Gaussian density of states

Let’s study an example where one can solve the saddle point Eq. (18), and solve for the Renyi entropies explicitly. Consider a system with volume V where the density of states $g(E)$ is a Gaussian as a function of the energy E :

$$g(E) = e^{V \ln 2 - E^2/2V}. \quad (22)$$

Thus, the microcanonical entropy density is given by

$$s(u) = \ln 2 - \frac{1}{2}u^2, \quad (23)$$

where $u \equiv E/V$ denotes the energy density. This expression also implies that the temperature $\beta(u) = -u$. As a practical application, for all systems whose energy-entropy relation $s(u)$ is symmetric under $u \rightarrow -u$, a Gaussian density of states will be a good approximation to the function $s(u)$ close to the infinite temperature. Therefore, the results derived can be thought of as a leading correction to the Renyi entropy in a high temperature series expansion for such systems.

Directly evaluating the expression in Eq. (11), one finds the following expression for S_2 (see Appendix F):

$$\overline{S}_2 = -\ln \left[\frac{1}{\sqrt{1-f^2}} e^{-V\gamma(f,u)} + \frac{1}{\sqrt{1-(1-f)^2}} e^{-V\gamma(1-f,u)} \right], \quad (24)$$

where

$$\gamma(f, u) = f \ln 2 - \frac{f}{1+f} u^2. \quad (25)$$

When $0 < f < \frac{1}{2}$ ($\frac{1}{2} < f < 1$), the first (second) term dominates in the thermodynamic limit. Thus, for $0 < f < \frac{1}{2}$,

$$\overline{S}_2 = fV \left(\ln 2 - \frac{u^2}{1+f} \right) = fV \left(\ln 2 - \frac{\beta^2}{1+f} \right). \quad (26)$$

Similarly, one can obtain Renyi entropy for arbitrary Renyi index n for $0 < f < \frac{1}{2}$ in the thermodynamic limit:

$$\overline{S}_n = fV \left[\ln 2 - \frac{n\beta^2}{2[1+(n-1)f]} \right]. \quad (27)$$

This expression illustrates several of the general properties discussed in the previous subsection. First we notice that \overline{S}_n is linear for arbitrary β only when $n = 1$, and therefore the von Neumann entropy follows the finite temperature Page curve. For $n \neq 1$, \overline{S}_n is linear in f only at the infinite temperature, and the nonlinear dependence on f becomes non-negligible as one moves away from the infinite temperature. Furthermore, the Renyi entropies are convex functions of V_A for $n > 1$ while they are concave for $n < 1$. As a demonstration, we plot Eq. (27) for different β with $n > 1$ (upper panel) and $n < 1$ (lower panel) in Fig. 2, where we clearly observe the concave and convex shape for Renyi entropies.

C. Comparison with ‘‘pure thermal’’ state

Recently, Ref. [15] also studied the entanglement entropies of chaotic systems using an approach which is similar in spirit to ours, but for a different class of states. They considered a canonical thermal pure quantum (CTPQ) state:

$$|\psi\rangle = \frac{1}{\text{tr} e^{-\beta H}} \sum_j z_j e^{-\beta H/2} |j\rangle, \quad (28)$$

where $\{|j\rangle\}$ form a complete orthonormal basis in the Hilbert space, and the coefficient z_j is a random complex number $z_j \equiv (x_j + iy_j)/\sqrt{2}$ with x_j and y_j denoting independent and identically distributed random variables from a Gaussian

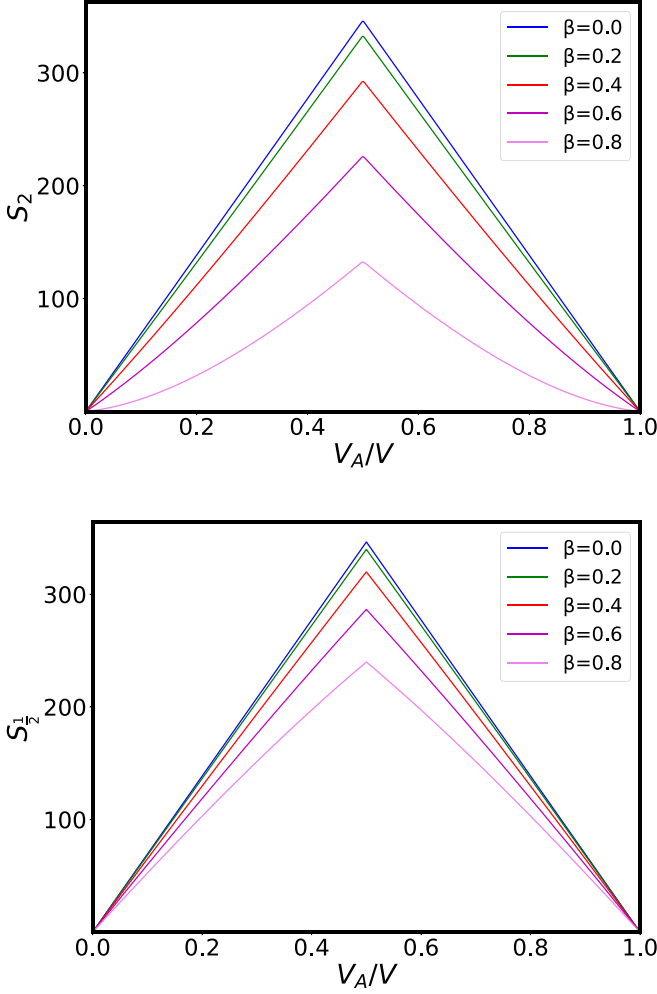


FIG. 2. The Renyi entropies S_2 (top) and $S_{1/2}$ (bottom) for a system of volume $V = 1000$ with Gaussian density of states [Eq. (27)]. The various lines plotted in descending order from the top correspond to $\beta = 0.0, 0.2, 0.4, 0.6, 0.8$ respectively.

distribution with zero mean and unit variance. They calculated the Renyi entropy of the CTPQ states and used the functional form thus obtained as a fitting function for Renyi entropies of chaotic eigenstates obtained via exact diagonalization. For reference, we write down the expression of the second Renyi entropy obtained in their paper:

$$\overline{S_{2,\text{CTPQ}}} = -\ln \frac{\text{tr}_A(\text{tr}_B e^{-\beta H})^2 + \text{tr}_B(\text{tr}_A e^{-\beta H})^2}{(\text{tr} e^{-\beta H})^2}. \quad (29)$$

Note the resemblance with our result Eq. (11). Despite the apparent similarity, the functional dependence of Renyi entropy obtained from Eq. (29) is actually quite different than our result, Eq. (20). In particular, for fixed V_A/V ($< 1/2$), as $V \rightarrow \infty$, one may verify that the volume law coefficient of the Renyi entropy $\overline{S_{n,\text{CTPQ}}}$ corresponding to the CTPQ state actually matches that of a thermal state: $\overline{S_{n,\text{CTPQ}}} = \frac{n}{n-1} V_A \beta [\mathfrak{f}(n\beta) - \mathfrak{f}(\beta)]$, and therefore follows the Page curve. This is in contrast to the Berry and EB states, which, as discussed above, have a distinct curvature dependence. One may also verify that the reduced density matrix in region A of

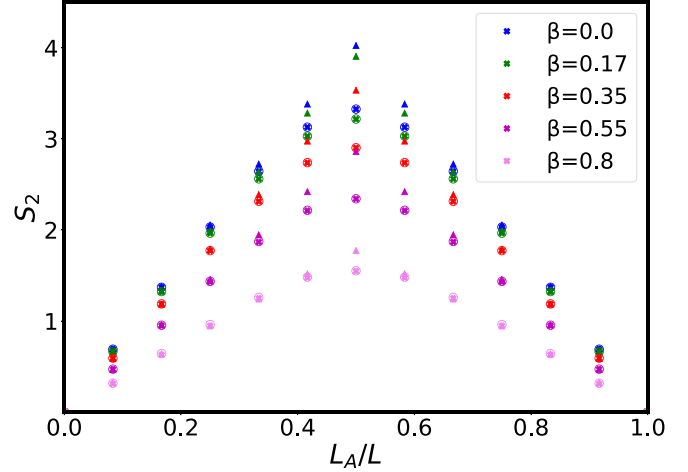


FIG. 3. Comparison of the three different ways to average over the random ensembles discussed in the text to obtain the second Renyi entropy. Triangles: $S_2^A(\overline{\rho_A})$. Crosses: $S_2^A(\overline{\text{tr} \rho_A^2})$. Open circles: $S_{2,\text{avg}}^A = -\ln[\text{tr}(\rho_A^2)]$. Note that $S_2^A(\overline{\text{tr} \rho_A^2})$ and $S_{2,\text{avg}}^A$ are essentially identical, as they should be (see Appendix B). The Hamiltonian is $H = -\sum_{i=1}^L Z_i + \varepsilon H_1$ for $L = 12$ and $\varepsilon = 0.1$, where H_1 is a real Hermitian random matrix. For each marker style, the data in descending order from the top correspond to $\beta = 0.0, 0.17, 0.35, 0.55, 0.8$.

a CTPQ state,

$$\rho_A \sim \frac{e^{-\beta H}}{\text{tr} e^{-\beta H}} \quad (30)$$

for any V_A/V in thermodynamic limit which implies that the energy variance $\sim V_A$ for all V_A/V and does not respect the fact that for an eigenstate, the energy variance should be symmetric around $V_A/V = 1/2$ (similar to Renyi entropies), and should vanish when $V_A/V \rightarrow 1$.

IV. COMPARISON OF ANALYTICAL PREDICTIONS WITH EXACT DIAGONALIZATION

In this section, we will compare our analytical predictions with numerical simulations on quantum spin-chain Hamiltonians. Recall that our analytical results are for $\overline{S_n} \stackrel{\text{def}}{=} \frac{1}{1-n} \ln(\text{tr} \rho_A^n)$, which is essentially identical to the more physical quantity, $S_{n,\text{avg}} = \frac{1}{1-n} \ln[\text{tr}(\rho_A^n)]$, as discussed at the beginning of Sec. III A and in Appendix B. See Fig. 3 for a demonstration. Due to this, we will continue to use the symbol $\overline{S_n}$ for Renyi entropies obtained from numerical simulations even though we are really calculating $S_{n,\text{avg}}$. In contrast, the quantity $S_n(\overline{\rho_A}) = \frac{1}{1-n} \ln[\text{tr}[(\overline{\rho_A})^n]]$, which incidentally equals the asymptotic expression for $\overline{S_n}$ in the thermodynamic limit [see Eqs. (10) and (15)], does not agree as well with $S_{n,\text{avg}}$ (Fig. 3).

We will compare the ED results with the analytical results for Berry, EB, and CTPQ states. Our approach will be different than the one in Ref. [15] where the analytical results for the CTPQ state were used only as a guide to fit the results of ED.

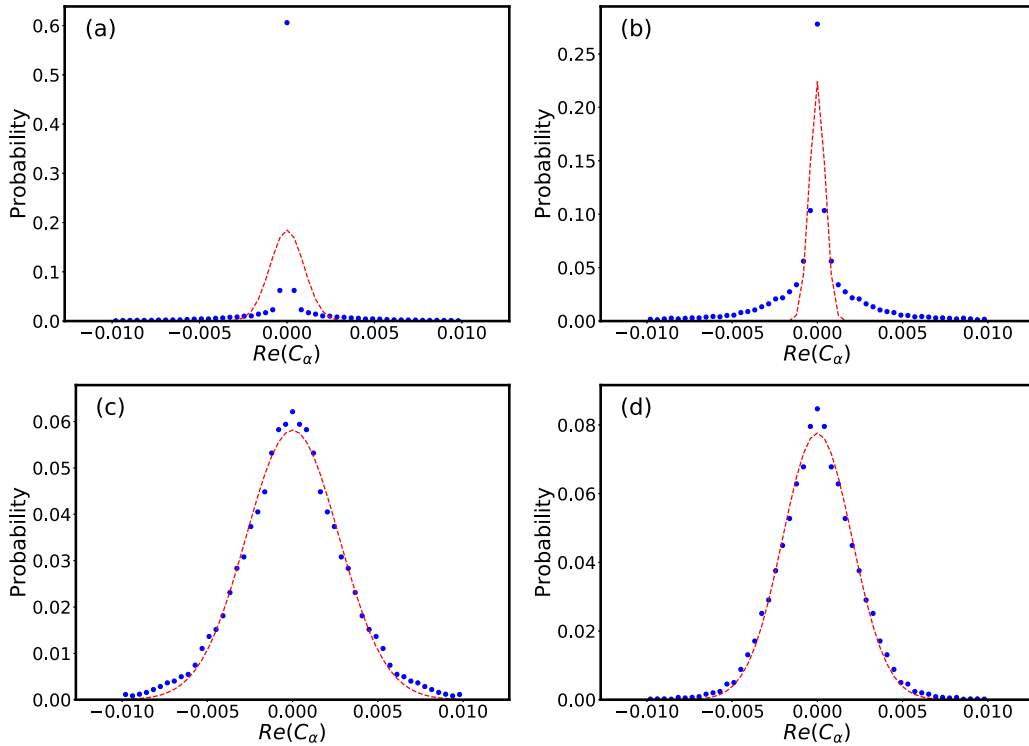


FIG. 4. Probability amplitudes for C_α [Eq. (8)] corresponding to the Hamiltonian in Eq. (31) with $L = 18$ when H_0 and H_1 are given by Eq. (32) for various values of the perturbation ε : (a) $\varepsilon = 0.01$, (b) $\varepsilon = 0.204$, (c) $\varepsilon = 0.404$, and (d) $\varepsilon = 0.724$. Blue dots: exact results from eigenstates. Red dashed lines: Gaussian fitting. We choose eigenstates at energy $E = 0$ and the width of energy window is $\Delta = 1$. The Gaussian distribution is obtained by least square fitting.

A. Nonintegrable spin-1/2 chain close to integrable regime

In this subsection we numerically study Renyi entropies for eigenstates of a nonintegrable Hamiltonian close to the classical limit, namely the Hamiltonians of the form in Eq. (7):

$$H = H_0 + \varepsilon H_1. \quad (31)$$

1. Spin-1/2 chain with local perturbation

Consider

$$H_0 = \sum_i^L -Z_i Z_{i+1} - Z_i, \quad H_1 = \sum_i^L X_i. \quad (32)$$

We first study the histogram of amplitudes C_α introduced in Eq. (8) for various values of ε to check the validity of Berry states. In Fig. 4, we observe that amplitudes approach a Gaussian probability distribution with increasing ε . Analytical and numerical estimates suggest that one requires $\varepsilon \gtrsim 1/L^\beta$ where β is some positive number to access the chaotic regime [17–20,23,24]. For example, a study of a Hamiltonian of a form similar to Eq. (32) in Ref. [20] found that for small ε , signatures of integrability persist, and one obtains a Lorentzian distribution for $\{C_\alpha\}$ while as one enters a regime where signatures of chaos (e.g., Wigner-Dyson level statistics) are visible, the coefficients follow a Gaussian distribution. This is consistent with our findings (Fig. 4) where, due to system size limitations, we require $\varepsilon \approx 0.4$ to see the onset of chaos. This implies that in the chaotic regime, the eigenstates of H cannot be simply obtained by randomly superposing eigenstates of H_0 since when ε is not infinitesimal, there

is no direct correspondence between the eigenstates of H and H_0 (i.e., the effect of H_1 is not restricted to simply randomize eigenstates of H_0). Therefore, we are unable to verify the validity of Eq. (8) for the accessible system sizes. Figure 5 compares the Renyi entropy of the eigenstates of H with those predicted by Berry conjecture when ε is smaller than ≈ 0.4 . Curiously, although we are not able to predict the full shape dependence of Renyi entropy using the Berry conjecture for the reasons just outlined, it still works rather well to predict the Renyi entropies for $V_A/V \ll 1$. This is perhaps not surprising, since physically, the crossover value of ε required to obtain features of chaos at smaller length scales should be smaller than the one required for chaos to set up globally.

2. Spin-1/2 chain with random nonlocal perturbation

Next we consider the Hamiltonian $H = H_0 + \varepsilon H_1$, where H_1 is a real Hermitian random matrix. The variance of the probability distribution function of the matrix element in H_1 is chosen such that the range of energy spectrum of H_1 is L . Our expectation is that the system size at which the crossover from integrability to chaos occurs is parametrically smaller when H_1 is nonlocal as compared to when it is local. In fact, a diagonal $N \times N$ matrix perturbed by a matrix chosen from a random Gaussian orthogonal ensemble (GOE) shows chaotic behavior when the strength of the perturbation [37,38] is $\gtrsim 1/\sqrt{N}$. Translating this to the many-body Hamiltonians with Hilbert space size \mathcal{H} , this indicates a crossover scale of $1/\sqrt{\mathcal{H}} = 2^{-L^d/2}$.

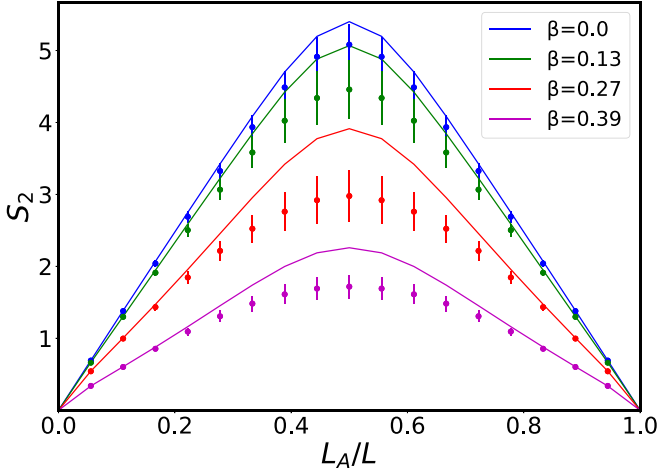


FIG. 5. Comparison of the second Renyi entropy S_2 for a Berry state, with those obtained from the exact diagonalization for the Hamiltonian $H = H_0 + \varepsilon H_1$ for $L = 20$ and $\varepsilon = 0.204$ where H_0 and H_1 are given by Eq. (32). The solid dots correspond to S_2 of eigenstates averaged over an energy window of width $\Delta E = 2$, and the vertical bars denote the standard deviation in S_2 in this energy window. Solid lines correspond to S_2 for the Berry state using Eq. (11). For each marker (line) style, the data in descending order from the top correspond to $\beta = 0.0, 0.13, 0.27, 0.39$.

As a demonstration, consider the case when $H_0 = -\sum_{i=1}^L Z_i$. As shown in Fig. 6, the coefficients C_α indeed behave as random Gaussian variables even when $\varepsilon = 0.1$. Furthermore, we verified that their variance equals e^{-S} , consistent with ETH. Note that despite the nonlocality of H , the equal time correlation functions of Berry states depend *solely* on H_0 , which is local. Due to this, the Berry states continue to satisfy properties expected from a local Hamiltonian, such as the validity of cluster decomposition for correlations of local operators.

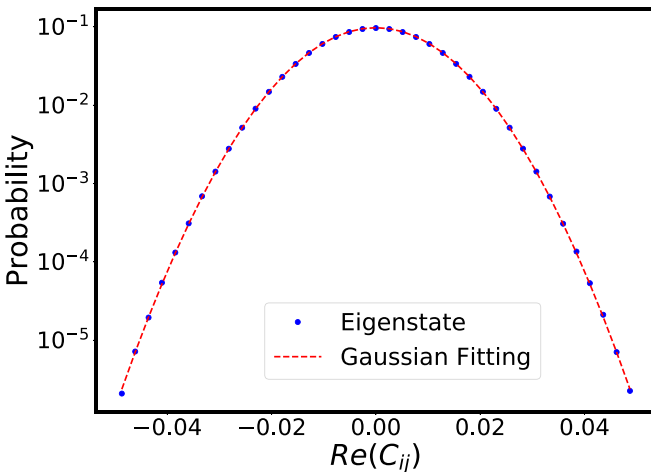


FIG. 6. Probability distribution of the amplitudes C_α [Eq. (8)] for a single eigenstate corresponding to inverse temperature $\beta = 0.26$ of the Hamiltonian $H = -\sum_{i=1}^L Z_i + \varepsilon H_1$, where H_1 is a real Hermitian random matrix. We choose $L = 16$ and $\varepsilon = 0.1$. The Gaussian distribution is obtained by least square fitting.

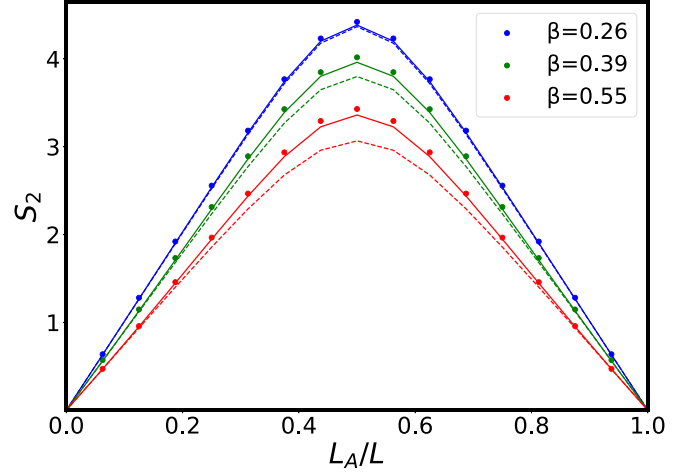


FIG. 7. Comparison of the second Renyi entropy S_2 of one-dimensional (1D) spin model with Hamiltonian $H = -\sum_{i=1}^L Z_i + \varepsilon H_1$ where H_1 is a random matrix. We choose $L = 16$ and $\varepsilon = 0.1$. The three plotted quantities correspond to Renyi entropy S_2 of eigenstates (solid dots), Berry states [Eq. (11)] (solid lines), and CTPQ states [Eq. (29)] (dashed lines). For each marker (line) style, the data in descending order from the top correspond to $\beta = 0.26, 0.39, 0.55$.

One advantage of working with the specific H_0 mentioned above is that one can calculate its density of states exactly, and therefore obtain analytical predictions for the Renyi entropies of the chaotic Hamiltonian H . In particular, the number of eigenstates of H_0 at energy E are

$$g = \frac{L!}{N_\uparrow! N_\downarrow!}, \quad (33)$$

where $N_\uparrow = \frac{L-E}{2}$ and $N_\downarrow = \frac{L+E}{2}$. Thus the microcanonical entropy $S^M = \ln(g)$ under Sterling's approximation is given by

$$S^M \approx L \ln(L) - \frac{L-E}{2} \ln \frac{L-E}{2} - \frac{L+E}{2} \ln \frac{L+E}{2}. \quad (34)$$

In fact, at high temperatures, the entropy density is same as that of the Gaussian model, Eq. (23), $s = S^M/L = \ln 2 - \frac{1}{2}\beta^2$.

Figure 7 shows the comparison of the Renyi entropies of the eigenstates of H at $\varepsilon = 0.1$ with the analytical predictions for a Berry state. We see that agreement is quite good for a wide range of temperatures.

In Fig. 7, we also compare the results with the expression obtained from a CTPQ state, Fig. 7. We see that they match well for small values of $f = L_A/L$. On the other hand, for $f = O(1)$, the Renyi entropy of a CTPQ state is smaller than the exact diagonalization results and the predictions from a Berry state. This is consistent with the fact that in the thermodynamic limit, a CTPQ state predicts linear dependence of the second Renyi entropy as a function of f , while for a Berry state, the second Renyi entropy is a convex function of f (Sec. III B).

3. Finite size scaling: Exact vs asymptotic predictions

As discussed in Sec. III, the expression for the n th Renyi entropy contains $n!$ terms, and only one of them contributes to the volume law coefficient in the thermodynamic

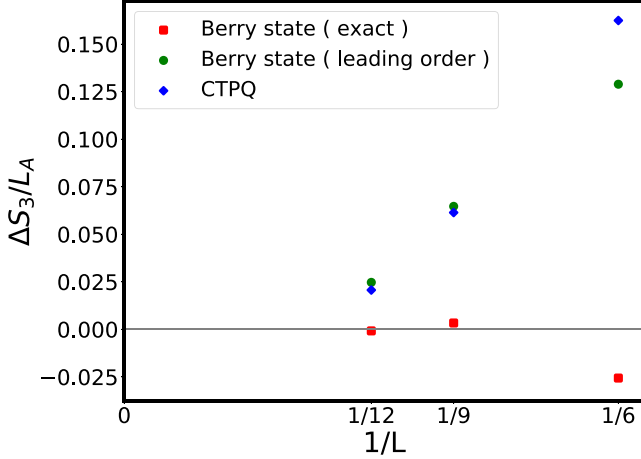


FIG. 8. Finite size scaling of the difference between the third Renyi entropy S_3 obtained from analytical expressions and exact diagonalization results for the eigenstates of a 1D spin model with Hamiltonian $H = -\sum_{i=1}^L Z_i + \varepsilon H_1$ where H_1 is a random matrix. Here $\varepsilon = 0.1$. A data point is obtained by averaging ΔS_3 for eigenstates in the range $0 < \beta < 0.5$. L_A is chosen to be $L/3$.

limit [compare Eqs. (14) and (15)]. The asymptotic result, Eq. (15), also matches the Renyi entropies $S_n^A(\rho_A)$ [Eq. (10)]. It is worthwhile to compare these two predictions, the exact and the asymptotic, with exact diagonalization results. Figure 8 compares the deviation of the exact result for S_3 corresponding to a Berry state [Eq. (14)] from the exact diagonalization, with the deviation of the asymptotic result [Eq. (15)] from the exact diagonalization. We notice that the exact result fares much better than the asymptotic one in a finite sized system. We also perform the finite size scaling of the deviation of the CTPQ state for S_3 from the exact diagonalization results. The extrapolation to thermodynamic limit indicates that the deviation becomes negative in the thermodynamic limit, which is again consistent with our prediction that S_3 for a chaotic system would be a convex function of L_A .

B. Nonintegrable spin-1/2 chain far from integrability

Next we study local Hamiltonians without any small parameter. As discussed in Sec. II, arguments based on ergodicity suggest that the bulk properties of a system can be described by EB states, Eq. (5). As a numerical test of Eq. (5), consider a one-dimensional spin-1/2 chain with the Hamiltonian

$$H = \sum_i^L -Z_i Z_{i+1} - Z_i + X_i, \tag{35}$$

where we impose the periodic boundary condition $i \equiv i + L$. Several works have already provided evidence in support of the validity of ETH in this model [8,14,39–42]. By diagonalizing H , we calculate the bipartite amplitude of eigenstates on the bases of tensor products of all eigenstates of H_A and $H_{\bar{A}}$ with A denoting the sites $i = 1, 2, \dots, L_A$ and \bar{A} denoting the sites $i = L_A + 1, L_A + 2, \dots, L$. Figure 9 shows the probability distribution of the bipartite amplitude on a semilog plot.

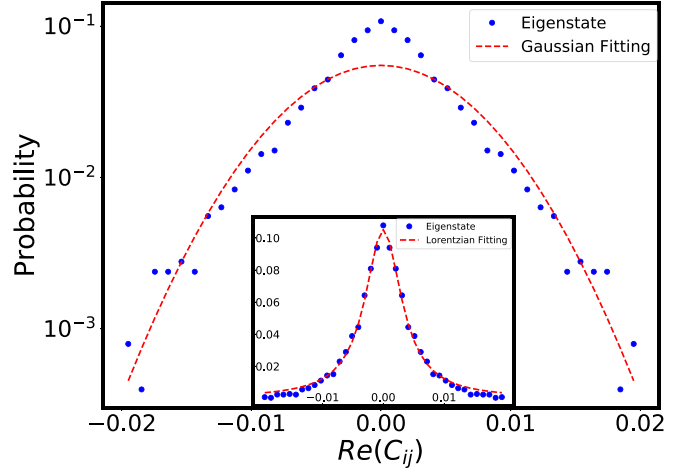


FIG. 9. Probability distribution of the bipartite amplitudes C_{ij} [Eq. (5)] when $|E\rangle$ corresponds to a single eigenstate of the Hamiltonian in Eq. (35) with inverse temperature $\beta = 0.18$. We choose $L = 16$ and the subsystem size $L_A = 8$. The energy window Δ that appears in Eq. (5) is chosen to be 2. The Gaussian distribution is obtained by least square fitting.

We find deviations from a Gaussian distribution and in fact the data fit a Lorentzian distribution better. We do not understand the origin of this deviation. They may be due to the surface term unaccounted for in the definition of EB states (5) which could be significant in a finite sized system. Nevertheless, as we discuss next, we find reasonable agreement for the Renyi entropies obtained from the EB state when compared to the exact diagonalization data.

The analytical prediction for Renyi entropy, say, for S_2 [Eq. (11)] involves the knowledge of the density of states of H_A and $H_{\bar{A}}$. One approximate way to proceed is $S_A^M(E_A) = s(E_A/V_A)L_A$ where $s(x)$ is the entropy density at energy density x obtained from the largest size accessible within ED (here $L = 20$). Alternatively, one can diagonalize H_A and $H_{\bar{A}}$ as well, and use the actual microcanonical density of states $S_A^M(E_A)$ and $S_{\bar{A}}^M(E - E_A)$ from such simulations. Here we chose this latter approach.

Figure 10 compares our analytical prediction of Renyi entropy with ED. For $\beta \lesssim 0.3$, the predictions match rather well with the ED results. The deviations from analytical predictions increase with decreasing temperature, which we attribute to the fact that for the system sizes accessible within ED, the spectrum is not dense enough at the corresponding energy densities leading to a poor estimate of the density of states. Furthermore, the ratio of thermal correlation length to the total system size also increases as temperature is lowered, leading to larger finite size effects. We also show the comparison with CTPQ states. We notice that even at relatively high temperatures, $\beta \gtrsim 0.3$, the predictions from CTPQ states fare less well when compared to the EB states.

We also perform the finite size scaling for Renyi entropies, Fig. 11, where ΔS_2 denotes the deviation of the analytical prediction from the exact diagonalization results. The upper panel shows the finite size scaling for S_2 while the lower panel shows the results for S_3 , where we also compare our asymptotic result [Eq. (15)] with the more accurate result

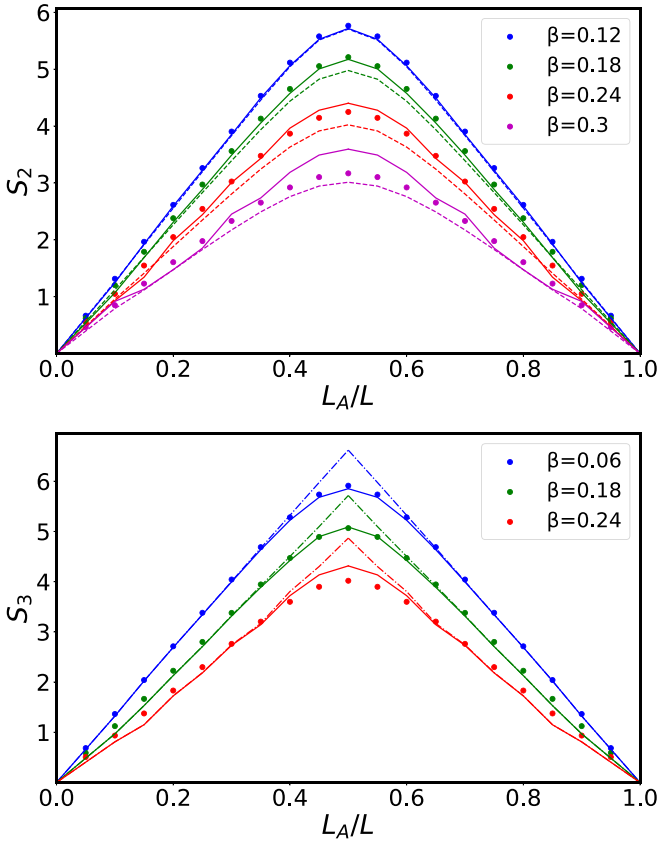


FIG. 10. Comparison of the second Renyi entropy S_2 and the third Renyi entropy S_3 obtained by different methods for the eigenstates of 1D nonintegrable Hamiltonian in Eq. (35) for $L = 20$. Top: Exact diagonalization (solid dots), ergodic bipartition states, Eq. (11) (solid lines), and CTPQ states, Eq. (29) (dashed lines). For each marker (line) style, the data in descending order from the top correspond to $\beta = 0.12, 0.18, 0.24, 0.3$. Bottom: Exact diagonalization (solid dots), exact expression for ergodic bipartition states, Eq. (14) (solid lines), leading order expression for ergodic bipartition states, Eq. (15) (dash-dot lines). For each marker (line) style, the data in descending order from the top correspond to $\beta = 0.06, 0.18, 0.24$.

[Eq. (14)]. Similar to the case of Berry states in the previous section, we again find that EB states fare better compared to the CTPQ states, and for the EB states, the exact expression fares better than the asymptotic one.

V. SUMMARY AND DISCUSSION

By employing arguments based on ergodicity, we derived a universal expression for the Renyi entropy for an arbitrary subsystem to system ratio which, we conjecture, applies to the finite-energy density eigenstates of chaotic many-body Hamiltonians. We found that the expression for the Renyi entropy does not match the Renyi entropy of the corresponding thermal ensemble unless $f = V_A/V$, the subsystem to total system ratio, approaches zero. For a general value of f , the Renyi entropy density S_n/V_A has a nontrivial dependence on f , and only in the case of von Neumann entropy $n \rightarrow 1$ is the density (i.e., the volume law coefficient) independent of f . The curvature $\frac{d^2 S_n}{df^2}$ is positive (negative) for $n > 1$

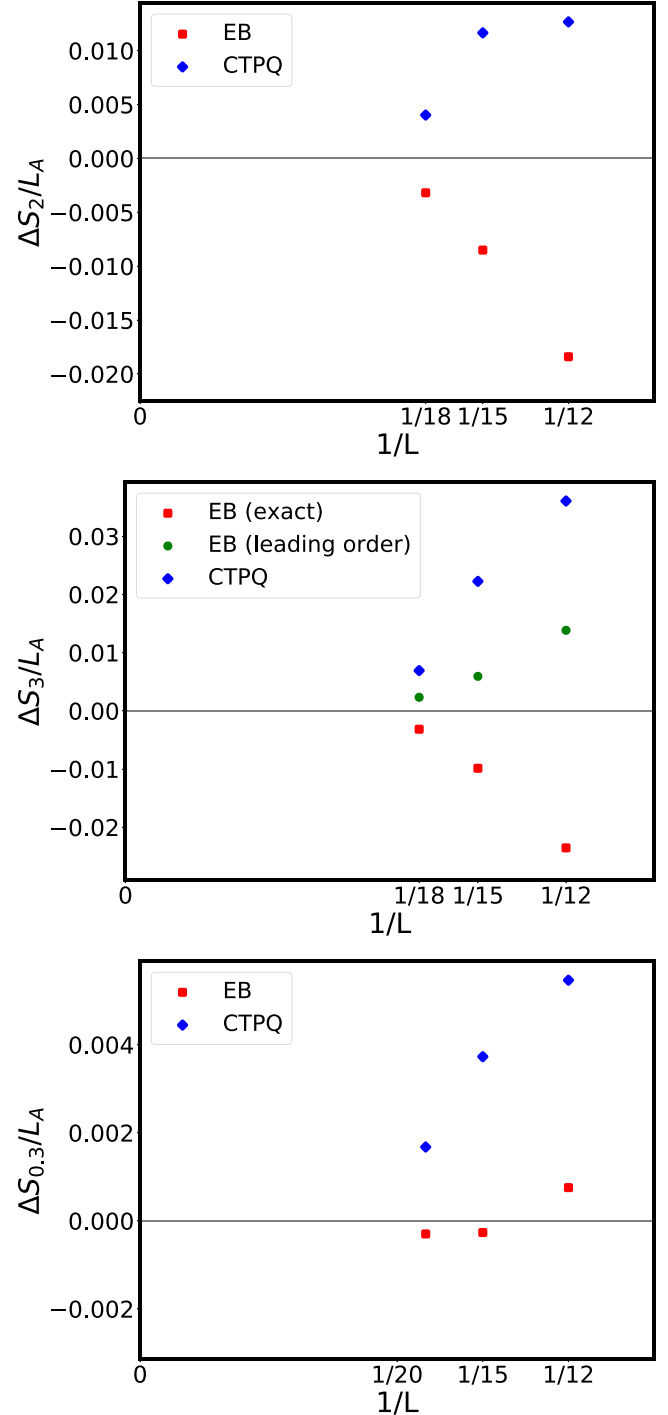


FIG. 11. Finite size scaling for $\Delta S_n/L_A$ for ergodic bipartition (EB) states and CTPQ states where ΔS_n is defined as the difference between the analytical expressions for the corresponding states (EB or CTPQ) and the exact diagonalization results. The Hamiltonian is given by Eq. (35) and eigenstates correspond to $\beta = 0.06$. L_A is chosen to be $L/3$ for all L . Note that in the middle panel, “EB (leading order)” refers to the expression in Eq. (15) while “EB (exact)” refers to Eq. (14). In the top panel we use the exact expression for EB states [Eq. (11)] while in the bottom panel, we use the leading order result [Eq. (15)] for EB states.

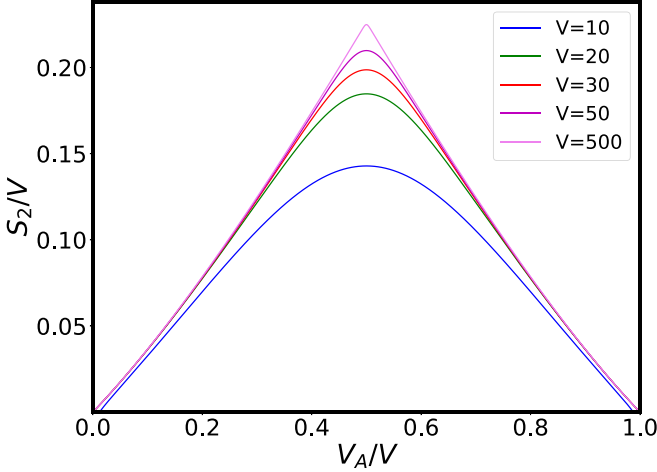


FIG. 12. Evolution of the shape of the Renyi entropy S_2 as the total system is increased for a system with Gaussian density of states [Eq. (24)] for inverse temperature $\beta = 0.6$. The various curves in ascending order correspond to $V = 10, 20, 30, 50, 500$ respectively. Note that as $V \rightarrow \infty$, the Renyi entropy is a convex function for all f , and has a cusp singularity at $f = 1/2$.

($n < 1$) and therefore the volume law coefficient for $n > 1$ is greater (less) than that of a corresponding thermal ensemble. Such dependence is quite different than the Renyi entropies corresponding to (a) the thermal density matrix as well as the CTPQ state [15,16], for which the Renyi entropy densities are independent of f ; (b) free fermion systems for which the von Neumann entropies (and hence all Renyi entropies $n > 1$) are concave functions of f [43,44]; (c) a random state in the Hilbert state [32,33], or systems without *any* conservation laws [41] for which all S_n are simply given by $Vf \ln(2)$ ($f < 1/2$) and do not have any curvature dependence. We compared our theoretical predictions for the Renyi entropy with exact diagonalization results on quantum spin chains, and found reasonable agreement for ergodic bipartition conjecture in the case of local Hamiltonians, and for the Berry conjecture in the case of local Hamiltonian perturbed by an infinitesimal random Hamiltonian.

In exact diagonalization studies on finite systems, the curvature dependence characteristic of the thermodynamic limit can be a bit challenging to observe. In fact, most of the curvature seen in finite size systems can be attributed to the subleading terms in S_n [e.g., the second term in the numerator of Eq. (11)] which do not contribute to the volume law coefficient at any fixed V_A/V in the thermodynamic limit. The presence of these terms in finite size systems can lead to the appearance that S_n for $n > 1$ is a concave function of V_A/V (see, e.g., Fig. 12). Further, the magnitude of the curvature vanishes at infinite temperature, and is proportional to β^2 at high temperatures. In exact diagonalization studies on finite systems, most states have $|\beta|$ below $O(1)$ (see Fig. 13), which also makes it harder to observe the curvature.

Our results show that Renyi entropy for a given subsystem to total system volume fraction $f = V_A/V$ depends on the density of states at an energy density that is itself a function of f . This allows one to obtain information about the full spectrum of the Hamiltonian by keeping the Renyi index

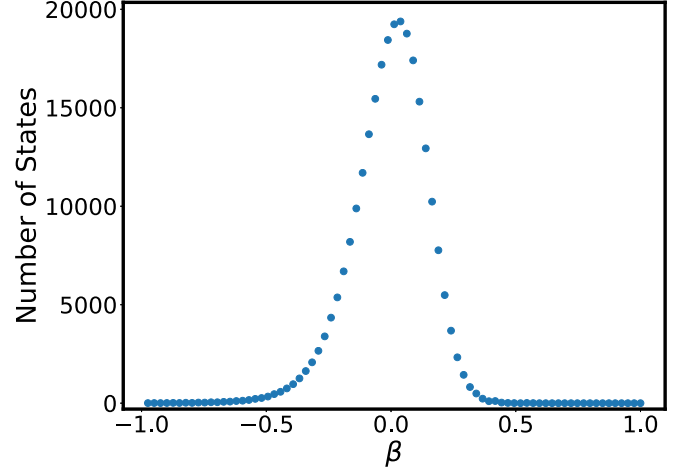


FIG. 13. The density of states as a function of the temperature of the eigenstates for an 18 site spin chain. The temperature for individual eigenstates $|E_n\rangle$ is evaluated by solving the equation $\frac{\text{tr}(H e^{-\beta(E_n)H})}{\text{tr}(e^{-\beta(E_n)H})} = E_n$.

n fixed and only varying f from a single eigenstate. To demonstrate this, we expand the microcanonical entropy $s(u)$ at an energy density corresponding to the infinite temperature $T \rightarrow \infty$: $s(u) = \ln 2 + \alpha_2 u^2 + \alpha_3 u^3 + \dots$, where we choose $u = 0$ corresponding to $T \rightarrow \infty$ without loss of generality. From Eq. (18), one can solve for the saddle point energy density $u_A^*(\{\alpha_i\})$ and $u_A^z(\{\alpha_i\})$, and plug them in Eq. (20) to obtain an equation relating $S_n, f, \{\alpha_i\}$. Suppose that one can measure S_n for various f given a single eigenstate; we then have a system of equations of $\{\alpha_i\}$ given from different (S_n, f) . By solving these equations, one can construct the whole function $s(u)$ to have the full spectrum (density of state as a function of energy density) just from a single eigenstate. Note that this is in strong contrast to the limit $V_A/V \rightarrow 0$ where S_n only encodes thermodynamical information at temperature β^{-1} and $(n\beta)^{-1}$.

Our results also provide a particularly simple prediction for Renyi entropies of chaotic eigenstates for systems where the entropy density $s(u)$ depends on the energy density u in a power law fashion, i.e., $s(u) = cu^\alpha$ where c is a constant. This is because in this case one can solve the saddle point equation [Eq. (18)] analytically. Consider, for example, a conformal field theory (CFT) in d space dimensions, where the exponent $\alpha = \frac{d}{d+1}$. A straightforward calculation yields

$$S_n = \frac{n}{(1-n)f} [\{ (1-f) + fn^{1/(\alpha-1)} \}^{1-\alpha} - 1] S_1, \quad (36)$$

where the von Neumann entanglement entropy $S_1 = cu^\alpha V f$, i.e., it follows the Page curve as expected ($f < 1/2$ of course). Remarkably, in a recent work [45], exactly the same expression was derived for holographic conformal field theories using a completely different method based on holographic duality [46,47].

The dependence of Renyi entropies on a subsystem to total system ratio sheds light on how to distinguish a mixed, thermal density matrix from a pure state which locally looks thermal. Besides being a basic question in quantum statistical mechanics, this question is also of central interest in the

“black hole information paradox” [48,49], where Hawking’s calculation [50] implies that the radiation emanating from an evaporating black hole resembles a thermal system, while at the same time, if one were to describe the evaporation process by a unitary evolution of a pure quantum state, then one expects that there must exist correlations that distinguish the state of the black hole from a thermal state. Our results indicate that the dependence of Renyi entropy S_n on V_A/V may be one way to distinguish a thermal state from a pure state of a black hole.

In this paper, we focused primarily on the volume law coefficient of the Renyi entropies. Reference [51] calculated the subleading contributions to the von Neumann entropy for the infinite temperature particle-number conserving states discussed in Ref. [8], and put in an upper bound that scales as \sqrt{V} for $V_A/V = 1/2$. In a similar spirit, it will be interesting to calculate the subleading contributions to the noninfinite temperature states introduced in this paper.

Recently, we noticed that a recent work, Ref. [52], also conjectures that states of the form Eq. (5) may represent eigenstates of chaotic Hamiltonians. Reference [52] argues that the average of von Neumann entropy over *all* eigenstates is linear in subsystem size at the leading order up to $V_A/V = 1/2$ with volume law coefficient $\ln(2)$ for a spin-1/2 system. This is consistent with our results, and follows from our general formula, Eq. (15), for individual eigenstates: the average will be dominated by eigenstates at the infinite temperature, whose entanglement at the leading order is indeed $V_A \ln(2)$ up to $V_A/V = 1/2$.

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APPENDIX A: SUBSYSTEM ENERGY FLUCTUATION IN AN ERGODIC BIPARTITION (EB) STATE

Consider an ergodic bipartition (EB) state defined by Eq. (5),

$$|E\rangle = \sum_{E_i^A + E_j^{\bar{A}} \in (E - \frac{1}{2}\Delta, E + \frac{1}{2}\Delta)} C_{ij} |E_i^A\rangle \otimes |E_j^{\bar{A}}\rangle; \quad (\text{A1})$$

the probability of finding an eigenstate $|E_i^A\rangle$ on region A is the diagonal element of reduced density matrix given by Eq. (2):

$$\langle E_i^A | \rho_A | E_i^A \rangle = \frac{1}{N} e^{S_{\bar{A}}(E - E_i^A)}, \quad (\text{A2})$$

from which we can derive the probability of finding a state with energy E_A by multiplying the density of state $e^{S_A(E_A)}$ on A :

$$P(E_A) \sim e^{S_A(E_A)} e^{S_{\bar{A}}(E - E_A)}. \quad (\text{A3})$$

This function has a peak at $E_A = \bar{E}_A$ determined by the saddle point equation,

$$\left. \frac{\partial S_A(E_A)}{\partial E_A} \right|_{E_A = \bar{E}_A} = \left. \frac{\partial S_{\bar{A}}(\bar{E}_A)}{\partial \bar{E}_A} \right|_{\bar{E}_A = E - \bar{E}_A}. \quad (\text{A4})$$

By expanding $P(E_A)$ around \bar{E}_A , $P(E_A)$ takes the Gaussian form:

$$P(E_A) \sim e^{-(E_A - \bar{E}_A)^2 / 2\Delta E^2}, \quad (\text{A5})$$

with

$$\Delta E^2 = cT^2 \frac{V_A V_{\bar{A}}}{V_A + V_{\bar{A}}} = cT^2 V f(1 - f), \quad (\text{A6})$$

where c denotes the specific heat per unit volume, T denotes the temperature, and $f \equiv V_A/V$.

APPENDIX B: PROOF THAT $|S_n^A(\overline{\text{tr } \rho_A^n}) - S_{n,\text{avg}}^A|$ IS EXPONENTIALLY SMALL IN THE TOTAL SYSTEM SIZE

Consider an ergodic bipartition (EB) ensemble defined by Eq. (5)

$$|E\rangle = \sum_{i,j} C_{ij} |E_i^A\rangle \otimes |E_j^{\bar{A}}\rangle, \quad (\text{B1})$$

where $\{C_{ij}\}$ is chosen from the probability distribution function

$$P(\{C_{ij}\}) \propto \delta\left(1 - \sum_{ij} |C_{ij}|^2\right) \prod_{i,j} \delta(E_i^A + E_j^{\bar{A}} - E), \quad (\text{B2})$$

where the index $i(j)$ in C_{ij} labels the state in $A(\bar{A})$. The reduced density matrix of A can be obtained by tracing out the Hilbert space in \bar{A} :

$$\rho_A = \text{tr}_{\bar{A}} |\psi\rangle\langle\psi| = \sum_{i,i'} |E_i^A\rangle\langle E_{i'}^A| \sum_j C_{ij} C_{i'j}^*. \quad (\text{B3})$$

In the main text we define two different averaging procedures for the Renyi entropy,

$$S_n^A(\overline{\text{tr } \rho_A^n}) = \frac{1}{1-n} \ln(\overline{\text{tr } \rho_A^n}), \quad S_{n,\text{avg}}^A = \frac{1}{1-n} \ln(\overline{\text{tr } \rho_A^n}), \quad (\text{B4})$$

and state that the difference between these two vanishes in the volume of the system. Here we provide the proof for this claim.

First

$$\text{tr } \rho_A^n = \overline{\text{tr } \rho_A^n} + (\text{tr } \rho_A^n - \overline{\text{tr } \rho_A^n}) = \overline{\text{tr } \rho_A^n} (1 + x), \quad (\text{B5})$$

where

$$x \equiv \frac{\text{tr } \rho_A^n}{\overline{\text{tr } \rho_A^n}} - 1. \quad (\text{B6})$$

Plugging Eq. (B5) into Eq. (B4), we have

$$S_{n,\text{avg}}^A = \frac{1}{1-n} \overline{\ln[\text{tr}(\rho_A^n)]} = S_n^A(\overline{\text{tr} \rho_A^n}) + \frac{1}{1-n} \overline{\ln(1+x)}, \quad (\text{B7})$$

where the last term, the difference between two averages, would be our main focus. By definition $\bar{x} = 0$, and

$$\overline{x^2} = \frac{\overline{(\text{tr} \rho_A^n)^2}}{\overline{\text{tr} \rho_A^n}^2} - 1. \quad (\text{B8})$$

Via Eq. (B3),

$$\begin{aligned} \rho_A^n &= \sum_{i_1, j_1, k_1} |E_{i_1}\rangle \langle E_{j_1}| C_{i_1 k_1} C_{j_1 k_1}^* \sum_{i_2, j_2, k_2} |E_{i_2}\rangle \langle E_{j_2}| C_{i_2 k_2} C_{j_2 k_2}^* \cdots \\ &\times \sum_{i_n, j_n, k_n} |E_{i_n}\rangle \langle E_{j_n}| C_{i_n k_n} C_{j_n k_n}^*. \end{aligned} \quad (\text{B9})$$

By taking the trace of the above formula, we get

$$\begin{aligned} \text{tr} \rho_A^n &= \sum_{i_1, j_1, k_1} \sum_{i_2, j_2, k_2} \cdots \sum_{i_n, j_n, k_n} \delta_{j_1, i_2} \delta_{j_2, i_3} \cdots \\ &\delta_{j_n, i_1} C_{i_1 k_1} C_{j_1 k_1}^* C_{i_2 k_2} C_{j_2 k_2}^* \cdots C_{i_n k_n} C_{j_n k_n}^*. \end{aligned} \quad (\text{B10})$$

Now we are going to calculate the $2n$ point correlation function, which contains $n!$ terms:

$$\begin{aligned} &\overline{C_{i_1 k_1} C_{j_1 k_1}^* C_{i_2 k_2} C_{j_2 k_2}^* \cdots C_{i_n k_n} C_{j_n k_n}^*} \\ &= \overline{C_{i_1 k_1} C_{j_1 k_1}^* \cdots C_{i_n k_n} C_{j_n k_n}^*} \\ &+ \text{all the other possible pairings.} \end{aligned} \quad (\text{B11})$$

Note that the above equality is only true when the dimension of the restricted Hilbert space $N \rightarrow \infty$ with n being finite such that Wick's theorem can hold. When we sum all the indices to calculate $\text{Tr} \rho_A^n$, the term with the maximal number of summation for the state in $\mathcal{H}_{\bar{A}}$ (labeled by k) will exponentially dominate all the other terms. Looking back to Eq. (B11), only first term contains no delta function constraint for k , and thus

$$\begin{aligned} \overline{\text{tr} \rho_A^n} &= \sum_{i_1, j_1, k_1} \sum_{i_2, j_2, k_2} \cdots \\ &\times \sum_{i_n, j_n, k_n} \left[\delta_{j_1, i_2} \delta_{j_2, i_3} \cdots \delta_{j_n, i_1} \frac{1}{N^n} \delta_{i_1, j_1} \cdots \delta_{i_n, j_n} + \cdots \right] \\ &= \frac{1}{N^n} \sum_i \sum_{k_1, \dots, k_n} \delta_{E_i^A + E_{k_1}^{\bar{A}}, E} \cdots \delta_{E_i^A + E_{k_n}^{\bar{A}}, E} + \cdots \\ &= \frac{\sum_{E_A} e^{S_A^M(E_A) + n S_{\bar{A}}^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_{\bar{A}}^M(E-E_A)} \right]^n} [1 + O(e^{-\alpha_1 V})], \end{aligned} \quad (\text{B12})$$

which gives

$$\overline{\text{tr} \rho_A^n}^2 = \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + n S_{\bar{A}}^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_{\bar{A}}^M(E-E_A)} \right]^n} \right]^2 [1 + O(e^{-\alpha_2 V})] \quad (\text{B13})$$

where α_1 and α_2 are positive order 1 constants. A similar calculation shows

$$\overline{(\text{tr} \rho_A^n)^2} = \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + n S_{\bar{A}}^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A) + S_{\bar{A}}^M(E-E_A)} \right]^n} \right]^2 [1 + O(e^{-\alpha_3 V})]. \quad (\text{B14})$$

Plugging Eqs. (B14) and (B13) into Eq. (B8),

$$\overline{x^2} = O(e^{-\alpha V}), \quad (\text{B15})$$

where α is a positive order 1 constant. This means that in thermodynamic limit $V \rightarrow \infty$, there is no fluctuation of x , and the precise statement is given by

$$\text{Prob}(|x| \geq \varepsilon) \leq \frac{\overline{x^2}}{\varepsilon^2} \quad (\text{B16})$$

via Chebyshev's inequality, and thus there does not exist x with finite distance away from zero in thermodynamics limit ($V \rightarrow \infty$), and an immediate consequence is that

$$\left| S_n^A(\overline{\text{tr} \rho_A^n}) - S_{n,\text{avg}}^A \right| = \frac{1}{1-n} \overline{\ln(1+x)} = O(e^{-\alpha V}) \quad (\text{B17})$$

and thus the difference between these two averages decreases exponentially in volume.

APPENDIX C: SECOND RENYI ENTROPY OF AN ERGODIC BIPARTITION (EB) STATE

Here we provide the calculation of the averaged second Renyi entropy of an EB state. From a technical standpoint, the calculations are similar to those in Ref. [15]. Consider an EB state in an energy window $I \equiv (E - \frac{1}{2}\Delta, E + \frac{1}{2}\Delta)$,

$$|E\rangle = \sum_{i,j} C_{ij} |E_i^A, E_j^{\bar{A}}\rangle, \quad (\text{C1})$$

where $\{C_{ij}\}$ is chosen from the probability distribution function,

$$P(\{C_{ij}\}) \propto \delta \left(1 - \sum_{ij} |C_{ij}|^2 \right) \prod_{i,j} \delta(E_i^A + E_j^{\bar{A}} - E). \quad (\text{C2})$$

Note that the first index i in C_{ij} labels the state in A while the second index j labels the states in \bar{A} . Now we can calculate the reduced density matrix of A :

$$\rho_A = \text{tr}_{\bar{A}} |E\rangle \langle E| = \sum_{i,i'} |E_i^A\rangle \langle E_{i'}^A| \sum_j C_{ij} C_{i'j}^*, \quad (\text{C3})$$

and ρ_A^2 is

$$\rho_A^2 = \sum_{i,k'} |E_i^A\rangle \langle E_{k'}^A| \sum_{i',j,l} C_{ij} C_{i'j}^* C_{i'l} C_{k'l}^*. \quad (\text{C4})$$

Then it is straightforward to calculate $\text{tr} \rho_A^2$:

$$\text{tr} \rho_A^2 = \sum_{i,j,k,l} C_{ij} C_{kl} C_{il}^* C_{kj}^*, \quad (\text{C5})$$

In order to calculate the average of the second Renyi entropy:

$$\overline{S_2} = -\ln[\overline{\text{tr} \rho_A^2}], \quad (\text{C6})$$

we perform the average for $C_{ij}C_{kl}C_{il}^*C_{kj}^*$ first:

$$\overline{C_{ij}C_{kl}C_{il}^*C_{kj}^*} = \frac{1}{N(N+1)} [\delta_{jl}\delta_{E_i^A+E_j^{\bar{A}},E}\delta_{E_k^A+E_l^{\bar{A}},E} + \delta_{ik}\delta_{E_i^A+E_j^{\bar{A}},E}\delta_{E_l^A+E_k^{\bar{A}},E}], \quad (\text{C7})$$

where N is the dimension of the Hilbert space in the restricted energy window. Next we calculate $\overline{\text{tr} \rho_A^2}$:

$$\begin{aligned} \overline{\text{tr} \rho_A^2} &= \frac{1}{N(N+1)} \left[\sum_{i,j,k} \delta_{E_i^A+E_j^{\bar{A}},E}\delta_{E_k^A+E_l^{\bar{A}},E} + \sum_{i,j,l} \delta_{E_i^A+E_j^{\bar{A}},E}\delta_{E_l^A+E_i^{\bar{A}},E} \right] \\ &= \frac{1}{N(N+1)} \left[\sum_{E_A} e^{2S_A^M(E_A)+S_A^M(E-E_A)} + \sum_{E_{\bar{A}}} e^{2S_{\bar{A}}^M(E_{\bar{A}})+S_{\bar{A}}^M(E-E_{\bar{A}})} \right] \\ &= \frac{1}{N(N+1)} \left[\sum_{E_A} e^{2S_A^M(E_A)+S_A^M(E-E_A)} + e^{S_A^M(E_A)+2S_{\bar{A}}^M(E-E_{\bar{A}})} \right], \end{aligned} \quad (\text{C8})$$

where we make the change of variable for the last term. Note that the above equation is manifestly symmetric between A and \bar{A} . Finally we can derive the second Renyi entropy of an EB state:

$$\overline{S_2} = -\ln \left\{ \frac{1}{N^2} \left[\sum_{E_A} e^{2S_A^M(E_A)+S_A^M(E-E_A)} + e^{S_A^M(E_A)+2S_{\bar{A}}^M(E-E_{\bar{A}})} \right] \right\} = -\ln \left[\frac{\sum_{E_A} e^{2S_A^M(E_A)+S_A^M(E-E_A)} + e^{S_A^M(E_A)+2S_{\bar{A}}^M(E-E_{\bar{A}})}}{\left[\sum_{E_A} e^{S_A^M(E_A)+S_{\bar{A}}^M(E-E_A)} \right]^2} \right], \quad (\text{C9})$$

where we have assumed N is large such that $N+1 \approx N$. Notice that when we take $V_A, V \rightarrow \infty$ with $\frac{V_A}{V} < \frac{1}{2}$, the first term in the numerator can be neglected, and thus

$$\overline{S_2} = -\ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A)+2S_{\bar{A}}^M(E-E_{\bar{A}})}}{\left[\sum_{E_A} e^{S_A^M(E_A)+S_{\bar{A}}^M(E-E_A)} \right]^2} \right]. \quad (\text{C10})$$

APPENDIX D: RENYI ENTROPY S_n OF AN ERGODIC BIPARTITION (EB) STATE

Equation (C3) shows the reduced density matrix obtained from an EB state:

$$\rho_A = \sum_{i,j,k} |E_i\rangle \langle E_j| C_{ik} C_{jk}^*, \quad (\text{D1})$$

where as usual the first index of C labels the eigenstate in \mathcal{H}_A and the second index of C labels the eigenstate in $\mathcal{H}_{\bar{A}}$.

Next we can calculate ρ_A^n :

$$\rho_A^n = \sum_{i_1, j_1, k_1} |E_{i_1}\rangle \langle E_{j_1}| C_{i_1 k_1} C_{j_1 k_1}^* \sum_{i_2, j_2, k_2} |E_{i_2}\rangle \langle E_{j_2}| C_{i_2 k_2} C_{j_2 k_2}^* \cdots \sum_{i_n, j_n, k_n} |E_{i_n}\rangle \langle E_{j_n}| C_{i_n k_n} C_{j_n k_n}^*. \quad (\text{D2})$$

By taking the trace of the above formula, we get

$$\text{tr} \rho_A^n = \sum_{i_1, j_1, k_1} \sum_{i_2, j_2, k_2} \cdots \sum_{i_n, j_n, k_n} \delta_{j_1, i_2} \delta_{j_2, i_3} \cdots \delta_{j_n, i_1} C_{i_1 k_1} C_{j_1 k_1}^* C_{i_2 k_2} C_{j_2 k_2}^* \cdots C_{i_n k_n} C_{j_n k_n}^*. \quad (\text{D3})$$

Now we are going to calculate the $2n$ point correlation function, which contains $n!$ terms:

$$\overline{C_{i_1 k_1} C_{j_1 k_1}^* C_{i_2 k_2} C_{j_2 k_2}^* \cdots C_{i_n k_n} C_{j_n k_n}^*} = \overline{C_{i_1 k_1} C_{j_1 k_1}^*} \cdots \overline{C_{i_n k_n} C_{j_n k_n}^*} + \text{all the other possible pairings}. \quad (\text{D4})$$

Note that the above equality is only true when the dimension of the restricted Hilbert space $N \rightarrow \infty$ with n being finite such that Wick's theorem can hold. When we sum all the indices to calculate $\text{tr} \rho_A^n$, the term with the maximal number of summation for the state in $\mathcal{H}_{\bar{A}}$ (labeled by k) will exponentially dominate all the other terms. Looking back to Eq. (D4), only the first term

contains no delta function constraint for k , and thus

$$\begin{aligned}\overline{\text{tr}} \rho_A^n &= \sum_{i_1, j_1, k_1} \sum_{i_2, j_2, k_2} \cdots \sum_{i_n, j_n, k_n} \delta_{j_1, i_2} \delta_{j_2, i_3} \cdots \delta_{j_n, i_1} \frac{1}{N^n} \delta_{i_1, j_1} \cdots \delta_{i_n, j_n} \\ &= \frac{1}{N^n} \sum_i \sum_{k_1, \dots, k_n} \delta_{E_i^A + E_{k_1}^{\bar{A}}, E} \cdots \delta_{E_i^A + E_{k_n}^{\bar{A}}, E} = \frac{1}{N^n} \sum_{E_A} e^{S_A^M(E_A) + nS_A^M(E-E_A)}.\end{aligned}\quad (\text{D5})$$

Finally we can obtain the Renyi entropy of order n in thermodynamic limit:

$$\overline{S}_n = \frac{1}{1-n} \ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + nS_A^M(E-E_A)}}{[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)}]^n} \right], \quad (\text{D6})$$

which is exactly equal to the Renyi entropy obtained from the maximally mixed state. In general we can derive the closed form of the Renyi entropy for arbitrary order without taking the thermodynamic limit by calculating Eq. (D4) explicitly, but for simplicity, we only present the exact result for $n = 3$:

$$\overline{S}_3 = -\frac{1}{2} \ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A) + 3S_A^M(E-E_A)} + 3e^{2S_A^M(E_A) + 2S_A^M(E-E_A)} + e^{S_A^M(E_A) + S_A^M(E-E_A)} + e^{3S_A^M(E_A) + S_A^M(E-E_A)}}{[\sum_{E_A} e^{S_A^M(E_A) + S_A^M(E-E_A)}]^3} \right]. \quad (\text{D7})$$

APPENDIX E: CURVATURE OF RENYI ENTROPY S_n

Here we show the Renyi entropy \overline{S}_n is convex for $n > 1$ while it is concave for $n < 1$. Recall that \overline{S}_n is given by Eq. (20),

$$\overline{S}_n = \frac{V}{1-n} [f s(u_A^*) + n(1-f) s(u_A^*) - n s(u)]. \quad (\text{E1})$$

By taking the derivative of Eq. (E1), we have

$$\begin{aligned}\frac{1-n}{V} \frac{\partial \overline{S}_n}{\partial f} &= s(u_A^*) + f \frac{\partial s(u_A^*)}{\partial u_A^*} \frac{\partial u_A^*}{\partial f} - n s(u_A^*) \\ &\quad + n(1-f) \frac{\partial s(u_A^*)}{\partial u_A^*} \frac{\partial u_A^*}{\partial f}.\end{aligned}\quad (\text{E2})$$

With the saddle point equation (18)

$$\frac{\partial s(u_A^*)}{\partial u_A^*} = n \frac{\partial s(u_A^*)}{\partial u_A^*} \quad (\text{E3})$$

and

$$\frac{\partial u_A^*}{\partial f} = \frac{1}{1-f} \left[u_A^* - u_A^* - f \frac{\partial u_A^*}{\partial f} \right] \quad (\text{E4})$$

obtained by differentiating the energy conservation condition $f u_A^* + (1-f) u_A^* = u$, Equation (E2) can be simplified as

$$\frac{(1-n)}{V} \frac{\partial \overline{S}_n}{\partial f} = s(u_A^*) - n s(u_A^*) + \frac{\partial s(u_A^*)}{\partial u_A^*} (u_A^* - u_A^*). \quad (\text{E5})$$

Now we differentiate Eq. (E5) with respect to f again:

$$\begin{aligned}\frac{(1-n)}{V} \frac{\partial^2 \overline{S}_n}{\partial f^2} &= \frac{\partial s(u_A^*)}{\partial u_A^*} \frac{\partial u_A^*}{\partial f} - n \frac{\partial s(u_A^*)}{\partial u_A^*} \frac{\partial u_A^*}{\partial f} \\ &\quad + \frac{\partial^2 s(u_A^*)}{\partial u_A^{*2}} \frac{\partial u_A^*}{\partial f} (u_A^* - u_A^*) \\ &\quad + \frac{\partial s(u_A^*)}{\partial u_A^*} \left(\frac{\partial u_A^*}{\partial f} - \frac{\partial u_A^*}{\partial f} \right).\end{aligned}\quad (\text{E6})$$

With Eqs. (E3) and (E4), Eq. (E6) can be simplified:

$$\frac{(1-n)}{V} \frac{\partial^2 \overline{S}_n}{\partial f^2} = \frac{\partial^2 s(u_A^*)}{\partial u_A^{*2}} \frac{\partial u_A^*}{\partial f} (u_A^* - u_A^*). \quad (\text{E7})$$

Now let's study the sign of the right-hand side. The first quantity $s''(u_A^*)$ is always negative due to the concavity of microcanonical entropy. The sign of the last quantity $u_A^* - u_A^*$ can also be shown via the concavity of microcanonical entropy and the saddle point equation (E3),

$$\text{sgn}(u_A^* - u_A^*) = \begin{cases} \text{sgn}(n-1) & \text{for } \beta > 0 \\ -\text{sgn}(n-1) & \text{for } \beta < 0 \end{cases}, \quad (\text{E8})$$

where $\beta \equiv \frac{\partial s(u)}{\partial u}$. See Fig. 14 for a graphical illustration.

As for the sign of the quantity in the middle $\frac{\partial u_A^*}{\partial f}$, we need to differentiate the saddle point equation (E3) with

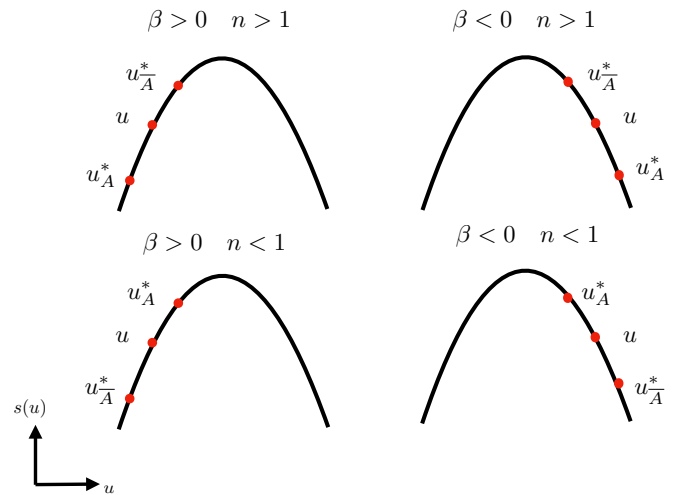


FIG. 14. Allowed relative positions of the energies u , u_A^* and u_A^* that solve Eq. (18). Note that the concavity of $s(u)$ curve, imposed by the non-negative value of specific heat, plays a crucial role.

respect to f :

$$\frac{\partial^2 s(u_A^*)}{\partial u_A^{*2}} \frac{\partial u_A^*}{\partial f} = n \frac{\partial^2 s(u_A^*)}{\partial u_A^{*2}} \frac{\partial u_A^*}{\partial f}. \quad (\text{E9})$$

This implies $\frac{\partial u_A^*}{\partial f}$ and $\frac{\partial u_{\bar{A}}^*}{\partial f}$ have the same sign. Combining this fact with the energy conservation condition Eq. (E4), we have

$$\text{sgn}\left(\frac{\partial u_A^*}{\partial f}\right) = \begin{cases} \text{sgn}(n-1) & \text{for } \beta > 0 \\ -\text{sgn}(n-1) & \text{for } \beta < 0. \end{cases} \quad (\text{E10})$$

Finally by combining Eqs. (E7), (E8), and (E10), and the concavity of the microcanonical entropy, we obtain the final result,

$$\frac{\partial^2 \bar{S}_n}{\partial f^2} > 0 \quad \text{for } n > 1, \quad \frac{\partial^2 \bar{S}_n}{\partial f^2} < 0 \quad \text{for } n < 1, \quad (\text{E11})$$

for all β and $f = V_A/V$.

APPENDIX F: RENYI ENTROPY FOR A SYSTEM WITH GAUSSIAN DENSITY OF STATES

1. Second Renyi entropy

Suppose that the probability density of finding a state with energy E takes the form

$$P(E) = \frac{1}{\sqrt{2\pi V}} e^{-E^2/2V}, \quad (\text{F1})$$

we can then derive the density of state by multiplying the total number of states in the Hilbert space:

$$D(E) \sim 2^V e^{-E^2/2V} = e^{V[\ln 2 - (1/2)(\frac{E}{V})^2]}, \quad (\text{F2})$$

which implies the microcanonical entropy density s is

$$s = \ln 2 - \frac{1}{2}u^2 \quad (\text{F3})$$

with u denoting the energy density. Also we can define the inverse temperature β ,

$$\beta = \frac{\partial s}{\partial u} = -u. \quad (\text{F4})$$

Given Eqs. (F2) or (F3), we can then calculate the number of states in A and \bar{A} with energy E_A and $E_{\bar{A}}$ respectively:

$$e^{S_A(E_A)} = 2^{V_A} P_A(E_A) \Delta = 2^{V_A} \frac{1}{\sqrt{2\pi V_A}} e^{-E_A^2/2V_A} \Delta, \quad (\text{F5})$$

$$e^{S_{\bar{A}}(E-E_A)} = 2^{V_{\bar{A}}} P_{\bar{A}}(E_{\bar{A}}) \Delta = 2^{V_{\bar{A}}} \frac{1}{\sqrt{2\pi V_{\bar{A}}}} e^{-E_{\bar{A}}^2/2V_{\bar{A}}} \Delta, \quad (\text{F6})$$

where Δ is the width of the energy window. First we calculate

$$\begin{aligned} \sum_{E_A} e^{S_A(E_A)} e^{S_{\bar{A}}(E-E_A)} &= \frac{2^{V_A+V_{\bar{A}}}}{\sqrt{4\pi^2 V_A V_{\bar{A}}}} \sum_{E_A} \Delta^2 e^{-E_A^2/2V_A - (E-E_A)^2/2V_{\bar{A}}} \\ &= \frac{2^{V_A+V_{\bar{A}}}}{\sqrt{\pi^2 V_A V_{\bar{A}}}} \Delta e^{-E^2/V} \sqrt{\frac{\pi}{\frac{1}{2V_A} + \frac{1}{2V_{\bar{A}}}}} \\ &= \frac{2^V}{\sqrt{2\pi V}} \Delta e^{-E^2/2V}, \end{aligned} \quad (\text{F7})$$

where we approximate $\sum_{E_A} \Delta$ by the continuous integral $\int dE_A$ and evaluate the Gaussian integral in the expression.

The other quantity we need to evaluate is

$$\begin{aligned} \sum_{E_A} e^{S_A(E_A)} e^{2S_{\bar{A}}(E-E_A)} &= \frac{2^{V_A+2V_{\bar{A}}}}{\sqrt{8\pi^3 V_A V_{\bar{A}}^2}} \sum_{E_A} \Delta^3 e^{-E_A^2/2V_A - (E-E_A)^2/V_{\bar{A}}} \\ &= \frac{2^{V_A+2V_{\bar{A}}}}{2\pi \sqrt{(2V_A + V_{\bar{A}})V_{\bar{A}}}} \Delta^2 e^{-E^2/(2V_A+V_{\bar{A}})}, \end{aligned} \quad (\text{F8})$$

and we also have

$$\begin{aligned} \sum_{E_A} e^{2S_A(E_A)} e^{S_{\bar{A}}(E-E_A)} &= \frac{2^{2V_A+V_{\bar{A}}}}{\sqrt{8\pi^3 V_A^2 V_{\bar{A}}}} \sum_{E_A} \Delta^3 e^{-E_A^2/V_A - (E-E_A)^2/2V_{\bar{A}}} \\ &= \frac{2^{2V_A+V_{\bar{A}}}}{2\pi \sqrt{(V_A + 2V_{\bar{A}})V_{\bar{A}}}} \Delta^2 e^{-E^2/(V_A+2V_{\bar{A}})}. \end{aligned} \quad (\text{F9})$$

With Eqs. (F7)–(F9), we can get the second Renyi entropy:

$$\begin{aligned} \bar{S}_2 &= -\ln \left[\frac{\sum_{E_A} e^{S_A^M(E_A)+2S_{\bar{A}}^M(E-E_A)} + e^{2S_A^M(E_A)+S_{\bar{A}}^M(E-E_A)}}{\left[\sum_{E_A} e^{S_A^M(E_A)+S_{\bar{A}}^M(E-E_A)} \right]^2} \right] \\ &= -\ln \left[\frac{1}{\sqrt{1-f^2}} e^{-V\gamma(f,u)} + \frac{1}{\sqrt{1-(1-f)^2}} e^{-V\gamma(1-f,u)} \right], \end{aligned} \quad (\text{F10})$$

where $u \equiv \frac{E}{V}$, $f \equiv \frac{V_A}{V}$, and

$$\gamma(f, u) = f \ln 2 - \frac{f}{1+f} u^2. \quad (\text{F11})$$

Notice that the S_2 is manifestly invariant under $f \rightarrow 1-f$, and is universal in the sense that it only depends on the energy density, and is capable of capturing the finite size correction of entanglement Renyi entropy.

In thermodynamic limit $V \rightarrow \infty$ with $f < 1/2$, we can then get

$$\bar{S}_2 = fV \left[\ln 2 - \frac{u^2}{1+f} \right] = fV \left[\ln 2 - \frac{\beta^2}{1+f} \right]. \quad (\text{F12})$$

2. Renyi entropy S_n in the limit $V \rightarrow \infty$

In thermodynamic limit $V \rightarrow \infty$, we can solve for the saddle point equation

$$\frac{\partial s(u_A^*)}{\partial u_A^*} = n \frac{\partial s(u_A^*)}{\partial u_A^*} \quad (\text{F13})$$

with $u_A^* = \frac{u^*}{1-f} - \frac{f}{1-f} u_A^*$, and then plug it in to Eq. (20),

$$\bar{S}_n = \frac{V}{1-n} [f s(u_A^*) + n(1-f) s(u_A^*) - n s(u)],$$

to derive n th Renyi entropy.

First from the saddle point equation, we get

$$u_A^* = n u_A^* = n \left(\frac{u}{1-f} - \frac{f}{1-f} u_A^* \right), \quad (\text{F14})$$

from which we can solve for u_A^* :

$$u_A^* = \frac{nu}{1 + (n-1)f}. \quad (\text{F15})$$

Finally we can then calculate the Renyi entropy for arbitrary Renyi index n :

$$\begin{aligned} \bar{S}_n &= \frac{V}{1-n} [fs(u_A^*) + n(1-f)s(u_A^*) - ns(u)] \\ &= \frac{V}{1-n} \left[f \left(\ln 2 - \frac{1}{2}(u_A^*)^2 \right) + n(1-f) \right. \\ &\quad \times \left. \left(\ln 2 - \frac{(u_A^*)^2}{2n^2} \right) - n \left(\ln 2 - \frac{u^2}{2} \right) \right] \\ &= fV \left[\ln 2 - \frac{nu^2}{2[1 + (n-1)f]} \right] \\ &= fV \left[\ln 2 - \frac{n\beta^2}{2[1 + (n-1)f]} \right]. \end{aligned} \quad (\text{F16})$$

When $n \rightarrow 1$, we have

$$\frac{\bar{S}_1}{fV} = \ln 2 - \frac{1}{2}\beta^2, \quad (\text{F17})$$

which is exactly the microcanonical entropy density.

APPENDIX G: SOME MATHEMATICAL RESULTS ON CORRELATION FUNCTIONS FOR RANDOM VECTORS

Suppose that we have a random vector X in \mathbb{R}^M with the probability distribution function being

$$P(\{x_i\}) \propto \delta \left(1 - \sum_{i=1}^M x_i \right)^2, \quad (\text{G1})$$

where $\{x_i\}$ denotes all the components of X . Note the probability measure is invariant under $O(M)$, which immediately indicates that

$$\langle x_i x_j \rangle = 0 \quad \forall i \neq j. \quad (\text{G2})$$

For the case where $i = j$, we recall the constraint:

$$\sum_{i=1}^M x_i^2 = 1. \quad (\text{G3})$$

When we take the average for the equation above, due to the $O(M)$ symmetry, $\langle x_i^2 \rangle = \langle x_j^2 \rangle \quad \forall i, j$, and thus we can get

$$\langle x_i^2 \rangle = \frac{1}{M}. \quad (\text{G4})$$

As for the four point function $\langle x_i x_j x_k x_l \rangle$, by imposing the $O(M)$ symmetry, we can write down the most general form:

$$\langle x_i x_j x_k x_l \rangle = A[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj}]. \quad (\text{G5})$$

Now in order to determine A , we contract the indices k, l first, meaning we set $k = l$ and then perform summation over k :

$$\langle x_i x_j \rangle = A \sum_{k=1}^M [\delta_{ij} + \delta_{ik}\delta_{jk} + \delta_{ik}\delta_{kj}] = A\delta_{ij}[M + 1 + 1]. \quad (\text{G6})$$

Recall that $\langle x_i x_j \rangle = \frac{1}{M}\delta_{ij}$, and thus A can be determined:

$$A = \frac{1}{M(M+2)}, \quad (\text{G7})$$

meaning the four point function is

$$\langle x_i x_j x_k x_l \rangle = \frac{1}{M(M+2)} [\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj}]. \quad (\text{G8})$$

Notice that Eq. (G8) looks very similar to Wick's theorem, but actually it is not:

$$\begin{aligned} \langle x_i x_j x_k x_l \rangle &= \frac{1}{M(M+2)} [\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj}] \\ &\neq \frac{1}{M^2} [\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj}] \\ &= \langle x_i x_j \rangle \langle x_k x_l \rangle + \langle x_i x_k \rangle \langle x_j x_l \rangle + \langle x_i x_l \rangle \langle x_k x_j \rangle. \end{aligned} \quad (\text{G9})$$

However we can notice that when we take $M \rightarrow \infty$, the difference between these two approaches is zero! This is not a coincidence since when we randomly pick a vector from \mathbb{R}^M with the only constraint being the magnitude of the vector and M is large, we can show that the probability distribution function for $\{x_i | i = 1, 2, \dots, s\}$ is Gaussian for $s \ll M$:

$$\begin{aligned} P(x_1, x_2, \dots, x_s) &= \prod_{i=s+1}^M \int_{-\infty}^{\infty} dx_i P(x_1, x_2, \dots, x_M) \\ &= \prod_{i=s+1}^M \int_{-\infty}^{\infty} dx_i \delta \left(1 - \sum_{i=1}^s x_i^2 - \sum_{i=s+1}^M x_i^2 \right) \\ &\propto \left[1 - \sum_{i=1}^s x_i^2 \right]^{(M-s-1)/2}, \end{aligned} \quad (\text{G10})$$

where we used fact that the $M-s$ dimensional integral is proportional to the surface area of the $M-s$ dimensional ball with radius $R = \sqrt{1 - \sum_{i=1}^s x_i^2}$. Then

$$\begin{aligned} P(x_1, x_2, \dots, x_s) &\sim \left[1 - \sum_{i=1}^s x_i^2 \right]^{(N-s-1)/2} \\ &\sim \left[1 - \frac{1}{N\sigma^2} \sum_{i=1}^s x_i^2 \right]^{N/2} \sim e^{-\sum_{i=1}^s x_i^2 / 2\sigma^2}, \end{aligned} \quad (\text{G11})$$

where the variance $\sigma^2 = \frac{1}{N}$. Therefore, the probability distribution function of the small number of degrees of freedom is indeed a Gaussian! Also note that the derivation above is just the standard derivation from microcanonical ensemble to canonical ensemble. For example, consider M particles in a box with total energy being E ; in a microcanonical ensemble we can write down the probability distribution for momenta $\{p_i\}$:

$$P(\{p_i\}) \propto \delta \left(E - \sum_{i=1}^M \frac{p_i^2}{2m} \right), \quad (\text{G12})$$

where we consider kinetic energy only for simplicity. Then if we look at the probability function for a small numbers of particles, we can derive the Boltzmann distribution for those particles via exactly the same calculation as above, which is indeed a Gaussian in momenta.

1. Correlation functions for a random state without imposing any constraint

Given a Hilbert space $\mathcal{H} = \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\overline{\mathcal{A}}}$ with $\text{Dim}(\mathcal{H}) \equiv N$, suppose we pick a state

$$|\psi\rangle = \sum_{i,j} C_{ij} |E_i^A, E_j^{\overline{A}}\rangle, \quad (\text{G13})$$

where $\{C_{ij}\}$ is chosen from the probability distribution function

$$P(\{C_{ij}\}) \propto \delta \left(1 - \sum_{ij} |C_{ij}|^2 \right) \quad (\text{G14})$$

with $i = 1, 2, \dots, \text{Dim}(\mathcal{H}_{\mathcal{A}})$ and $i = 1, 2, \dots, \text{Dim}(\mathcal{H}_{\overline{\mathcal{A}}})$ respectively. Since $C_{ij} = u_{ij} + iv_{ij}$, a random pure state is equivalent to a vector in \mathbb{R}^M ($M = 2N$) with the length of the vector being 1, meaning it can be regarded as a point on S^{M-1} with the probability measure

$$P(\{u_{ij}\}, \{v_{ij}\}) \propto \delta \left(1 - \sum_{ij} u_{ij}^2 - \sum_{ij} v_{ij}^2 \right). \quad (\text{G15})$$

We may want to calculate the two point function:

$$\begin{aligned} \langle C_{ij} C_{kl} \rangle &= \langle (u_{ij} + iv_{ij})(u_{kl} + iv_{kl}) \rangle \\ &= \langle u_{ij} u_{kl} \rangle - \langle v_{ij} v_{kl} \rangle + i \langle u_{ij} v_{kl} \rangle + i \langle v_{ij} u_{kl} \rangle \\ &= \langle u_{ij} u_{kl} \rangle - \langle v_{ij} v_{kl} \rangle, \end{aligned} \quad (\text{G16})$$

where the last two terms vanish since u_{ij} and v_{kl} are different components $\forall i, j, k, l$ of a vector in \mathbb{R}^M . On the other hand,

$$\langle u_{ij} u_{kl} \rangle = \langle u_{ij} u_{kl} \rangle = \frac{1}{M} \delta_{ik} \delta_{jl}, \quad (\text{G17})$$

and thus we conclude

$$\langle C_{ij} C_{kl} \rangle = 0 \quad \forall i, j, k, l. \quad (\text{G18})$$

Let's consider another two point function $\langle C_{ij} C_{kl}^* \rangle$:

$$\begin{aligned} \langle C_{ij} C_{kl}^* \rangle &= \langle (u_{ij} + iv_{ij})(u_{kl} - iv_{kl}) \rangle = \langle u_{ij} u_{kl} \rangle + \langle v_{ij} v_{kl} \rangle \\ &= \frac{2}{M} \delta_{ik} \delta_{jl} = \frac{1}{N} \delta_{ik} \delta_{jl}. \end{aligned} \quad (\text{G19})$$

Note that the above result can also be recognized as

$$\langle C_{ij} C_{kl}^* \rangle = \delta_{kj} \delta_{il} \langle |C_{ij}|^2 \rangle = \frac{1}{N} \delta_{ik} \delta_{jl}. \quad (\text{G20})$$

The lesson here is that C_{ij} is only correlated with its conjugate counterpart.

We can also consider the four point function:

$$\begin{aligned} \langle C_{ij} C_{kl} C_{mn}^* C_{pq}^* \rangle &= \langle (u_{ij} + iv_{ij})(u_{kl} + iv_{kl}) \\ &\quad \times (u_{mn} - iv_{mn})(u_{pq} - iv_{pq}) \rangle. \end{aligned} \quad (\text{G21})$$

There are 16 terms in the expansion, but the terms with an odd number of u vanish. Thus,

$$\begin{aligned} \langle C_{ij} C_{kl} C_{mn}^* C_{pq}^* \rangle &= \langle u_{ij} u_{kl} u_{mn} u_{pq} \rangle - \langle u_{ij} u_{kl} v_{mn} v_{pq} \rangle \\ &\quad + \langle u_{ij} u_{mn} v_{kl} v_{pq} \rangle + \langle u_{ij} u_{pq} v_{kl} v_{mn} \rangle \\ &\quad + \langle u_{kl} u_{mn} v_{ij} v_{pq} \rangle + \langle u_{kl} u_{pq} v_{ij} v_{mn} \rangle \\ &\quad - \langle u_{mn} u_{pq} v_{ij} v_{kl} \rangle + \langle v_{ij} v_{kl} v_{mn} v_{pq} \rangle, \end{aligned} \quad (\text{G22})$$

where the first line and the last line correspond to the term with four and zero numbers of u , and the C_2^4 terms in between are from choosing two u and two v . Via Eq. (G8), the first and the last term are

$$\begin{aligned} \langle u_{ij} u_{kl} u_{mn} u_{pq} \rangle &= \langle v_{ij} v_{kl} v_{mn} v_{pq} \rangle \\ &= \frac{1}{M(M+2)} [\delta_{ik} \delta_{jl} \delta_{mp} \delta_{nq} + \delta_{im} \delta_{jn} \delta_{kp} \delta_{lq} \\ &\quad + \delta_{ip} \delta_{jq} \delta_{km} \delta_{ln}], \end{aligned} \quad (\text{G23})$$

while six terms in the middle are

$$\begin{aligned} &-\langle u_{ij} u_{kl} v_{mn} v_{pq} \rangle + \langle u_{ij} u_{mn} v_{kl} v_{pq} \rangle + \langle u_{ij} u_{pq} v_{kl} v_{mn} \rangle \\ &\quad + \langle u_{kl} u_{mn} v_{ij} v_{pq} \rangle + \langle u_{kl} u_{pq} v_{ij} v_{mn} \rangle - \langle u_{mn} u_{pq} v_{ij} v_{kl} \rangle \\ &= \frac{2}{M(M+2)} [\delta_{ik} \delta_{jl} \delta_{mp} \delta_{nq} + \delta_{im} \delta_{jn} \delta_{kp} \delta_{lq} \\ &\quad + \delta_{ip} \delta_{jq} \delta_{km} \delta_{ln}]. \end{aligned} \quad (\text{G24})$$

Combining the result of Eqs. (G23) and (G24), the four point function can be calculated

$$\begin{aligned} \langle C_{ij} C_{kl} C_{mn}^* C_{pq}^* \rangle &= \frac{4}{M(M+2)} [\delta_{im} \delta_{jn} \delta_{kp} \delta_{lq} + \delta_{ip} \delta_{jq} \delta_{km} \delta_{ln}] \\ &= \frac{1}{N(N+1)} [\delta_{im} \delta_{jn} \delta_{kp} \delta_{lq} + \delta_{ip} \delta_{jq} \delta_{km} \delta_{ln}]. \end{aligned} \quad (\text{G25})$$

To check this result, we can calculate $\text{tr} \rho_A^2$ without energy constraint, and we get back to the same answer as in Ref. [33]:

$$\overline{\text{tr} \rho_A^2} = \frac{\text{Dim}(\mathcal{H}_{\mathcal{A}}) + \text{Dim}(\mathcal{H}_{\overline{\mathcal{A}}})}{\text{Dim}(\mathcal{H}_{\mathcal{A}}) \text{Dim}(\mathcal{H}_{\overline{\mathcal{A}}}) + 1}. \quad (\text{G26})$$

From this result we can calculate the second Renyi entropy,

$$\overline{S_2} = -\text{Intr} \rho_A^2 = \text{In}[\text{Dim}(\mathcal{H}_{\mathcal{A}})], \quad (\text{G27})$$

when we take both $\text{Dim}(\mathcal{H}_{\mathcal{A}})$ and $\text{Dim}(\mathcal{H}_{\overline{\mathcal{A}}})$ to infinity while the ratio $\text{Dim}(\mathcal{H}_{\mathcal{A}})/\text{Dim}(\mathcal{H}_{\overline{\mathcal{A}}}) < 1$.

Via Jensen's inequality, we have

$$\overline{S_2} = \text{In}[\text{Dim}(\mathcal{H}_{\mathcal{A}})] \leq \overline{S_1} \leq \text{In}[\text{Dim}(\mathcal{H}_{\mathcal{A}})] \quad (\text{G28})$$

and thus the entanglement entropy $\overline{S_1}$ is also maximal:

$$\overline{S_1} = \text{In}[\text{Dim}(\mathcal{H}_{\mathcal{A}})], \quad (\text{G29})$$

which is the answer from Page's calculation [32].

2. Correlation functions for a random state at a fixed energy

Consider a pure state in a small energy window with energy E :

$$|\psi\rangle = \sum_{i,j} C_{ij} |E_i^A, E_j^{\bar{A}}\rangle, \quad (\text{G30})$$

where $\{C_{ij}\}$ is chosen from the probability distribution function

$$P(\{C_{ij}\}) \propto \delta\left(1 - \sum_{ij} |C_{ij}|^2\right) \prod_{i,j} \delta(E_i^A + E_j^{\bar{A}} - E), \quad (\text{G31})$$

with $i = 1, 2, \dots, \text{Dim}(\mathcal{H}_{\mathcal{A}})$ and $i = 1, 2, \dots, \text{Dim}(\mathcal{H}_{\bar{\mathcal{A}}})$ respectively. Due to the energy conservation, the two point function will be

$$\langle C_{ij} C_{kl}^* \rangle = \frac{1}{N} \delta_{ik} \delta_{jl} \delta_{E_i^A + E_j^{\bar{A}}, E}, \quad (\text{G32})$$

and the four point function is

$$\langle C_{ij} C_{kl} C_{mn}^* C_{pq}^* \rangle = \frac{1}{N(N+1)} \left[\delta_{im} \delta_{jn} \delta_{kp} \delta_{lq} \delta_{E_i^A + E_j^{\bar{A}}, E} \delta_{E_k^A + E_l^{\bar{A}}, E} + \delta_{ip} \delta_{jq} \delta_{km} \delta_{ln} \delta_{E_i^A + E_j^{\bar{A}}, E} \delta_{E_k^A + E_l^{\bar{A}}, E} \right]. \quad (\text{G33})$$

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