Entanglement and the sign structure of quantum states

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Many-body quantum eigenstates of generic Hamiltonians at finite-energy density typically satisfy the "volume law" of entanglement entropy: the von Neumann entanglement entropy and the Renyi entropies for a subregion scale in proportion to its volume. Here we provide a connection between the volume law and the sign structure of eigenstates. In particular, we ask the following question: Can a positive wave function support a volume law entanglement? Remarkably, we find that a typical random *positive* wave function exhibits a *constant law* for Renyi entanglement entropies S_n for $n > 1$, despite arbitrary large-amplitude fluctuations. We also provide evidence that the modulus of the finite-energy density eigenstates of generic local Hamiltonians shows similar behavior.

I. INTRODUCTION

The intricate sign structure of quantum states plays an important role in fields as disparate as quantum chaos [1,2], quantum Monte Carlo simulations [3,4], and semiclassical quantum mechanics [5]. In this paper, we point out that the sign structure is also important for understanding the qualitative behavior of entanglement entropy in finite-energy density eigenstates of a generic quantum many-body system.

In sharp contrast to the celebrated "area-law" scaling in the quantum ground states for the von Neumann entanglement entropy S_{vN} [6,7], and the Renyi entanglement entropies S_n with $S_{vN}, S_n \sim \ell_A^{d-1}$ in d spatial dimensions, the finite-energy density eigenstates instead typically satisfy a "volume law" scaling, $S_{vN}, S_n \sim \ell_A^d$, where ℓ_A is the linear size of the subregion for which entanglement is being calculated [8–10]. For a generic, nonlocalized [11–15], nonintegrable system, where the equivalence between microcanonical and canonical ensembles is expected to hold true vis-a-vis the "eigenstate thermalization hypothesis" (ETH) [16–20], the volume law scaling of entanglement is equivalent to the extensivity of thermal entropy. In particular, in these systems, the von Neumann entanglement entropy S_{vN} of an eigenstate with energy density e equals $s_{thermal}(e)V_A$, where $s_{thermal}(e)$ is the thermal entropy density and $V_A \sim \ell_A^d$ is the volume of region A. In this paper, we ask the following: What feature(s) in a quantum state are responsible for the volume law scaling? We provide evidence that the sign structure of wave functions [21] is essential for obtaining volume law scaling for Renyi entanglement entropies S_n for $n > 1$. In particular, we show that a generic *positive* wave function in the Hilbert space, despite arbitrary large-amplitude fluctuations, typically only shows a *constant law*: $S_n \sim s_n$ for $n > 1$, where s_n are finite positive numbers. We also provide evidence that the same holds true for the modulus of finite-energy density eigenstates of local Hamiltonians.

At a heuristic level, the aforementioned volume law entanglement for excited states results from the random structure of eigenstates at finite-energy density, which necessitates an $O(e^{s_{thermal}\ell_A^d})$ number of eigenvectors to faithfully represent the reduced density matrix for a region of size ℓ_A, where $s_{thermal}$ is the corresponding entropy density. This is in contrast to the ground-state wave functions, which typically have a much more "rigid" structure, thus typically requiring a much smaller number $\sim O(e^{\ell_A^{d-1}})$ of eigenvectors. This motivates us to explore the concept of ensemble of wave functions, which will be important for our discussion throughout. Specifically, consider the set of wave functions of the form

$$|\psi\rangle = \sum_C \psi(C) |C\rangle, \tag{1}$$

where $|C\rangle$ is a basis vector in a certain local (i.e., real-space) basis and $\psi(C)$ are picked from a specific random distribution subject to the normalization condition $\sum_C |\psi(C)|^2 = 1$. Given such an ensemble, one may ask the following: What are the average entanglement entropies $\langle S_n\rangle, \langle S_{vN}\rangle$? As shown several decades ago by Lubkin [8], if $\psi(C)$ are random real or random complex numbers with respect to the unitarily invariant Haar measure [i.e., the vector $\vec{\psi}(C)$ is distributed uniformly over a sphere of the size of the total Hilbert space], then $\langle S_{vN}\rangle, \langle S_n\rangle$ are maximal: $\langle S_{vN}\rangle = \langle S_n\rangle = \ln(|\mathcal{H}_A|) \sim V_A$, where $|\mathcal{H}_A|$ is the size of the Hilbert space for region A while $\overline{A}$ denotes the complement of subregion A, and we have assumed that the ratio $\frac{V_A}{V_{\overline{A}}} < 1$ while both $V_A, V_{\overline{A}} \to \infty$. Due to ETH, an eigenstate of a lattice model at "infinite temperature" (i.e., at an energy density e such that $\frac{\partial s_{thermal}}{\partial e} = 0$) also satisfies $S_{vN} = S_n = \ln(|\mathcal{H}_A|) \sim V_A$ and, therefore, in this respect, resembles a typical member of the ensemble in Eq. (1).

In this paper, we develop a relation between random ensembles and entanglement with an eye on the sign structure of many-body eigenstates. Does any arbitrary random ensemble yield a volume law entanglement, or does one require a more specific structure to the states comprising the ensemble? For example, as discussed in Ref. [22], a "sign-random" wave function, where $\psi(C) = \pm 1$ with equal probability, recovers the full infinite-temperature entanglement entropy, $\langle S_n\rangle = \ln(|\mathcal{H}_A|)$, despite no fluctuations in the amplitude $|\psi(C)|$. This motivates us to ask the following: Would a random ensemble where the wave function is allowed to fluctuate in amplitude, but not in its sign, show a volume law entanglement? A naive guess is that this is indeed the case—one can clearly construct wave functions which are positive in a local basis and have volume law S_n for arbitrary n. For example, consider

a "long-range triplet" (LRT) state for a spin-1/2 system: $|\psi_{\mathrm{LRT}}\rangle = \prod_i (|\uparrow\rangle_i|\downarrow\rangle_{j(i)} + |\downarrow\rangle_i|\uparrow\rangle_{j(i)})$, where $j(i)$ denotes the triplet partner of the ith spin and is chosen so that the distance $|i - j(i)|$ is of the order of the total system size for each i. Such a state can be easily demonstrated to have a volume law S_n for all n. Surprisingly, our analysis of random positive ensembles shows that this naive caricature of volume law wave functions is misleading: on average, positive states show a *constant law* Renyi entanglement entropy for Renyi index $n > 1$ whose magnitude does not depend on the size of the Hilbert space in region A. Therefore, states such as $|\psi_{\mathrm{LRT}}\rangle$ which are positive and have a volume law entropy are extremely rare. We also study physical Hamiltonians and find that they also agree with the aforementioned constant law when entanglement is computed for the modulus of finite-energy density eigenstates.

II. AVERAGE ENTANGLEMENT ENTROPY FOR RANDOM POSITIVE ENSEMBLES

In order to understand the role of sign structure in generating entanglement, we ask the following: What is the average entanglement entropy of a wave function which, in a given local basis, has only positive coefficients that are drawn from a specific random distribution? This may seem an ill-motivated question since a physical finite-energy density state (e.g., a finite-energy density eigenstate) will generically not be expandable with positive coefficients in a local basis. Furthermore, even if one restricts oneself to an ensemble of wave functions that have positive coefficients in a local basis, a change of basis will generically not maintain positiveness of the coefficients. However, we find that the analysis of a random ensemble where the coefficients are positive in a fixed, chosen basis will lead to insights that are more generally applicable. We will examine the role of the choice of basis in Sec. III where we study eigenstates of physical Hamiltonians.

Given an ensemble of wave functions, one may define at least three different measures of entanglement, depending on how one performs the averaging:

$$S_n(\langle \rho_A \rangle) = -\frac{1}{n-1} \ln(\mathrm{tr} \langle \rho_A \rangle^n), \qquad (2)$$

$$S_n(\langle \mathrm{tr}\, \rho_A^n \rangle) = -\frac{1}{n-1} \ln\left(\langle \mathrm{tr}\, \rho_A^n \rangle\right), \qquad (3)$$

$$\langle S_n(\rho_A) \rangle = -\frac{1}{n-1} \langle \ln\left(\mathrm{tr}\, \rho_A^n\right) \rangle. \qquad (4)$$

Here, n is any positive real number. Of these three, $\langle S(\rho_A) \rangle$ is the easiest to interpret physically and hardest to access analytically, while $S_n(\langle \rho_A \rangle)$ may seem the least physical, but is the easiest one to calculate. For brevity, we will sometimes denote $\langle S_n(\rho_A) \rangle$ as $\langle S_n \rangle$.

Let us therefore consider a wave function,

$$||\psi|\rangle = \sum_C |\psi(C)| |C\rangle, \qquad (5)$$

where $\{C\}$ spans the Hilbert space, and $\langle \psi | \psi \rangle = 1$. The random coefficients $\psi(C)$ are distributed uniformly on the sphere $S^{|\mathcal{H}_A||\mathcal{H}_{\overline{A}}|-1}$ or $S^{2|\mathcal{H}_A||\mathcal{H}_{\overline{A}}|-1}$, depending on whether $\psi(C)$ are real or complex, with the distinction between the two cases (i.e., real versus complex) being inconsequential for any of

our results. Since the expansion coefficients $|\psi(C)|$ in the basis $|C\rangle$ are positive, we will refer to this ensemble as the "random positive ensemble" (RPE). We will also study a less general case where the coefficients $\psi(C)$ in Eq. (5) are Slater determinants formed out of single-particle plane-wave states, while the corresponding wave vectors are chosen at random from a uniform distribution over a Brillouin zone.

A simple calculation (Appendix A1) shows that in general, $S_n(\langle \rho_A \rangle)$ for the wave function $||\psi|\rangle$ in Eq. (5) is given by

$$
\begin{aligned}
&S_n(\langle \rho_A \rangle) \\
&= \frac{1}{1-n} \ln\left[(|\mathcal{H}_A| - 1)\left(\frac{1-g}{|\mathcal{H}_A|}\right)^n + \left(g + \frac{1-g}{|\mathcal{H}_A|}\right)^n \right],
\end{aligned}
$$
(6)

where $g = \frac{\langle |\psi(C)| \rangle^2}{\langle |\psi(C)|^2 \rangle}$ and $|\mathcal{H}_A|$ denotes the size of the Hilbert space for subregion A. The expression for the von Neumann entropy is obtained by taking the limit $n \to 1$ in the above equation. For ease of presentation, below we will denote $\ln(|\mathcal{H}_A|)$ by ℓ_A^d, where d is the spatial dimension and ℓ_A is proportional to the linear extend of the region A. The actual physical length differs from ℓ_A only by an $O(1)$ multiplicative factor that depends on the size of the local Hilbert space, which we ignore.

Let us consider the two aforementioned cases separately:

(a) *Random positive ensemble* (RPE). As mentioned above, this is the case for a state $|\psi|$, where ψ is an infinite-temperature state which satisfies ETH. A simple calculation (Appendix A2) shows that for this case, the parameter $g = 2/\pi$. This implies that in the asymptotic limit $V, V_A \to \infty$ with $V_A \leqslant V_{\overline{A}}$, one obtains

$$
S_n(\langle \rho_A \rangle) = \begin{cases} \frac{n}{n-1} \ln\left(\frac{\pi}{2}\right) & \text{if } n > 1, \\ \left(1 - \frac{2}{\pi}\right) \ell_A^d & \text{if } n = 1, \\ \ell_A^d & \text{if } n \leqslant 1, \end{cases}
$$
(7)

with $S_1 \equiv S_{\mathrm{vN}}$, the von Neumann entanglement entropy. Thus, all of the Renyi entropies for $n > 1$ satisfy a *constant law*, in sharp contrast to the ensemble of complex or real wave functions which satisfy a volume law with maximal coefficient: $S_n = \ell_A^d$. At the same time, the asymptotic scaling of S_n for $n < 1$ remains exactly the same as the one for the random complex or random real ensemble, while S_{vN} displays a reduced volume law prefactor.

The contrasting behavior for $n > 1$ and $n \leqslant 1$ signals a finite-temperature phase transition in the (averaged) entanglement Hamiltonian, $H_\rho = -\ln(\langle \rho_A \rangle)$, for the positive ensemble. Indeed, $\langle \rho_A \rangle$ has $|\mathcal{H}_A| - 1$ number of degenerate eigenvectors with a rather small eigenvalue of magnitude $\frac{(1-\frac{2}{\pi})}{|\mathcal{H}_A|}$, and a single eigenvector with a large eigenvalue $\frac{2}{\pi} + \frac{(1-\frac{2}{\pi})}{|\mathcal{H}_A|}$ which results in the phase transition at a temperature $1/n = 1$ for the entanglement Hamiltonian (see Appendix A1 for details).

We also calculated the two other measures of average entanglement for the RPE: $S_n(\langle \mathrm{tr}\, \rho_A^n \rangle)$ and the most physically relevant $\langle S_n(\rho_A) \rangle$. As shown analytically in Appendix B, the result for $S(\langle \mathrm{tr}\, \rho_A^n \rangle)$ matches exactly with those for $S_n(\langle \rho_A \rangle)$ in Eq. (7). Finally, we numerically calculate $\langle S_n(\rho_A) \rangle$ for the RPE
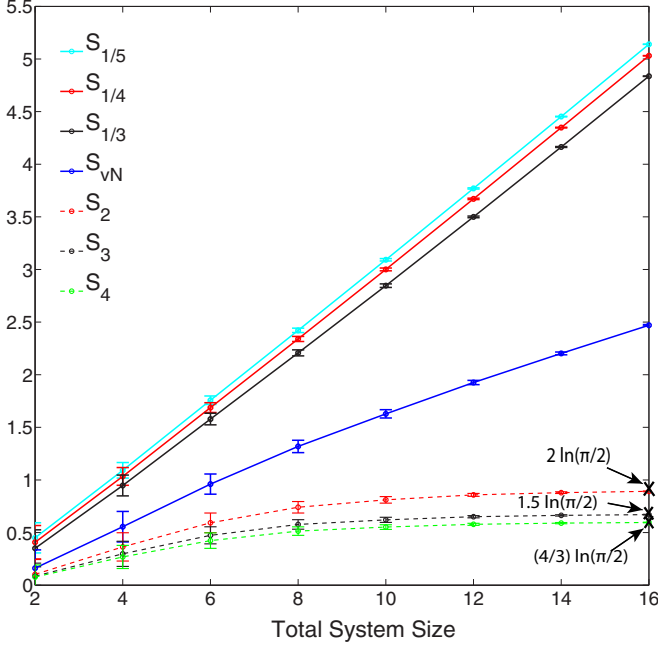
FIG. 1. (Color online) Average entanglement entropies $\langle S_n(\rho_A)\rangle$ corresponding to the random positive ensemble. Region A is half the total system size. $\langle S_n\rangle$ for $n > 1$ ($n \leqslant 1$) shows a constant law (volume law) whose values match the analytical results for $S_n(\langle\rho_A\rangle)$ for the same ensemble (see text for details). The "error bars" shown correspond to the variance of $S_n(\rho_A)$. n increases from top to bottom in the figure.

FIG. 2. (Color online) Renyi entanglement entropy $\langle S_2(\rho_A)\rangle$ corresponding to a wave function $\psi = |\det(M)|$, where M is a matrix whose elements are plane-wave states with random wave vectors (blue solid curve) or a matrix whose elements are ± 1 with equal probability (red dashed curve). In the former case, we find $S_2 \approx \frac{3}{4} \ln(\ell_A)$, while in the latter case, $S_2 \approx \ln(\ell_A)$. The total system size is fixed at 60 sites, while ℓ_A varies from 1 to 20 sites. The error bars reflect the Monte Carlo sampling standard deviation, and not the actual variance of S_2 over the random ensemble.

for a total Hilbert space size $|\mathcal{H}_A||\mathcal{H}_{\bar{A}}|$ up to 2^{16} (see Fig. 1) and find nearly perfect agreement with Eq. (7). Therefore, for the RPE, all three measures of entanglement, $S_n(\langle\rho_A\rangle), S_n(\langle\text{tr } \rho_A^n\rangle)$ and $\langle S_n(\rho_A)\rangle$, agree with one another.

(b) $\psi(C) =$ *random Slater determinant.* In this case, the original wave function is $\psi(C) = \det(e^{i\vec{k}_i \cdot \vec{r}_j(C)})$, up to normalization, where the vector $\vec{k}$ is chosen from a uniform distribution over the one-dimensional (1D) Brillouin zone, and the vector $\vec{r}(C)$ denotes the configuration C in real space (this is equivalent to choosing complex numbers of unit modulus with a uniformly distributed argument). Since ψ corresponds to an integrable system, namely free fermions on a 1D lattice, this case is nongeneric, although still instructive. The results of Refs. [23,24] imply that for a total system size of length L, the equality between the von Neumann entropy and thermal entropy for such a wave function holds only in the limit $\ell_A/L \to 0$, while $L \to \infty$ (unlike the case of RPE where it holds as long as $\ell_A \leqslant L/2$, while $L \to \infty$).

The numerical results for $\langle S_2(\rho_A)\rangle$ corresponding to the wave function $||\psi|\rangle$ in Eq. (5) are shown in Fig. 2. These results are calculated using the quantum Monte Carlo sampling discussed in Ref. [25]. We find that $\langle S_2\rangle \sim \alpha \ln(\ell_A)$, with $\alpha \sim \frac{3}{4}$, which is reminiscent of the $S_n \sim c \ln(\ell_A)$ for $(1+1)$D conformal field theories at zero temperature (c is the central charge), although, in contrast, the logarithmic scaling should hold in all dimensions since there is no notion of locality. Therefore, the positive random Slater determinant does not support a volume law entanglement either, although the entanglement is larger compared to the RPE discussed above.
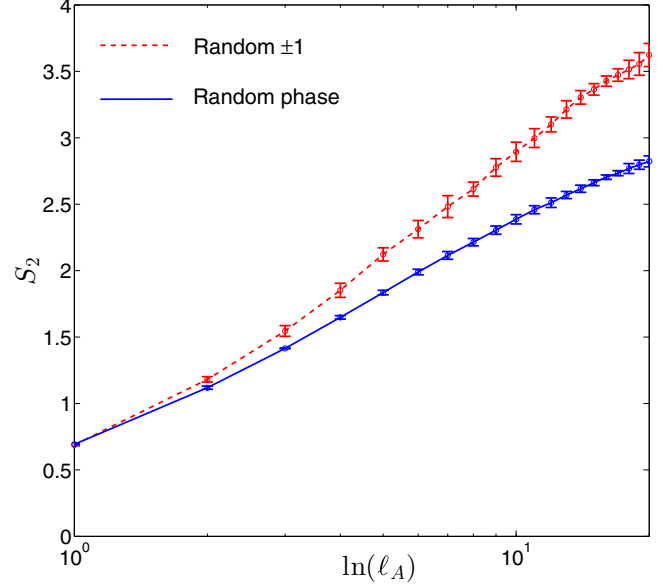
A partial understanding of the logarithmic scaling of $\langle S_2\rangle$ is obtained by analytically calculating $S_n(\langle\rho_A\rangle)$. As is obvious from Eq. (6), $S_n(\langle\rho_A\rangle)$ is independent of ℓ_A and depends only on L, the total system size. Therefore, unlike the case of RPE above where all three measures of entanglement [Eq. (4)] were asymptotically independent of the ratio ℓ_A/L, here we do not expect $S_n(\langle\rho_A\rangle)$ to capture the full ℓ_A/L dependence of $\langle S_n(\rho_A)\rangle$. Nonetheless, it may still capture the correct scaling behavior of $\langle S_n(\rho_A)\rangle$ when $\ell_A = rL$, with r nonzero and fixed, so that there is only one scale in the problem. We have checked that this is indeed the case for a specific ensemble where $\psi(C)$ is a determinant of a matrix with random ± 1 entries. We chose this particular ensemble because the probability distribution function for the modulus of determinant for this ensemble was recently calculated in Ref. [26] (see also Ref. [27]) which allows us to calculate $S_n(\langle\rho_A\rangle)$ analytically via Eq. (6). We find that the parameter g in Eq. (6) scales as $g \sim 1/\sqrt{L}$, in contrast to the RPE where it was a constant (see Appendix A2 for details). Therefore, for this particular ensemble, we find

$$S_n(\langle\rho_A\rangle) = \begin{cases} \ln(\ell_A) & \text{if} \quad n > 1, \\ \ell_A^d & \text{if} \quad n \leqslant 1, \end{cases} \tag{8}$$

when $\ell_A = rL$ with r nonzero and fixed. As already hinted above, we find that the physically more relevant $\langle S_2(\rho_A)\rangle$ shows exactly the same scaling behavior, including the prefactor of unity for the logarithm: $\langle S_2(\rho_A)\rangle = \ln(\ell_A)$ (see Fig. 2). Even though the prefactor of the logarithm is slightly different than the case when $\psi(C) = \det(e^{i\vec{k}_i \cdot \vec{r}_j(C)})$ with $\vec{k}$

random (1 instead of $\frac{3}{4}$), the qualitative behavior evidently remains unchanged. We expect the scaling $\langle S_n \rangle \propto \ln(\ell_A)$, when $n > 1$, and $\langle S_n \rangle \propto \ell_A^d$, when $n \leqslant 1$, to hold in general dimensions, akin to Eq. (8).

In passing, we mention that we also studied a case where only a fraction f of $\vec{k}$ points is chosen randomly while the rest are contiguous. Not surprisingly, as $f \to 0$, the coefficient of the logarithm in the equation $\langle S_2 \rangle \propto \ln(\ell_A)$ for the wave function $|\psi|$ approaches $\frac{1}{4}$, since when all k points are contiguous, the $|\det(e^{i\vec{k}_i \cdot \vec{r}_j})|$ corresponds to the conformally invariant ground state of a 1D hard-core bosonic system [28] whose entanglement entropy is $S_n = \frac{c}{6}(1 + \frac{1}{n})\ln(\ell_A)$ [29,30].

III. RELATION TO PHYSICAL HAMILTONIANS

The results of the previous section indicate that the sign structure is essential to obtain volume law entanglement for the Renyi entropies corresponding to a generic state in the Hilbert space. Here we provide further evidence for this statement by studying eigenstates of a nonintegrable Hamiltonian. Specifically, consider the following Hamiltonian for a spin-1/2 chain:

$$H = \Sigma_i \left(-\sigma_i^z \sigma_{i+1}^z + h_x \sigma_i^x + h_z \sigma_i^z \right), \qquad (9)$$

where the σ's are spin-1/2 Pauli matrices and we impose periodic boundary conditions. We set $h_x = h_z = 1$; we verified that the qualitative features of our results remain true for other parameters as well as long as the Hamiltonian stays nonintegrable.

We diagonalized the above Hamiltonian for system sizes up to 12 sites and investigated eigenstates close to infinite temperature by averaging over 1/8th of the total number of eigenstates around the part of the $S_{vN}(E)$ curve where $\frac{\partial S_{vN}}{\partial E} = 0$, with E being the energy eigenvalue. Akin to the random ensembles studied in the previous section, we focus on the entanglement structure of the modulus of these infinite-temperature eigenstates. We first calculate entanglement in the σ^z basis and discuss the basis dependence in detail below. As shown in Fig. 3, we find clear evidence for a constant law for $\langle S_n \rangle$ when $n > 1$ and volume law for $n < 1$ and for $\langle S_{vN} \rangle$, akin to the RPE. This is in accordance with the fact that the Hamiltonian H in Eq. (9) is nonintegrable and is expected to satisfy ETH. The numerical values of the constant law are also very close to those found for the RPE.

As cautioned earlier, unlike the entanglement for an actual eigenstate ψ, the entanglement corresponding to its modulus $|\psi|$ in general depends on the choice of the local basis. Therefore, we next study the basis dependence of our results, again close to the infinite temperature. In particular, we consider the Hamiltonian

$$H'(\theta) = U^\dagger(\theta) H U(\theta), \qquad (10)$$

where $U(\theta)$ denotes a global rotation of spins around the $\hat{y}$ axis by an angle θ with $H'(\theta = 0) \equiv H$. We obtain the eigenstates ψ_α of $H'(\theta)$ in the σ^z basis and study the entanglement entropies corresponding to $|\psi_\alpha|$. We find that both qualitatively and quantitatively, the results are rather insensitive to the choice of basis. This is not completely surprising—assuming ETH holds, the coefficients $\psi(C)$ corresponding to the wave
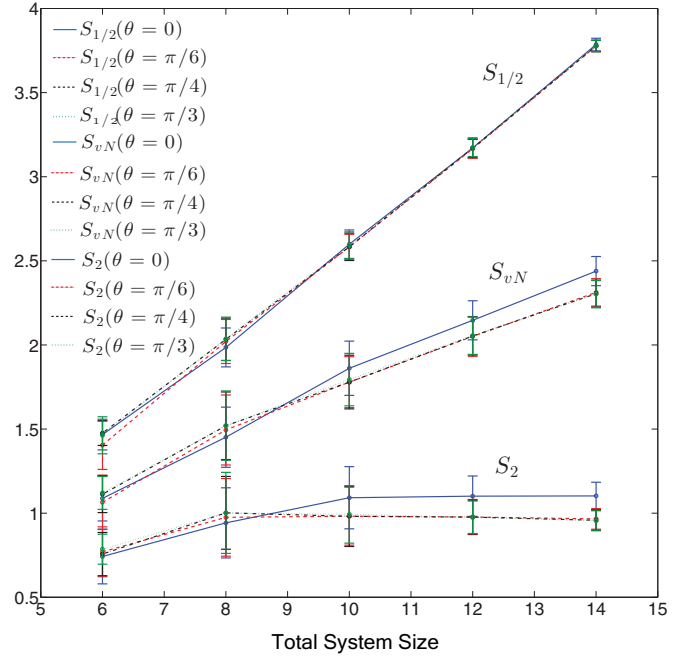

FIG. 3. (Color online) $\langle S_n \rangle$ for several n corresponding to the modulus of the eigenstates of the Hamiltonian in Eq. (9) close to the infinite temperature. The entanglement bipartition divides the total system into two equal halves. The plots for different θ correspond to the global rotation of the local basis by an angle θ along the $\hat{y}$ axis (recall that the entanglement for $|\psi|$ is basis dependent). The qualitative behavior is found to be exactly the same as that for the random positive ensemble (RPE), as in Fig. 1.

functions of H are distributed uniformly over the sphere the size of Hilbert space, and a global rotation does not alter the random distribution.

We also studied the Renyi entropies of wave functions away from the infinite temperature. Our numerics indicate that the constant law for the Renyi entropies continues to hold *away from* infinite temperature. This is also consistent with our quantum Monte Carlo results (not shown) for $\langle S_2(|\psi|) \rangle$, where we chose a variational wave function ψ such that, when expanded in a local basis, its sign structure is random while the amplitudes are not distributed uniformly on the sphere $S^{N_A N_B - 1}$, thus mimicking a finite-temperature state. As $T \to 0$, we expect that one recovers the area-law entanglement for $|\psi|$ generically—this is obvious for bosonic Hamiltonians whose ground state is positive in a local basis, though we expect it to be true more generally (see also Ref. [25]).

IV. CONCLUDING REMARKS

Our main result is that the Renyi entropies $\langle S_n(|\psi|) \rangle$, $n > 1$, do not scale with volume, and instead show a constant law when ψ is either a random wave function, or an eigenstate of a physical Hamiltonian close to infinite temperature. This is related to the fact that the off-diagonal elements of $\langle \rho_A(|\psi|) \rangle$ in any local basis are of the same magnitude as the diagonal elements. In contrast, the off-diagonal elements of $\langle \rho(\psi) \rangle$ are exponentially smaller in subsystem size compared to the diagonal elements leading to volume law Renyi entropies.

A slightly different perspective is obtained by noting that the Renyi entropies S_n for integer $n > 1$ may be decomposed into a "sign" and a "modulus" contribution [25]. For example,

$$S_2(\psi) = S_2(|\psi|) + S_2^{\text{sign}}(\psi), \qquad (11)$$

where $S_2(|\psi|)$ is the Renyi entropy corresponding to $|\psi|$, while $S_2^{\text{sign}}(\psi)$ is defined via

$$e^{-S_2^{\text{sign}}(\psi)} = \sum_{C_1 C_2} \rho_{C_1, C_2} \text{sign}$$
$$\times [\psi(C_1)\psi(C_2)\psi(Sw_A C_1)\psi(Sw_A C_2)], \quad (12)$$

where $\sum_{C_1 C_2}$ denotes the sum over configurations in two copies of the system, $\psi(Sw_A C_1)$ and $\psi(Sw_A C_2)$ are wave functions that are obtained by swapping the field configuration in subregion A for $\psi(C_1)$ with those for $\psi(C_2)$, and ρ_{C_1, C_2} is the probability density defined by $\rho_{C_1, C_2} = |\psi(C_1)||\psi(C_2)||\psi(Sw_A C_1)||\psi(Sw_A C_2)|$. Above, we have assumed that the wave function is real; the corresponding expression for complex wave functions is very similar (see Ref. [25]). At infinite temperature, all configurations are equally likely, and therefore one may approximate $S_2^{\text{sign}}(\psi)$ as $S_2[\text{sign}(\psi)]$. Furthermore, assuming ETH holds, $\text{sign}(\psi)$ will be completely random at infinite temperature and, therefore, $S_2^{\text{sign}}(\psi)$ equals the second Renyi entropy for the "sign-random" wave function discussed in Ref. [22]. For a given real-space basis vector in the Hilbert space, such a wave function takes values of either $+1$ or -1 with equal probability. As shown in Ref. [22], the Renyi entropy for a sign-random wave function is maximal, i.e., when $V_A \leqslant V_{\bar{A}}$, $S_2[\text{sign}(\psi)] = \ln(\mathcal{H}_A) = \ell_A^d$, consistent with our detailed calculations which show that $S_2(|\psi|)$ does not contribute to the volume law entanglement *at all* and, as far as the contribution to the volume law entanglement is concerned, one may equate $S_2(\psi)$ with $S_2^{\text{sign}}(\psi)$. This discussion applies to S_n for any integer $n \geqslant 2$.

As a potential application of our results, one may consider writing down variational wave functions ψ for highly excited states [e.g., the ground state of $(H - E)^2$ would be an excited state of H with energy E]. How might one verify that such wave functions have the correct entanglement structure? For a finite-energy density eigenstate, calculating Renyi entropies $S_n(\psi)$ ($n \geqslant 2$) using Monte Carlo [25] is extremely expensive from a computational standpoint, since one needs to calculate $\text{tr}[\rho_A^n(\psi)]$, which scales as e^{-V_A} where V_A is the volume of region A. On the other hand, our results imply that $S_n(|\psi|)$ is straightforward to calculate since its computational complexity does not scale with the system size at all due to the constant law. Indeed, this is the reason that we were able to perform Monte Carlo calculations for some of the results presented in this paper. Therefore, $S_n(|\psi|)$ can provide an insight into the entanglement structure of such highly excited states while still being computationally accessible.

Our result is reminiscent of the relation between the number of nodes and the kinetic energy in elementary quantum mechanics—typically, more nodes result in higher kinetic energy and, as we argued in the many-body context, higher entanglement entropy as well. This is not too surprising given that entropy and energy are directly related via $dE = T\,dS$ (recall that ETH implies that entanglement entropy equals the thermal entropy). We also note that ground states of bosonic systems are often nodeless in an appropriate local basis, which correlate with the fact that ground states typically do not exhibit volume law scaling of entanglement. Furthermore, as corroborated numerically in Ref. [25], even for systems with a Fermi surface which show a multiplicative logarithm violation of area law, the modulus of the wave function only shows an area-law entanglement. On that note, it will be interesting to explore the differences in the nodal structure for bosons and fermions in the excited states, and their manifestations in the corresponding entanglement structure.

We note that the essential role played by the random sign structure in obtaining the volume law also manifests itself in states that do not satisfy ETH. Consider a many-body localized phase where eigenstates obey an area law for the von Neumann entanglement entropy (and, consequently, area-law Renyi entropies as well). As recently argued, there exist quasilocal unitary bases in which eigenstates can be expanded with positive coefficients [31–35]. This is consistent with the intuition developed in this paper that a volume law Renyi entropy indicates that generically, there exists no local basis in which the wave function can be expanded with positive coefficients. Similar reasoning applies to the area law obeying ground states of systems that satisfy Marshall sign such as the ground states of the Heisenberg antiferromagnet on bipartite lattices.

In this paper, we focused on wave-function ensembles and eigenstates of local Hamiltonians to understand the connection between quantum entanglement and the sign structure of quantum states. It might also be interesting to understand the role of sign structure in quantum dynamics. An elementary insight along this direction follows from comparing the real-time versus the imaginary-time evolution of a quantum state. For a system that satisfies ETH, the real-time evolution of a direct product state will eventually lead to a state whose entanglement entropy equals the thermal entropy [17]. In contrast, the *imaginary*-time evolution corresponds to projection onto the ground-state wave function which would typically satisfy area-law entanglement (up to logarithmic corrections). This is reminiscent of the contrast between the random complex ensemble and the positive random ensemble considered in this paper. We leave further exploration along this direction to the future.

APPENDIX A: DETAILS OF CALCULATIONS FOR $\langle \rho_A \rangle$

1. Entanglement spectrum of $\langle \rho_A \rangle$

The reduced density matrix for the wave function $||\psi\rangle = \sum_C |\psi(C)||C\rangle$, where $\psi(C)$ are chosen from a random

ensemble, is given by

$$
\begin{aligned}
\rho_A(C_A, C_A') &= \frac{\sum_{C_{\overline{A}}} |\psi(C_A, C_{\overline{A}})| |\psi(C_A', C_{\overline{A}})|}{\sum_{C_A, C_{\overline{A}}} |\psi(C_A, C_{\overline{A}})|^2} \\
&= \delta_{C_A, C_A'} \frac{\sum_{C_{\overline{A}}} |\psi(C_A, C_{\overline{A}})|^2}{\sum_{C_A, C_{\overline{A}}} |\psi(C_A, C_{\overline{A}})|^2} \\
&\quad + (1 - \delta_{C_A, C_A'}) \frac{\sum_{C_{\overline{A}}} |\psi(C_A, C_{\overline{A}})| |\psi(C_A', C_{\overline{A}})|}{\sum_{C_A, C_{\overline{A}}} |\psi(C_A, C_{\overline{A}})|^2}.
\end{aligned}
$$

One may now perform an average over the random ensemble to obtain $\langle \rho_A \rangle$:

$$
\langle \rho_A \rangle = \delta_{C_A, C_A'} \frac{1}{|\mathcal{H}_A|} + g \frac{(1 - \delta_{C_A, C_A'})}{|\mathcal{H}_A|}, \tag{A1}
$$

where $g = \frac{\langle |\psi(C)| \rangle^2}{\langle |\psi(C)|^2 \rangle}$ and $|\mathcal{H}_A|$ denotes the size of the Hilbert space in subregion A. The simple structure of $\langle \rho_A \rangle$ readily allows one to diagonalize it: there is a single eigenvector with eigenvalue $\lambda = g + \frac{1-g}{\mathcal{H}_A}$, and $|\mathcal{H}_A| - 1$ degenerate eigenvectors with eigenvalue $\frac{1-g}{\mathcal{H}_A}$. This leads to the result for the Renyi entropies in Eq. (6).

The huge gap in the entanglement spectrum between the single lowest-lying eigenvalue and the rest of the states leads to a finite-temperature phase transition for the entanglement Hamiltonian $H_\rho = -\ln(\langle \rho_A \rangle)$ at unit temperature, as reflected in the qualitative difference between the scaling of the Renyi entropies $S_n(\langle \rho_A \rangle)$ depending on whether $n \leqslant 1$ (volume law) or $n > 1$ (constant law).

2. Calculation of parameter g for random wave-function ensembles

As is evident from the discussion above, the entanglement entropies $S_n(\langle \rho_A \rangle)$ for a particular choice of ensemble depend crucially on the parameter g. Let us consider the two cases discussed in the main text separately.

(a) *Random positive ensemble* (RPE). In this case, $\psi(C)$ is distributed randomly and uniformly on S^N, where $N = 2|\mathcal{H}_A||\mathcal{H}_{\overline{A}}| - 1$ or $|\mathcal{H}_A||\mathcal{H}_{\overline{A}}| - 1$, depending on whether the wave function is complex or real, where the latter case might be relevant to time-reversal invariant systems (for example).

The parameter g is given by

$$
g = \frac{\langle |\vec{\psi}| \rangle^2}{\langle |\vec{\psi}|^2 \rangle}, \tag{A2}
$$

where $\vec{\psi}$ is an N-component vector and the average is taken over a uniform distribution. We employ the following polar coordinates for our calculation:

$$
\begin{aligned}
\psi_1 &= \cos(\phi_1), \\
\psi_2 &= \sin(\phi_1) \cos(\phi_2), \\
\psi_3 &= \sin(\phi_1) \sin(\phi_2) \cos(\phi_3), \\
&\cdots \\
\psi_N &= \sin(\phi_1) \sin(\phi_2) \ldots \sin(\phi_{N-2}) \sin(\phi_{N-1}),
\end{aligned} \tag{A3}
$$

where the angles ϕ_1 to ϕ_{N-2} lie between 0 and π, while ϕ_{N-1} lie between 0 and 2π. To calculate the expression in (A2), it

suffices to restrict ϕ_1 to ϕ_{N-2} to the interval $[0, \pi/2]$ and ϕ_{N-1} to $[0, \pi)$, and replace $|\psi| \to \psi$ since all the coordinates are positive within this restricted domain.

The denominator in Eq. (A2) is calculable trivially: $\langle |\vec{\psi}|^2 \rangle = \frac{1}{N}$, since $\sum_{i=1}^N |\psi_i|^2 = 1$. On the other hand, $\langle |\psi| \rangle$ is given by

$$
\begin{aligned}
\langle |\psi| \rangle &= \frac{\int d\phi_1 \, \cos(\phi_1) \sin^{N-2}(\phi_1)}{\int d\phi_1 \, \sin^{N-2}(\phi_1)} \\
&= \begin{cases} \frac{1}{N-1} \frac{2}{\pi} \frac{(N-2)!!}{(N-3)!!} & \text{if} \quad N \text{ is even,} \\[2ex] \frac{1}{N-1} \frac{(N-2)!!}{(N-3)!!} & \text{if} \quad N \text{ is odd.} \end{cases}
\end{aligned} \tag{A4}
$$

When $N \gg 1$, one may approximate the factorials in Eq. (A4) using Sterling's formula $n! \approx \sqrt{2\pi n} (\frac{n}{e})^n$, and one finds

$$
\langle |\psi| \rangle \approx \sqrt{\frac{2}{\pi N}}, \tag{A5}
$$

irrespective of whether N is even or odd (as one might expect). Combining Eq. (A5) with $\langle |\vec{\psi}|^2 \rangle = \frac{1}{N}$, one finds that $g = 2/\pi$, which leads to Eq. (7) in the main text.

(b) $\psi(C) = \det(M)$ *where M is a matrix with random ± 1 entries.* Recall that to obtain Renyi entropies, one requires the ratio $\frac{\langle |\det(M)| \rangle^2}{\langle |\det(M)|^2 \rangle}$. Clearly, the denominator $\langle |\det(M)|^2 \rangle = L!$, where L is the size of the matrix L (=the total number of particles). One might have naively guessed that the numerator $= \langle |\det(M)| \rangle^2$ scales in the same fashion with L. However, this turns out to be incorrect. The problem of the expectation value of the modulus of a determinant was studied recently in the mathematics literature by Nguyen and Vu in Ref. [26]. They found that $\ln |\det(M)|$ is normal distributed with mean $\ln[\sqrt{(L-1)!}]$, and variance $\sqrt{\frac{\ln(L)}{2}}$. From this, one finds that $\langle |\det(M)| \rangle^2 \sim (L-1)! \sqrt{L}$, and, therefore, the Renyi entropies $S_n(\langle \rho_A \rangle) \sim \ln(L)$ for $n > 1$, while they continue to follow a volume law for $n < 1$ and for the von Neumann entropy [Eq. (8)]. As discussed in the main text, this result yields the correct scaling of $\langle S_n \rangle$ only when ℓ_A / L is a nonzero constant as $L \to \infty$, so that there remains only one length scale in the problem.

APPENDIX B: CALCULATION OF $S_n(\langle \text{tr} \, \rho_A^n \rangle)$

By definition, $\langle \text{tr} \rho_A^n \rangle$ for the wave function $||\psi| \rangle$ in Eq. (5) is given by

$$
\begin{aligned}
\langle \text{tr} \rho_A^n \rangle = \sum_{\{A_i, \overline{A}_i\}} \langle |\psi(C_{A_1} C_{\overline{A}_1})| |\psi(C_{A_2} C_{\overline{A}_1})| \, |\psi(C_{A_2} C_{\overline{A}_2})| \\
\ldots |\psi(C_{A_n} C_{\overline{A}_n})| \, |\psi(C_{A_1} C_{\overline{A}_n})| \rangle.
\end{aligned} \tag{B1}
$$

A bit of thought will convince the reader that the leading contribution to the above expression (in the limit where the size of the Hilbert space is taken to infinity) comes from the terms where all A_i's and $\overline{A}_i$'s are *distinct*. Interestingly, such a contribution does not exist for the average over a random real or complex wave function [8]. This is because if the wave function was allowed to take both positive and negative values, and if all $A_i, \overline{A}_i$ are distinct, then the contributions would cancel

out pairwise. This crucial difference leads to a qualitatively different behavior of entanglement entropy $S_n(\langle \mathrm{tr}\, \rho_A^n \rangle)$ for a positive wave function.

The above average, to the leading order, is

$$\langle \mathrm{tr}\, \rho_A^n \rangle \approx \prod_{i=0}^{n-1} (|\mathcal{H}_A| - i)(|\mathcal{H}_{\overline{A}}| - i) \times \left\langle \prod_{i=1}^{2n} x_i \right\rangle, \quad (B2)$$

where x_i are the first $2n$ Cartesian coordinates of the Euclidean embedding of the unit sphere $S^{|\mathcal{H}_A||\mathcal{H}_{\overline{A}}|-1}$, and we have assumed that the wave function ψ is real. The combinatorial prefactor multiplying $\langle \prod_{i=1}^{2n} x_i \rangle$ can be obtained by imposing the constraint on the expression in Eq. (B1) that all the configurations are distinct. $\langle \prod_{i=1}^{2n} x_i \rangle$ can be calculated conveniently via spherical polar coordinates. One finds

$$\left\langle \prod_{i=1}^{2n} x_i \right\rangle = \left(\frac{2}{\pi}\right)^n \left[\prod_{i=1}^{n} (|\mathcal{H}_A||\mathcal{H}_{\overline{A}}| + 2n - 2i) \right]^{-1}. \quad (B3)$$

Putting everything together, and taking the limit $|\mathcal{H}_A|, |\mathcal{H}_{\overline{A}}| \gg n$, one finds that at the leading order,

$$\langle \mathrm{tr}\, \rho_A^n \rangle \approx \left(\frac{2}{\pi}\right)^n. \quad (B4)$$

Therefore, $S_n(\langle \mathrm{tr}\, \rho_A^n \rangle)$ for n integer $(n > 1)$ is given by

$$S_n\!\left(\langle \mathrm{tr}\, \rho_A^n \rangle\right) = \frac{n}{n-1} \ln\!\left(\frac{\pi}{2}\right), \quad (B5)$$

which precisely matches the results for $S_n(\langle \rho_A \rangle)$ and $\langle S_n(\rho_A) \rangle$ discussed in the main text. Even though we only discussed the case where ψ is real, the above calculation trivially generalizes to the case when ψ is complex, and the answer [Eq. (B5)] remains unchanged.

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