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Universal entanglement of mid-spectrum eigenstates of chaotic local Hamiltonians

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Abstract

In systems governed by chaotic local Hamiltonians, my previous work [7] conjectured the universality of the average entanglement entropy of all eigenstates by proposing an exact formula for its dependence on the subsystem size. In this note, I extend this result to the average entanglement entropy of a constant fraction of eigenstates in the middle of the energy spectrum. The generalized formula is supported by numerical simulations of various chaotic spin chains.

1. Introduction

In systems governed by chaotic local Hamiltonians, my previous work [7] conjectured the universality of eigenstate entanglement by proposing an exact formula for its dependence on the subsystem size. This formula was derived from an analytical argument based on an assumption that characterizes the chaoticity of the system, and is supported by numerical simulations.

For simplicity, Ref. [7] only considered the average entanglement entropy of all eigenstates explicitly. Due to the recent interest [6], in this note I extend the result to the average entanglement entropy of a constant fraction of eigenstates in the middle of the energy spectrum. The extension is straightforward and does not require any essentially new ideas beyond those in Ref. [7].

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For completeness and for the convenience of the reader, definitions and derivations are presented in full so that this note is technically self-contained, although this leads to substantial text overlap with the original paper [7]. It is not necessary to consult Ref. [7] before or during reading this note. However, in this note I do not discuss the conceptual aspects of the work. Such discussions are in Ref. [7].

I recommend related works [14,9,10], which use a similar approach to study other aspects of eigenstate entanglement.

The rest of this note is organized as follows. Section 2 gives basic definitions and a brief review of random-state entanglement. Section 3 presents the main result. Section 4 provides numerical evidence for this analytical result in various chaotic spin chains. The main text of this note should be easy to read, for most of the technical details are deferred to Appendix A.

2. Preliminaries

Definition 1 *(entanglement entropy).* The entanglement entropy of a bipartite pure state ρ_{AB} is defined as the von Neumann entropy

$$S(\rho_A) = -\operatorname{tr}(\rho_A \ln \rho_A) \tag{1}$$

of the reduced density matrix $\rho_A = \operatorname{tr}_B \rho_{AB}$.

Theorem 1 *(conjectured and partially proved by Page [11]; proved in Refs. [4,12,13]). Let ρ_{AB} be a bipartite pure state chosen uniformly at random with respect to the Haar measure. In average,*

$$S(\rho_A) = \sum_{k=d_B+1}^{d_A d_B} \frac{1}{k} - \frac{d_A - 1}{2d_B} = \ln d_A - \frac{d_A}{2d_B} + O(1/d), \tag{2}$$

where $d_A \le d_B$ are the dimensions of subsystems A and B, respectively, and $d = d_A d_B$ is the dimension of the total Hilbert space. For an equal bipartition $d_A = d_B$,

$$S(\rho_A) = \ln d_A - 1/2 + O(1/d). \tag{3}$$

Let $\gamma \approx 0.577216$ be the Euler–Mascheroni constant. The second step of Eq. (2) uses the formula

$$\sum_{k=1}^{d_B} \frac{1}{k} = \ln d_B + \gamma + \frac{1}{2d_B} + O(1/d_B^2). \tag{4}$$

Let $\operatorname{erf} : \mathbb{R} \cup \{\pm\infty\} \to [-1, 1]$ be the error function

$$\operatorname{erf} x := \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, \mathrm{d}t. \tag{5}$$

Let $\operatorname{erf}^{-1} : [-1, 1] \to \mathbb{R} \cup \{\pm\infty\}$ be the inverse error function such that both $\operatorname{erf}^{-1} \circ \operatorname{erf}$ and $\operatorname{erf} \circ \operatorname{erf}^{-1}$ are identity maps.

3. Universal eigenstate entanglement

Consider a chain of N spin-1/2's governed by a local Hamiltonian

$$H = \sum_{i=1}^{N-1} H_i, \tag{6}$$

where H_i represents the nearest-neighbor interaction between spins at positions i and $i+1$. For concreteness, we use open boundary conditions, but our argument also applies to other boundary conditions. Assume without loss of generality that $\operatorname{tr} H_i = 0$ (traceless) so that the mean energy of H is 0. We do not assume translational invariance. In particular, $\|H_i\|$ may be site dependent but should be $\Theta(1)$ for all i.

Suppose that the Hamiltonian (6) is chaotic in a sense to be made precise below. We provide an analytical argument for

Conjecture 1 *(universal eigenstate entanglement). Assume without loss of generality that N is even. Consider the spin chain as a bipartite quantum system $A \otimes B$. Subsystem A consists of spins at positions $1, 2, \ldots, N/2$. For a constant $0 < \nu \le 1$, let Λ be such that H has $\nu 2^N$ eigenvalues in the interval $[-\Lambda, \Lambda]$. The average entanglement entropy of the eigenstates in this energy interval is*

$$\bar{S} = \frac{N-1}{2}\ln 2 + \frac{2(e^{-(\operatorname{erf}^{-1}\nu)^2} - 1)}{\nu\pi} + \frac{(e^{-(\operatorname{erf}^{-1}\nu)^2} + 2\nu - 2)\operatorname{erf}^{-1}\nu}{2\nu\sqrt{\pi}} \tag{7}$$

in the thermodynamic limit $N \to +\infty$.

Remark. It is straightforward to extend Eq. (7) to the case where the subsystem size is an arbitrary constant fraction of the system size.

We split the Hamiltonian (6) into three parts: $H = H_A + H_\partial + H_B$, where $H_{A(B)}$ contains terms acting only on subsystem $A(B)$, and $H_\partial = H_{N/2}$ is the boundary term. Let $\{|j\rangle_A\}_{j=1}^{2^{N/2}}$ and $\{|k\rangle_B\}_{k=1}^{2^{N/2}}$ be complete sets of eigenstates of H_A and H_B with corresponding eigenvalues $\{\epsilon_j\}$ and $\{\varepsilon_k\}$, respectively. Since H_A and H_B are decoupled from each other, product states $\{|j\rangle_A|k\rangle_B\}$ form a complete set of eigenstates of $H_A + H_B$ with eigenvalues $\{\epsilon_j + \varepsilon_k\}$. Due to the presence of H_∂, a (normalized) eigenstate $|\psi\rangle$ of H with eigenvalue E is a superposition

$$|\psi\rangle = \sum_{j,k=1}^{2^{N/2}} c_{jk}|j\rangle_A|k\rangle_B. \tag{8}$$

The locality of H_∂ implies a strong constraint stating that the population of $|j\rangle_A|k\rangle_B$ is significant only when $\epsilon_j + \varepsilon_k$ is close to E.

Lemma 1. *There exist constants $c, \Delta > 0$ such that*

$$\sum_{|\epsilon_j+\varepsilon_k-E|\ge\Lambda} |c_{jk}|^2 \le ce^{-\Lambda/\Delta}. \tag{9}$$

Proof. This is a direct consequence of Theorem 2.3 in Ref. [1]. □

In chaotic systems, we expect

Assumption 1. The expansion (8) of a generic eigenstate $|\psi\rangle$ is a random superposition subject to the constraint (9).

This assumption is consistent with, but goes beyond, the semiclassical approximation Eq. (16) of Ref. [3].

We now show that Assumption 1 implies Conjecture 1. Consider the following simplified setting. Let M_j be the set of computational basis states with j spins up and $N-j$ spins down, and $U_j \in \mathcal{U}(|M_j|) = \mathcal{U}(\binom{N}{j})$ be a Haar-random unitary on span M_j. Define $M'_j = \{U_j|\phi\rangle : \forall|\phi\rangle \in M_j\}$ so that $M := \bigcup_{j=0}^{N} M'_j$ is a complete set of eigenstates of the Hamiltonian

$$H = \sum_{i=1}^{N} \sigma_i^z. \tag{10}$$

The energy of a state in M is defined with respect to this Hamiltonian.

The set M captures the essence of Assumption 1. Every state in M satisfies

$$\sum_{|\epsilon_j+\varepsilon_k-E|\geq 1} |c_{jk}|^2 = 0, \tag{11}$$

which is a hard version of the constraint (9). The random unitary U_j ensures that Eq. (8) is a random superposition. Thus, we establish Conjecture 1 by

Proposition 1. *The average entanglement entropy of the $\nu 2^N$ states in M in the middle of the energy spectrum is given by Eq. (7) in the thermodynamic limit $N \to +\infty$.*

4. Comparison with numerics

In this section, we compare Eq. (7) with the numerical results in the literature [15,5,6]. All these numerical results are obtained by exact diagonalization. They are limited to relatively small system sizes $N \leq 20$ and suffer from non-negligible finite-size effects. Although they cannot confirm Conjecture 1 conclusively, they are quite suggestive: Eq. (7) is supported by numerical simulations of various (not necessarily translation-invariant) chaotic spin chains for various values of ν.

Sometimes an incorrect analytical formula with one or more fitting parameters can fit the numerical data well when the number of data points is limited. We do not need to worry about such false positives here, for Eq. (7) does not contain any fitting parameters.

4.1. $\nu = 1$

The original paper [7] considered the case $\nu = 1$ or the average entanglement entropy of all eigenstates. In this case, Eq. (7) becomes

$$\bar{S} = \frac{N-1}{2}\ln 2 - \frac{2}{\pi} \approx \frac{N}{2}\ln 2 - 0.983193. \tag{12}$$

This is the special case $f = 1/2$ of Eq. (12) in Ref. [7].

Table 1
ΔS, defined by subtracting the right-hand side of Eq. (7) from that of Eq. (3), as a function of ν.

ν	0^+	$1/16$	$1/8$	$1/4$	$1/2$	1
ΔS	0.096574	0.097582	0.100563	0.112324	0.160362	0.483193

Let $\sigma_i^x, \sigma_i^y, \sigma_i^z$ be the Pauli matrices at site i. In the spin-1/2 chain

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + g\sigma_i^x + h\sigma_i^z \tag{13}$$

with $(g, h) = (-1.05, 0.5)$ [2] and $((5+\sqrt{5})/8, (1+\sqrt{5})/4)$ [8], the average entanglement entropy of all eigenstates was calculated up to the system size $N = 18$. The numerical results support Eq. (12). See Fig. 1 of Ref. [7].

4.2. $\nu = 0^+$

In fact, the original paper [7] also presented the result of the case $\nu = 0^+$ or the entanglement entropy of the eigenstates at the mean energy of the Hamiltonian. In this case, Eq. (7) becomes

$$\bar{S} = \frac{N-1}{2}\ln 2 - \frac{1}{4} \approx \frac{N}{2}\ln 2 - 0.596574. \tag{14}$$

This is the special case $J = 0$ of Eq. (35) in Ref. [7], and is slightly less than random-state entanglement (3).[1]

In the spin-1/2 chain (13) with $(g, h) = (0.9045, 0.8090)$, the entanglement entropy of the eigenstate with energy closest to 0 was calculated for the system size $N = 20$ [5]. The numerical result is $10\ln 2 - 0.635769$,[2] which is closer to Eq. (14) than to Eq. (3).

Let $\{h_i\}$ be a set of independent random variables uniformly distributed on the interval $[-1, 1]$. In the spin-1/2 chain

$$H = \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + 0.2\sigma_i^x + h_i\sigma_i^z, \tag{16}$$

the entanglement entropy of an eigenstate with energy close to 0 was calculated for the system size $N = 16$ [15]. The numerical result, averaged over 10 samples of $\{h_i\}$, is $8\ln 2 - 0.5733 \pm 0.0015$, which is closer to Eq. (14) than to Eq. (3).

4.3. $0 < \nu < 1$

Let ΔS be the difference between the right-hand sides of Eqs. (3) and (7). Its values as a function of ν are listed in Table 1.

[1] If the size of the smaller subsystem is a constant $f < 1/2$ fraction of the system size,

$$\bar{S} = fN\ln 2 + \frac{f + \ln(1-f)}{2} \tag{15}$$

in the thermodynamic limit $N \to +\infty$. This is the special case $J = 0$ of Eq. (31) in Ref. [7].

[2] We thank the authors of Ref. [5] for sharing the exact value of the data point at $\beta = 0.0$ and $L_A = 10$ in their Fig. 3.

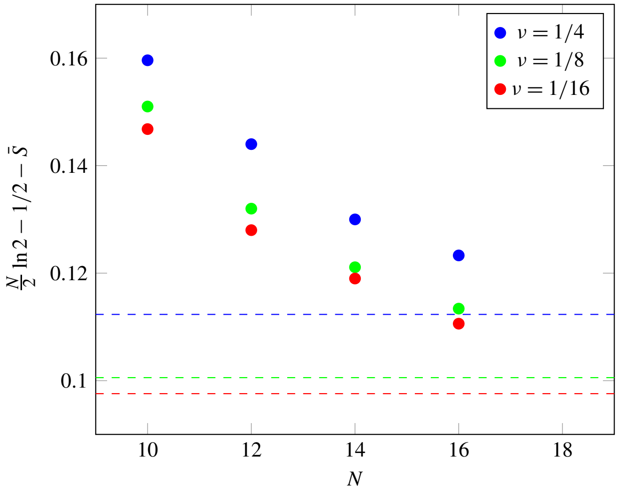

Fig. 1. Difference between random-state entanglement (3) and $\bar{S}$ as a function of the system size N for $\nu = 1/4$ (blue), $1/8$ (green), $1/16$ (red) in the spin chain (17). The dots are numerical results from Fig. 7 of Ref. [6]. The dashed lines are our model-independent theoretical results in the thermodynamic limit (Table 1). Although one cannot conclude whether the dots approach the dashed lines of the same color as $N \to +\infty$, the trend looks promising.

In the spin-$1/2$ chain

$$H = \sum_i 5\sigma_i^x\sigma_{i+1}^x + 15\sigma_i^y\sigma_{i+1}^y + 9\sigma_i^z\sigma_{i+1}^z + 5\sigma_i^x\sigma_{i+2}^x + 15\sigma_i^y\sigma_{i+2}^y + 9\sigma_i^z\sigma_{i+2}^z + 4\sigma_i^x + 16\sigma_i^z, \tag{17}$$

the average entanglement entropy $\bar{S}$ of the $\nu = 1/4$, $1/8$, $1/16$ fraction of eigenstates in the middle of the energy spectrum was calculated up to the system size $N = 16$ [6]. As shown in Fig. 1, the numerical results semi-quantitatively support Eq. (7).

CRediT authorship contribution statement

Yichen Huang: Conceptualization, Formal analysis, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Proof of Proposition 1

Let L_j (R_j) be the set of computational basis states of subsystem A (B) with j spins up and $N/2 - j$ spins down so that

$$|L_j| = |R_j| = \binom{N/2}{j}, \quad M_j = \bigcup_{k=\max\{0,j-N/2\}}^{\min\{N/2,j\}} L_k \times R_{j-k}. \tag{18}$$

Thus, any (normalized) state $|\psi\rangle$ in M'_j can be decomposed as

$$|\psi\rangle = \sum_{k=\max\{0,j-N/2\}}^{\min\{N/2,j\}} c_k|\phi_k\rangle, \tag{19}$$

where $|\phi_k\rangle$ is a normalized state in $\operatorname{span} L_k \otimes \operatorname{span} R_{j-k}$. Let ρ_A and $\sigma_{k,A}$ be the reduced density matrices of $|\psi\rangle$ and $|\phi_k\rangle$ for A, respectively. It is easy to see

$$\rho_A = \bigoplus_{k=\max\{0,j-N/2\}}^{\min\{N/2,j\}} |c_k|^2\sigma_{k,A} \implies S(\rho_A) = \sum_{k=\max\{0,j-N/2\}}^{\min\{N/2,j\}} |c_k|^2 S(\sigma_{k,A}) - |c_k|^2 \ln |c_k|^2. \tag{20}$$

Since $|\psi\rangle$ is a random state in $\operatorname{span} M_j$, each $|\phi_k\rangle$ is a (Haar-)random state in $\operatorname{span} L_k \otimes \operatorname{span} R_{j-k}$. Theorem 1 implies that in average,

$$S(\sigma_{k,A}) = \ln \min\{|L_k|, |R_{j-k}|\} - \frac{\min\{|L_k|, |R_{j-k}|\}}{2\max\{|L_k|, |R_{j-k}|\}}. \tag{21}$$

In average, the population $|c_k|^2$ is proportional to the dimension of $\operatorname{span} L_k \otimes \operatorname{span} R_{j-k}$:

$$|c_k|^2 = |L_k||R_{j-k}|/|M_j|. \tag{22}$$

The deviation of $|c_k|^2$ (from the mean) for a typical state $|\psi\rangle \in \operatorname{span} M_j$ is exponentially small. In the thermodynamic limit, j, k can be promoted to continuous real variables so that $|M_j|, |L_k|$ follow normal distributions with means $N/2$, $N/4$ and variances $N/4$, $N/8$, respectively. Let

$$J := j/\sqrt{N} - \sqrt{N}/2, \quad K := k/\sqrt{N} - \sqrt{N}/4. \tag{23}$$

We have

$$|L_k| = 2^{N/2+1}e^{-4K^2}/\sqrt{\pi N}, \quad |R_{j-k}| = 2^{N/2+1}e^{-4(J-K)^2}/\sqrt{\pi N}, \tag{24}$$

$$|M_j| = 2^{(N+1)/2}e^{-2J^2}/\sqrt{\pi N}, \quad |c_k|^2 = \sqrt{8}e^{2J^2-4K^2-4(J-K)^2}/\sqrt{\pi N}. \tag{25}$$

Consider the case that $j \le N/2$ and $k \le j/2$ (i.e., $J \le 0$ and $K \le J/2$) so that $|L_k| \le |R_{j-k}|$. Hence,

$$S(\sigma_{k,A}) = \left(\frac{N}{2} + 1\right)\ln 2 - \frac{\ln(\pi N)}{2} - 4K^2 - \frac{e^{4J^2-8JK}}{2}. \tag{26}$$

Substituting Eqs. (25), (26) into Eq. (20),

$$
\begin{aligned}
S(\rho_A) &= 2\int_{-\infty}^{j/2} |c_k|^2 S(\sigma_{k,A})\,\mathrm{d}k - \int_{-\infty}^{+\infty} |c_k|^2 \ln|c_k|^2\,\mathrm{d}k \\
&= \left(\frac{N}{2}+1\right)\ln 2 - \frac{\ln(\pi N)}{2} - \frac{1}{4} + J\sqrt{\frac{2}{\pi}} - J^2 - \frac{e^{2J^2}\left(1-\operatorname{erf}(-\sqrt{2}J)\right)}{2} \\
&\quad + \frac{1+\ln(\pi N/8)}{2} \\
&= \frac{N-1}{2}\ln 2 + \frac{1}{4} + J\sqrt{\frac{2}{\pi}} - J^2 - \frac{e^{2J^2}\left(1-\operatorname{erf}(-\sqrt{2}J)\right)}{2}.
\end{aligned}
\tag{27}
$$

This is the average entanglement entropy of a random state in span M_j for $j \le N/2$. For $j > N/2$, Eq. (27) remains valid upon replacing J by $-J$. We determine the energy cutoff Λ such that $\nu 2^N$ states in M have energies in the interval $[-\Lambda, \Lambda]$:

$$
2\sqrt{\frac{2}{\pi}}\int_{-\Lambda}^{0} e^{-2J^2}\,\mathrm{d}J = \nu \implies \Lambda = \frac{\operatorname{erf}^{-1}\nu}{\sqrt{2}}.
\tag{28}
$$

Averaging over these $\nu 2^N$ states in M,

$$
\begin{aligned}
\bar{S} &= \frac{N-1}{2}\ln 2 + \frac{2}{\nu}\sqrt{\frac{2}{\pi}}\int_{-\Lambda}^{0} e^{-2J^2}\left(\frac{1}{4} + J\sqrt{\frac{2}{\pi}} - J^2 - \frac{e^{2J^2}\left(1-\operatorname{erf}(-\sqrt{2}J)\right)}{2}\right)\mathrm{d}J \\
&= \frac{N-1}{2}\ln 2 + \frac{2(e^{-(\operatorname{erf}^{-1}\nu)^2}-1)}{\nu\pi} + \frac{(e^{-(\operatorname{erf}^{-1}\nu)^2}+2\nu-2)\operatorname{erf}^{-1}\nu}{2\nu\sqrt{\pi}}.
\end{aligned}
\tag{29}
$$

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