arXiv:1708.08607v1 [quant-ph] 29 Aug 2017

Universal eigenstate entanglement of chaotic local Hamiltonians

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April 6, 2018

Abstract

In systems governed by "chaotic" local Hamiltonians, we conjecture the universality of eigenstate entanglement (defined as the average entanglement entropy of all eigenstates) by proposing an exact formula for its dependence on the subsystem size. This formula is derived from an analytical argument based on a plausible assumption, and is supported by numerical simulations.

1 Introduction

Entanglement, a concept of quantum information theory, has been widely used in condensed matter and statistical physics to provide insights beyond those obtained via "conventional" quantities. For ground states of local Hamiltonians, it characterizes quantum criticality [39, 26, 7, 8] and topological order [25, 27, 9, 22]. The scaling of entanglement [14] reflects physical properties (e.g., correlation decay [5, 6, 18]) and is quantitatively related to the classical simulability of quantum many-body systems [38, 34, 29, 17, 20].

Besides ground states, it is also important to understand the entanglement of excited eigenstates. A lot of progress has been made for various classes of local Hamiltonians. In many-body localized systems, one expects an area law in the sense that eigenstate entanglement between a subsystem and its complement scales as the boundary (area) rather than the volume of the subsystem [4, 36, 23]. In any translation-invariant free-fermion system, the average entanglement entropy of all eigenstates obeys a volume law with non-maximal coefficients due to the integrability of the model [40].

Here we consider "chaotic" quantum many-body systems. We are not able to specify the precise meaning of being chaotic, for there is no unique definition of quantum chaos. Intuitively, this class of systems should include non-integrable models in which energy is the only local conserved quantity. For such systems, there are some widely accepted opinions [12, 33, 13, 10, 16]:

1. For a subsystem smaller than half of the system size, the bipartite entanglement entropy of an eigenstate is the thermodynamic entropy of the thermal state with the same energy density.

2. For entanglement properties, an eigenstate at the mean energy density (of the Hamiltonian) is indistinguishable from a random (pure) state.

3. For entanglement properties, a generic eigenstate is indistinguishable from a random state.

We briefly explain the reasonings behind these opinions. The eigenstate thermalization hypothesis (ETH) states that for expectation values of local observables, a single eigenstate resembles the thermal state with the same energy density [11, 37, 31]. Opinion 1 is a variant of ETH for entropy. It should be noted that there are models that satisfy ETH for local observables but not for entropy.

We remind the reader that the entanglement entropy of a random state is nearly maximal [30]. Opinion 2 follows from Opinion 1 as the thermal state at the mean energy density is the maximally mixed state. Furthermore, Opinion 3 follows from Opinion 2 because a generic eigenstate has nearly the mean energy density (Lemma 3 in Ref. [21]).

These opinions concern the scaling of entanglement only to leading order. A more ambitious goal is to find the exact value of eigenstate entanglement. We conjecture that the average entanglement entropy of all eigenstates is universal (model-independent), and propose a formula for its dependence on the subsystem size. This formula is derived from an analytical argument based on an assumption characterizing the chaoticity of the model. It is also supported by numerical simulations of a non-integrable spin chain.

The formula implies that by taking into account sub-leading corrections not captured in Opinion 3, a generic eigenstate is distinguishable from a random state in the sense of being less entangled. Indeed, this implication can be proved rigorously for any (not necessarily chaotic) local Hamiltonian. The proof also solves an open problem of Keating et al. [24].

The paper is organized as follows. Section 2 is a very brief review of random-state entanglement. Section 3 proves that for any (not necessarily chaotic) local Hamiltonian, the average entanglement entropy of all eigenstates is smaller than that of random states. Sections 4 and 5 provide an analytical argument and numerical evidence, respectively, for the universality of eigenstate entanglement in chaotic systems. The main text of this paper should be easy to read, for all technical details are deferred to Appendices A and B.

2 Entanglement of random states

We begin with a very brief review of random-state entanglement. For simplicity, we use the natural logarithm throughout this paper.

Definition 1 (entanglement entropy)**.** The entanglement entropy of a bipartite (pure) state $\rho_{AB} = |\psi\rangle\langle\psi|$ is defined as the von Neumann entropy of the reduced density matrix $\rho_A = \operatorname{tr}_B \rho_{AB}$:

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

It is the Shannon entropy of ρ_A's eigenvalues, which form a probability distribution because $\rho_A \geq 0$ (positive semidefinite) and $\operatorname{tr} \rho_A = 1$ (normalization).

Theorem 1 (conjectured and partially proved by Page [30]; proved in Refs. [15, 32, 35])**.** *Let ρ_{AB} be a bipartite pure state chosen uniformly at random (with respect to the Haar measure). In average,*

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

where $d_A \leq d_B$ are the local dimensions of the subsystems A and B, respectively.

Let $\gamma \approx 0.577$ be Euler's constant. In the second step of Eq. (2), we used the formula

$$\sum_{k=1}^{d_B} \frac{1}{k} = \ln d_B + \gamma + O(1/d_B). \tag{3}$$

Note for experts: A concentration bound proved in Ref. [19] using Levy's lemma (below) shows that the deviation of $S(\rho_A)$ (from the mean value) for a typical state ρ_{AB} is exponentially small in the system size.

Lemma 1 (Levy's lemma [28])**.** *Let $f : S^k \to \mathbf{R}$ be a real function defined on a unit k-sphere with Lipschitz constant $O(1)$ (with respect to the Euclidean norm), and a point $x \in S^k$ chosen uniformly at random (with respect to the Haar measure). Then,*

$$\Pr(|f(x) - \bar{f}| > \delta) \leq e^{-\Omega(k\delta^2)}, \tag{4}$$

where $\bar{f}$ is the mean value of f.

3 Rigorous bounds on eigenstate entanglement

This section proves a rigorous upper bound on the average entanglement entropy of all eigenstates. The result holds for any (not necessarily chaotic) local Hamiltonian, and allows us to distinguish a generic eigenstate from a random state.

For ease of presentation, consider a chain of n spin-1/2's governed by a local Hamiltonian

$$H = \sum_{i=1}^{n} H_i, \quad H_i := H'_i + H'_{i,i+1}, \tag{5}$$

where H'_i is an on-site term acting on the spin i, and $H'_{i,i+1}$ represents nearest-neighbor interactions between the spins i and $i+1$. We use periodic boundary conditions by identifying the indices i and $(i \mod n)$. Suppose H'_i and $H'_{i,i+1}$ are linear combinations of one- and two-local Pauli operators, respectively, so that $\operatorname{tr} H'_i = \operatorname{tr} H'_{i,i+1} = 0$ (traceless) and $\operatorname{tr}(H_i H_{i'}) = 0$ for $i \neq i'$. We assume translational invariance and $\|H_i\| = 1$ (unit operator norm). Let $\{|j\rangle\}_{j=1}^{d}$ for $d = 2^n$ be a complete set of translationally invariant eigenstates of H with the corresponding eigenvalues $\{E_j\}$.

Lemma 2. *Consider the spin chain as a bipartite quantum system $A \otimes B$. The subsystem A consists of spins with indices 1,2,...,m. Without loss of generality, assume m is even and $f := m/n \leq 1/2$. Let $\rho_{j,A}$ be the reduced density matrix of $|j\rangle$ on A. Then,*

$$S(\rho_{j,A}) \leq m \ln 2 - f E_j^2/(4n). \tag{6}$$

See Appendix A for the proof of Lemma 2. We are ready to prove the main result of this section:

Theorem 2. *In the setup of Lemma 2,*

$$\frac{1}{d} \sum_{j=1}^{d} S(\rho_{j,A}) \leq m \ln 2 - f \langle H_1^2 \rangle / 4, \tag{7}$$

where $\langle \cdots \rangle := d^{-1} \operatorname{tr} \cdots$ denotes the expectation value of an operator at infinite temperature.

Proof. It follows from Lemma 2 and the observation that

$$\frac{1}{d} \sum_{j=1}^{d} E_j^2 = \langle H^2 \rangle = \sum_{i,i'=1}^{n} \langle H_i H_{i'} \rangle = \sum_{i=1}^{n} \langle H_i^2 \rangle = n \langle H_1^2 \rangle. \tag{8}$$

Note that the assumption $\|H_1\| = 1$ implies $1/4 \leq \langle H_1^2 \rangle \leq 1$. □

For $2 \leq m = O(1)$, Theorem 2 gives the upper bound

$$\frac{1}{d}\sum_{j=1}^{d} S(\rho_{j,A}) \leq m\ln 2 - \Theta(1/n). \tag{9}$$

A lower bound can be easily derived from Theorem 1 in Ref. [24]

$$\frac{1}{d}\sum_{j=1}^{d} S(\rho_{j,A}) \geq m\ln 2 - \Theta(1/n). \tag{10}$$

Therefore, both bounds are tight. This answers an open question in Section 6.1 of Ref. [24].

As a side remark, in the absence of translational invariance a similar result can be obtained by averaging over all ways of "cutting" a region of length m. Here, we allow $\|H_i\|$ to be site-dependent but require $\|H_i\| = \Theta(1)$ for any i.

Corollary 1. *The average entanglement entropy of a random eigenstate for a random consecutive region of size m is upper bounded by $m\ln 2 - \Theta(f)$.*

Proof. We follow the proof of Theorem 2. The inequality of square and arithmetic means

$$n\sum_{i=1}^{n} |\langle j|H_i|j\rangle|^2 \geq \left(\sum_{i=1}^{n}\langle j|H_i|j\rangle\right)^2 = E_j^2. \tag{11}$$

is the only new ingredient. The details are left to the reader as an exercise. □

It is very straightforward to extend all results in this section to higher spatial dimensions.

4 Eigenstate entanglement of "chaotic" Hamiltonians

Suppose the Hamiltonian (5) is chaotic in a sense specified below. This section provides an analytical argument for

Conjecture 1 (Universal eigenstate entanglement)**.** *Consider the spin chain as a bipartite quantum system $A \otimes B$. The subsystem A consists of spins with indices 1,2,...,m. For a fixed constant $f := m/n \leq 1/2$, the average entanglement entropy of all eigenstates is*

$$m\ln 2 + (\ln(1-f))/2 - 2\delta_{f,1/2}/\pi \tag{12}$$

in the thermodynamic limit $n \to +\infty$, where δ is the Kronecker delta function.

We decompose the Hamiltonian (5) into three parts: $H = H_A + H_\partial + H_B$, where $H_{A(B)}$ includes the terms acting only on the subsystem $A(B)$, and $H_\partial = H'_{m,m+1} + H'_{n,1}$ consists of the cross terms. Let $\{|j\rangle_A\}_{j=1}^{2^m}$ and $\{|k\rangle_B\}_{k=1}^{2^{n-m}}$ be complete sets of eigenstates of H_A and H_B with the corresponding eigenvalues $\{\epsilon_j\}$ and $\{\varepsilon_k\}$, respectively. As H_A, 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 $\{\epsilon_j + \varepsilon_k\}$.

The term H_∂ has the effect of mixing product states in the sense that a (normalized) eigenstate $|\psi\rangle$ of H with energy E is a superposition

$$|\psi\rangle = \sum_{j=1}^{2^m}\sum_{k=1}^{2^{n-m}} c_{jk}|j\rangle_A|k\rangle_B. \tag{13}$$

The locality of H_∂ imposes a strong constraint, which states that the population of $|j\rangle_A|k\rangle_B$ is negligible unless $\epsilon_j + \varepsilon_k$ is close to E.

Lemma 3 ([1])**.** *There exist constants $c, \Delta > 0$ such that*

$$\sum_{|\epsilon_j+\varepsilon_k-E|\geq\Lambda} |c_{jk}|^2 \leq ce^{-\Lambda/\Delta}. \tag{14}$$

In chaotic systems, it is tempting to expect

Assumption 1. The expansion (13) is a random linear combination subject to the constraint (14).

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

$$H = \sum_{i=1}^{n} \sigma_i^z. \tag{15}$$

It should be clear that the set M captures the essential aspects of Assumption 1. The constraint imposed by the subspace span M_j is a "hard" variant of Eq. (14):

$$\sum_{|\epsilon_j+\varepsilon_k-E|\geq 1/2} |c_{jk}|^2 = 0. \tag{16}$$

The random unitary U_j guarantees that the expansion (13) is a random linear combination. Thus, Conjecture 1 is established by the following proposition proved in Appendix B.

Proposition 1. *The average entanglement entropy of all states in M is given by Eq. (12).*

5 Numerics

To provide numerical evidence for Conjecture 1, we consider the spin-1/2 chain [3]

$$H = \sum_{i=1}^{n} H_i, \quad H_i := \sigma_i^z\sigma_{i+1}^z + g\sigma_i^x + h\sigma_i^z, \quad g = -1.05,\ h = 0.5 \tag{17}$$

with periodic boundary conditions ($\sigma_{n+1}^z := \sigma_1^z$), where $\sigma_i^x, \sigma_i^y, \sigma_i^z$ are the Pauli matrices at the site i. This model is non-integrable in the sense of Wigner-Dyson level statistics [3]. We compute the average entanglement entropy of all eigenstates by exact diagonalization in each momentum sector.

Figure 1 shows the numerical result, which semi-quantitatively supports Conjecture 1. Noticeable deviations from Eq. (12) are expected due to significant finite-size effects. However, the trend appears to be that the difference between theory and numerics decreases for larger system sizes.

Acknowledgments

We would like to thank Fernando G.S.L. Brandão and Xiao-Liang Qi for interesting discussions.

We acknowledge funding provided by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (NSF Grant PHY-1125565) with support of the Gordon and Betty Moore Foundation (GBMF-2644). Additional funding support was provided by NSF DMR-1654340.

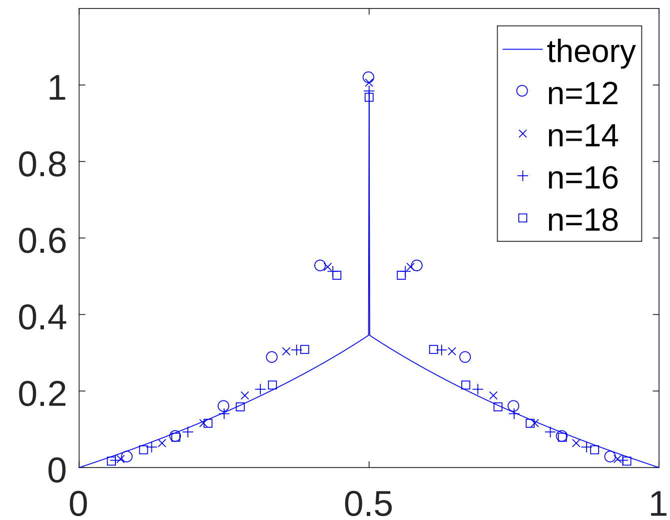

Figure 1: Numerical check of Conjecture 1. The horizontal axis is the fraction f of spins in one subsystem. To be aesthetically pleasing, we allow $0 < f < 1$ so that the plot is reflection-symmetric about $f = 1/2$. The symbols represent values obtained by subtracting the average entanglement entropy of all eigenstates from $\min\{f, 1-f\}n \ln 2$. Different symbols correspond to different system sizes. The curve is the theoretical prediction given by Eq. (12).

A Proof of Lemma 2

Let $\epsilon_j := \langle j|H_i|j\rangle = E_j/n$ so that $|\epsilon_j| \le 1$. Let $\rho_{j,i}$ be the reduced density matrix of $|j\rangle$ on the spins i and $i+1$. Let I_4 be the identity matrix of dimension 4×4. Let $\|X\|_1 = \operatorname{tr}\sqrt{X^\dagger X}$ be the trace norm. As H_i is traceless, $|\epsilon_j|$ provides a lower bound on the deviation of $\rho_{j,i}$ from the maximally mixed state:

$$|\epsilon_i| = |\operatorname{tr}(\rho_{j,i}H_i)| = |\operatorname{tr}((\rho_{j,i}-I_4/4)H_i)| \le \|\rho_{j,i}-I_4/4\|_1\|H_i\| = \|\rho_{j,i}-I_4/4\|_1 = \sum_{k=1}^{4}|\lambda_k-1/4|, \quad (18)$$

where λ_k's are the eigenvalues of $\rho_{j,i}$. An upper bound on $S(\rho_{j,i})$ is given by

$$\max\left\{-\sum_{k=1}^{4} p_k \ln p_k\right\}; \quad \text{s. t.} \quad \sum_{k=1}^{4} p_k = 1, \quad \sum_{k=1}^{4} |p_k - 1/4| \ge \epsilon_j. \quad (19)$$

As the Shannon entropy is concave, it suffices to compare the values in three cases:
(i) $p_1 = p_2 = 1/4 + \epsilon_j/4$, $p_3 = p_4 = 1/4 - \epsilon_j/4$;
(ii) $p_1 = 1/4 + \epsilon_j/2$, $p_2 = p_3 = p_4 = 1/4 - \epsilon_j/6$;
(iii) $p_1 = 1/4 - \epsilon_j/2$, $p_2 = p_3 = p_4 = 1/4 + \epsilon_j/6$.
For $|\epsilon_j| \ll 1$, the Taylor expansion shows that Case (i) "dominates," and one can prove

$$S(\rho_{j,i}) \le 2\ln 2 - \epsilon_j^2/2. \quad (20)$$

Furthermore, we have checked numerically that this inequality holds for any $|\epsilon_j| \le 1$. Therefore,

$$S(\rho_{j,A}) \le \sum_{k=0}^{m/2-1} S(\rho_{j,2k+1}) \le m\ln 2 - m\epsilon_j^2/4 = m\ln 2 - \frac{fE_j^2}{4n} \quad (21)$$

due to the subadditivity [2] of the von Neumann entropy.

B Proof of Proposition 1

Without loss of generality, assume m and n are even. Let L_j (R_j) be the set of states with j spins up and $m-j$ ($n-m-j$) spins down in the computational basis of the subsystem A (B) so that

$$|L_j| = \binom{m}{j}, \quad |R_j| = \binom{n-m}{j}, \quad \text{and} \quad M_j = \bigcup_{k=\max\{0,m-n+j\}}^{\min\{m,j\}} L_k \otimes R_{j-k}. \tag{22}$$

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

$$|\psi\rangle = \sum_{k=\max\{0,m-n+j\}}^{\min\{m,j\}} c_k|\phi_k\rangle, \tag{23}$$

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

$$\rho_A = \bigoplus_{k=\max\{0,m-n+j\}}^{\min\{m,j\}} |c_k|^2\sigma_{k,A} \implies S(\rho_A) = \sum_{k=\max\{0,m-n+j\}}^{\min\{m,j\}} |c_k|^2 S(\sigma_{k,A}) - |c_k|^2 \ln|c_k|^2. \tag{24}$$

As $|\psi\rangle$ is a random state in span M_j, each $|\phi_k\rangle$ is a random state distributed uniformly (with respect to the Haar measure) in $\operatorname{span}\{L_k \otimes R_{j-k}\}$. Equation (2) implies that in average,

$$S(\sigma_{k,A}) = \ln\min\{|L_k|, |R_{j-k}|\} - \min\{|L_k|, |R_{j-k}|\}/(2\max\{|L_k|, |R_{j-k}|\}). \tag{25}$$

Furthermore, in average, $|c_k|^2$ is proportional to $\dim\operatorname{span}\{L_k \otimes R_{j-k}\}$:

$$|c_k|^2 = |L_k||R_{j-k}|/|M_j|. \tag{26}$$

Lemma 1 implies that the deviation (from the mean value) of $|c_k|^2$ for a typical state $|\psi\rangle \in \operatorname{span} M_j$ is exponentially small. Hence, we may compute $S(\rho_A)$ by substituting Eq. (26) into Eq. (24). Let

$$J := j/\sqrt{n} - \sqrt{n}/2 \le 0, \quad K := k/\sqrt{n} - f\sqrt{n}/2. \tag{27}$$

In the thermodynamic limit, J (K) can be promoted to a continuous variable in $\mathbf{R}$, and its binomial distribution approaches Gaussian with zero mean and variance $1/4$ ($f/4$). In particular,

$$|L_k| = \sqrt{2}d^f e^{-2K^2/f}/\sqrt{f\pi n}, \quad |R_{j-k}| = \sqrt{2}d^{1-f}e^{-2(J-K)^2/(1-f)}/\sqrt{(1-f)\pi n}, \tag{28}$$

$$|M_j| = \sqrt{2}de^{-2J^2}/\sqrt{\pi n}, \quad |c_k|^2 = \sqrt{2}e^{2J^2-2K^2/f-2(J-K)^2/(1-f)}/\sqrt{f(1-f)\pi n}. \tag{29}$$

For any fixed constant $f < 1/2$, the condition $|L_k| \ll |R_{j-k}|$ almost always holds so that

$$S(\sigma_{k,A}) = (m + 1/2)\ln 2 - \ln(f\pi n)/2 - 2K^2/f. \tag{30}$$

Equation (24) leads to

$$S_j := S(\rho_A) = \int_{-\infty}^{+\infty} |c_k|^2(S(\sigma_{k,A}) - \ln|c_k|^2)\mathrm{d}k = \left(m + \frac{1}{2}\right)\ln 2 - \frac{\ln(f\pi n)}{2} + \frac{f - 4fJ^2 - 1}{2}$$
$$+ (1 + \ln(f - f^2) + \ln(\pi n/2))/2 = m\ln 2 + f(1 - 4J^2)/2 + \ln(1-f)/2. \tag{31}$$

Averaging over all states in M_j',

$$\frac{1}{d}\sum_{j=0}^{n}|M_j|S_j \approx m\ln 2+\frac{\ln(1-f)}{2}+\frac{f}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-2J^2}(1-4J^2)\mathrm{d}J = m\ln 2+\frac{\ln(1-f)}{2}. \tag{32}$$

For $f=1/2$, we first consider the situation $J\le 0$ and $K\le J/2$ (i.e., $j\le n/2$ and $k\le j/2$) so that $|L_k|\le|R_{j-k}|$. In this case,

$$S(\sigma_{k,A}) = (m+1)\ln 2-\ln(\pi n)/2-4K^2-e^{4J^2-8JK}/2. \tag{33}$$

Let

$$\operatorname{erfc} x = \frac{2}{\sqrt{\pi}}\int_{x}^{+\infty}e^{-t^2}\mathrm{d}t \tag{34}$$

be the complementary error function. Equation (24) leads to

$$S_j := S(\rho_A) = 2\int_{-\infty}^{j/2}|c_k|^2 S(\sigma_{k,A})\mathrm{d}k-\int_{-\infty}^{+\infty}|c_k|^2\ln|c_k|^2\mathrm{d}k = \left(\frac{n}{2}+1\right)\ln 2-\frac{\ln(\pi n)}{2}-\frac{1}{4}+J\sqrt{\frac{2}{\pi}}$$
$$-J^2-\frac{e^{2J^2}\operatorname{erfc}|\sqrt{2}J|}{2}+\frac{1+\ln(\pi n/8)}{2} = \frac{n-1}{2}\ln 2+\frac{1}{4}+J\sqrt{\frac{2}{\pi}}-J^2-\frac{e^{2J^2}\operatorname{erfc}|\sqrt{2}J|}{2}. \tag{35}$$

This is the mean value of the entanglement entropy of a state in M_j' with $j\le n/2$. For $j>n/2$, it suffices to replace J by $-J$ in the formula. Averaging over all states in M_j',

$$\frac{1}{d}\sum_{j=0}^{n}|M_j|S_j \approx \frac{n-1}{2}\ln 2+\sqrt{\frac{8}{\pi}}\int_{-\infty}^{0}e^{-2J^2}\left(\frac{1}{4}+J\sqrt{\frac{2}{\pi}}-J^2-\frac{e^{2J^2}\operatorname{erfc}|\sqrt{2}J|}{2}\right)\mathrm{d}J = \frac{n-1}{2}\ln 2-\frac{2}{\pi}. \tag{36}$$

We obtain Eq. (12) by combining Eqs. (32) and (36).

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