Ensemble equivalence and eigenstate thermalization from clustering of correlation

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Clustering of an equilibrium bipartite correlation is widely observed in non-critical many-body quantum systems. Herein, we consider the thermalization phenomenon in generic finite systems exhibiting clustering. We demonstrate that such classes of systems exhibit the ensemble equivalence between microcanonical and canonical ensembles even for subexponentially small energy shell with respect to the system size. Most remarkably, in low-energy regime, the thermalization for single eigenstate is proven. Our results provide a key insight into the precise analysis of the eigenstate thermalization via the clustering property.

Introduction.— Thermalization in an isolated quantum system is a fundamental phenomenon that is directly connected to the arrow of time in nature. The first study on this phenomenon dates back to von Neumann’s study in 1929 [1]. Recently, this subject has been revived, fueled by relevant experiments of cold atomic systems [2] and a new concept resulting from the quantum information theory [3]. The studies have now become interdisciplinary, including statistical physics, quantum information theory, and experiments.

Subjects on thermalization are primarily divided into two categories, i.e., equilibration dynamics from an initial state to a steady state, and the thermodynamic properties of the steady state. Concerning the second category, the eigenstate thermalization hypothesis (ETH) is a central subject that guarantees the thermodynamic property of an isolated quantum system. The ETH states that an expectation value of any local observable needs to approach the thermodynamic ensemble average in the long-time limit, hence, more detailed information is desired with analytical approaches.

Here, \( \langle \Omega \rangle_U,\Delta \) and \( \langle \Omega \rangle_\beta \) are the averages with respect to the microcanonical and the corresponding canonical ensembles in Eq. (1), respectively. In this context, the ETH is defined by setting \( \Delta \to +0 \) so that the energy window contains only one eigenstate (i.e., \( \mathcal{N}_{U,\Delta} = 1 \)). The emergence of the ensemble equivalence is key for accessing the ETH. It is noteworthy that the weak version of the ETH [6] has been recently proven together with the argument on the realization of the ensemble equivalence [7].

In spite of its deep and direct connection to the thermalization phenomenon, the ensemble equivalence in finite systems has not been studied comprehensively until recently [8–11] (See also [12–14] for classical cases). Bråndao and Cramer employed the technique of information theory and proved the ensemble equivalence by considering the finite-size effect for the first time [15]. More recently, Tasaki reconsidered a similar setup that considers the structure of the Massieu function and demonstrated the ensemble equivalence for \( \Delta_c \sim O(n^{-1/2}) \) at high-temperature regimes [16]. Although these demonstrate remarkable progress, a number of open questions are still unanswered. The critical questions include how small we can take the energy width \( \Delta \) to obtain the ensemble equivalence and whether it is possible or not that a significant reduction in the energy width \( \Delta \) eventually results in the ETH. Many numerical calculations indicate that nonintegrability is necessary to obtain the ETH for the high-temperature regime. However, this is a general and vague concept; hence, more detailed information is desired with analytical approaches.

We herein consider a system class that satisfies the clustering property for the canonical distribution. The clustering property implies that two local observables are exponentially uncorrelated as the distance between them is increased (see the definition 1). By utilizing the clustering property, we demonstrate that the ensemble equivalence holds for sub-exponentially small energy width with respect to the system size, i.e., \( \Delta \sim e^{-O(n^{\gamma})} \) (\( \gamma < 1 \)). More remarkably, the eigenstate thermalization is rigorously proved for low-lying energy eigenstates near the ground state. This implies that low-lying eigenstates behave as the ground state and yield the same value for local observables. Notably, we do not assume the nonintegrability of the systems.
eral, integrable systems can demonstrate clustering, and hence the eigenstate thermalization can be valid even in integrable systems. Our findings provide one general condition towards the ETH in the low-energy regime.

Setup. — We consider a \((1/2)\)-quantum spin system defined on a \(d\)-dimensional hypercubic lattice. The Hamiltonian consists of \(n\) local terms:

\[
H = \sum_{i=1}^{n} H_i, \quad \|H_i\| \leq 1
\]  

with \(\cdot\) the operator norm. The local Hamiltonian \(H_i\) contains spin operators that act nontrivially on spins \(j\) with the distance \(\text{dist}(i, j) \leq \ell_0\), where \(\text{dist}(i, j)\) is the Manhattan distance. The translation invariance of the Hamiltonian is not assumed here. Subsequently, without generality loss, we set the energy of the ground state to zero. In addition, we assume that the system satisfies the clustering property for the canonical distribution that is defined as follows:

**Definition 1.** Let \(A, B\) be arbitrary operators with a unit norm supported on subsets \(X\) and \(Y\), respectively. We say that a density matrix \(\rho\) satisfies the \((r, \xi)\)-clustering if

\[
|\text{tr}(\rho A X B Y) - \text{tr}(\rho A X) \text{tr}(\rho B Y)| \leq e^{-\text{dist}(X,Y)/\xi}
\]

for \(\text{dist}(X,Y) \geq r\), where \(r\) and \(\xi\) are fixed constants. Here, the distance between the subsets \(\text{dist}(X,Y)\) is defined as \(\text{dist}(X,Y) = \min_{i \in X, j \in Y} \text{dist}(i,j)\).

In one dimension, the clustering of the canonical ensemble has been proven at arbitrary temperatures \([17, 18]\), whereas in higher dimensions, the clustering holds above a threshold temperature \([19-22]\). Even in low-temperature phases, the clustering property is expected to be satisfied if the system is away from the critical temperature. Note that no direct connection exists between the clustering property and nonintegrability of the system; hence, even integrable systems can exhibit clustering. Thus, the clustering property typically appears in non-critical many-body quantum systems. Furthermore, the clustering property is in general connected to the Chernoff-Hoeffding-type concentration inequality for macroscopic observables \([23, 24]\), which is crucial in this study at the mathematical level.

**Main results.** — We consider the microcanonical and canonical averages of local observables in the system with the clustering property. Let \(\Omega\) be a local operator:

\[
\Omega = \sum_{i=1}^{n} \Omega_i, \quad \|\Omega_i\| \leq 1
\]

where \(\Omega_i\) is composed of spin operators that act on spins \(j\) with the distance \(\text{dist}(i, j) \leq \ell\). For equilibrium distribution \(\rho\) exhibiting the clustering property, we describe the two theorems below. For presentational simplification, we present the results for \(\ell \geq r\). To concentrate on the physics given by the theorems, we provide the proofs in the supplementary material \([25]\).

**Theorem 1.** We measure the energy with the unit of the energy width \(\Delta\), and relate the inverse temperature to the energy as \(U = \nu \Delta\), where \(\nu\) is an integer maximizing \(e^{-\nu \Delta} \mathcal{N}_{U, \Delta}\) \([16]\). If the canonical ensemble \(\rho\) satisfies the \((r, \xi)\)-clustering, under the condition \(\Delta \ll 1/\beta\), the microcanonical ensemble \(\rho_{U, \Delta}\) satisfies the following:

\[
(1/n)(\langle \Omega \rangle_{U, \Delta} - \langle \Omega \rangle) \leq (1/\sqrt{n}) \max(c_1 A_1, c_2 A_2),
\]

\[
A_1 = [\log((\sqrt{n}/\Delta))^{(d+1)/2}]
\]

\[
A_2 = [\ell^d \log(\sqrt{n}/\Delta)]^{1/2},
\]

where the constants \(c_1\) and \(c_2\) depend on \(d, r, \xi\), and \(\ell_0\).

Imposing \(A_1, A_2 \ll \mathcal{O}(n^{1/2})\), the system size dependence of the lower bound of the energy width \(\Delta_c\) for obtaining the ensemble equivalence is given by

\[
\Delta_c \sim \exp\left(-\mathcal{O}(n^{1/(d+1)})\right).
\]

This implies that even a subexponentially small energy width is sufficient to guarantee the ensemble equivalence. This system-size dependence is a significant improvement from the state-of-the-art estimation \(\mathcal{O}(n^{-1/2})\) in \([15, 16]\). Furthermore, we can quantitatively improve the argument on the weak version of the ETH \([6, 7]\). The weak ETH argues that the variance in the energy shell,

\[
\frac{1}{N^{d+3}} \sum_{E \in (\mathcal{E}(U, \Delta), \mathcal{E}(U, \Delta))} [\langle E | \Omega | E \rangle - \langle \Omega \rangle_{U, \Delta}]^2
\]

approaches zero with the system size \(n\). Our new estimation leads to the finite-size effect of the variance as \(\log(d+1)/n\) provided that \(\Delta = 1/\text{poly}(n)\) \([25]\). It is noteworthy that recent calculations by Alba \([26]\) showed an example that expresses the variance of \(\mathcal{O}(1/n)\). This implies that our estimation is the best general upper bound on the weak ETH up to a logarithmic correction.

Despite a significant reduction in the energy width, large numbers of energy eigenstates still exist within the energy shell; hence, one cannot access the true eigenstate thermalization. In the following, we show the theorem for a single eigenstate to access the eigenstate thermalization in a low-energy regime.

**Theorem 2.** Let \(\beta^*\) be an inverse temperature for which the canonical ensemble \(\rho_{\beta^*}\) satisfies \((r, \xi)\)-clustering. Then, any energy eigenstate \(|E\rangle\) satisfies

\[
(1/n)|\langle E | \Omega | E \rangle - \langle \Omega \rangle_{\beta^*}| \leq (1/\sqrt{n}) \max(c_1 B_1, c_2 B_2),
\]

\[
B_1 = [\beta^* E + \log Z_{\beta^*}]^{(d+1)/2},
\]

\[
B_2 = [\ell^d (\beta^* E + \log Z_{\beta^*})]^{1/2},
\]

where the constants \(c_1, c_2\) depend on \(d, r, \xi\), and \(\ell_0\).

Because we set the energy of the ground state to zero, the quantity \(\log Z_{\beta^*}\) has always a positive value \([27]\). We emphasize that the theorem above is valid for an arbitrary eigenstate. Next, we discuss that the theorem results in eigenstate thermalization in the low-energy regime. To this end, we first consider the eigenstate whose energy \(E\) is \(\mathcal{O}(1)\), which is the same energy scale as that in the local site Hamiltonian (See Eq. (3)). As the total energy increases linearly as the system size from the extensivity, this choice of eigenstate is equivalent to analyzing an extremely low-temperature regime.
in the thermodynamic limit. Next, we choose the inverse temperature $\beta^*$ according to the system size as $\beta^* \propto \log n$; this implies that one can eventually replace $\langle \Omega \rangle_{\beta^*}$ by $\langle \Omega \rangle_{\infty}$ in the thermodynamic limit [25].

In addition, suppose that we consider the system that shows $\log Z_{\beta^*} \sim O(1)$ [28]. This leads to a vanished right-hand side in the thermodynamic limit, implying eigenstate thermalization in the sense that low-lying eigenstates with $E = O(1)$ (more precisely, one can extend the regime to $E \lesssim n^{1/(d+1)}$) are indistinguishable from the ground state as long as the local observables are measured.

A possible realistic situation for obtaining this scenario is given by a system satisfying the following relation in terms of the number of eigenstates in an energy shell $[\varepsilon - 1, \varepsilon]$ for the low-energy regime:

$$\mathcal{N}_{\varepsilon,1} \leq n^{\varepsilon}.$$  \hspace{1cm} (9)

This behavior is ubiquitous in many systems, as discussed in [29–31]. Furthermore, we demonstrate this with a specific model below. It is straightforward to demonstrate that the quantity $\log Z_{\beta^*}$ with $\beta^* \propto \log n$ becomes the order of 1 in the thermodynamic limit [32].

Numerical demonstration on eigenstate thermalization based on theorem 2.— To obtain a better understanding on the realization of eigenstate thermalization, we consider a simple integrable model as a specific example. It is noteworthy that the clustering property has no direct connection to the nonintegrability of the dynamics; hence, it can be realized even in an integrable system. In addition, the relation on the number of eigenstates at the low-energy regime (9) is discussed below. Let us consider the $xy$ model with a magnetic field:

$$H = \sum_{i=1}^{n} [(3/4)\sigma_i^x \sigma_{i+1}^x + (1/4)\sigma_i^y \sigma_{i+1}^y] + h \sum_{i=1}^{n} \sigma_i^z,$$  \hspace{1cm} (10)

where $\sigma_i^\alpha (\alpha = x, y, z)$ is the $\alpha$-component of the Pauli matrix at the site $i$. We here consider the gapped case with $h > 1$. Through the Jordan–Wigner transformation [33, 34], the Hamiltonian is diagonalized into the Fermionic representation $H = \sum_{k=1}^{n} 2\epsilon_k c_k^\dagger c_k$, where $c_k$ is a positive eigenmode energy for the $k$th mode [35] and $c_k^\dagger$ is the creation operator (we adjust the energy of the ground state to zero). An arbitrary eigenstate is expressed in the following form:

$$|E\rangle = \prod_{k=1}^{n} [c_k^\dagger]^{q_k} |0\rangle,$$  \hspace{1cm} (11)

where $|0\rangle$ is the vacuum state. In this representation, the ground state is identical to the vacuum state. For $h > 1$, each eigenmode energy $\epsilon_k$ is of the order 1. Hence, the number of eigenstates for low-energy excitations of the order 1 can be estimated through a simple combinatorial argument. This estimation justifies the relation (9) [36].

The theorem 2 is valid for the system with the clustering property. Hence, we must verify this in the present model. In general, the ground state in the one-dimensional gapped system shows an exponential decay in the correlation of separated observables [37]. We anticipate this property to be shared by the excited states as well. We numerically verify the clustering property in the canonical ensemble for the case $h = 3/2$, in which we consider the mutual information between two separated spins. For a given density matrix $\rho$, the mutual information $I_{ij}(\rho)$ between the sites $i$ and $j$ is defined as $I_{ij}(\rho) = S(\rho_i) + S(\rho_j) - S(\rho_{i,j})$, where $S(\rho)$ is the von Neumann entropy of the density matrix $\rho$, and $\rho_i$ and $\rho_{i,j}$ are reduced density matrices of one site $i$ and two sites $i,j$, respectively. We first verify that $I_{ij}(\rho_{i,j})$ shows an exponential decay as a function of distance $|i-j|$, which is demonstrated in the inset of Fig. 1 (a). Using the data for many temperatures, we calculate the $\beta$-dependence of the correlation length $\xi(\beta)$ and present a plot in the primary graph of Fig. 1 (a). This plot strongly indicates the realization of the clustering property even at the extremely low-temperature regime.

Having obtained a strong evidence of the clustering property and the energy dependence of the number of states (9), we can now directly observe an evidence of the emergence of the eigenstate thermalization. Let $\mathcal{E}_s$ be the set of all the eigenstates (11) with $\sum_{k=1}^{n} k \leq s$. The set includes low-lying excited states whose energy is of the order 1. Hence, we consider a deviation on the local thermodynamic property between the eigenstates in the $\mathcal{E}_s$ set and the ground state. Hence, we define the following two quantities:

$$f_s(n) := \max_{|E\rangle \in \mathcal{E}_s} \left|\left\langle [E]M_z|0\right\rangle - \langle 0|M_z|0\rangle\right|,$$  \hspace{1cm} (12)

$$g_s(n) := \max_{|E\rangle \in \mathcal{E}_s} \left\|\rho_{m+1} - \rho_{m+1}^{0}\right\|_1,$$

where we use magnetization as a local observable, i.e.,

$$M_{z} = \sum_{i=1}^{n} \sigma_{i}^{z},$$

$m = \lfloor n/2 \rfloor$. The matrices $\rho_{m+1}$ and $\rho_{m+1}^{0}$ are the reduced density matrices at the sites $m, m+1$ of the density matrix $|E\rangle\langle E|$ and the ground state $|0\rangle\langle 0|$, respectively. The quantity $f_s(n)$ measures the deviation in terms of local observable (magnetization) between eigenstates in the set $\mathcal{E}_s$ and the ground state. The quantity $g_s(n)$ measures the distance between the reduced density matrices of an eigenstate in $\mathcal{E}_s$ and the ground state. In Fig. 1 (b) and (c), we show $f_s(n)$ and $g_s(n)$ for $s = 3, 5, 7$ as a function of the system size $n$. The figures show the systematic decays of these quantities as the system size increases. This is a direct and clear indication of the emergence of eigenstate thermalization. The decay rate in this specific case is faster than $n^{-1/2}$ of the theorem 2. This implies that the convergence behavior of the eigenstate thermalization inferred from the theorem is not optimum for this specific case.

Remark on the eigenstate thermalization in the low-energy regime.— A condition that results in the eigenstate thermalization is the behavior of the density of eigenstates (9). As mentioned in Refs. [29–31], this behavior is ubiquitous in many-body systems with gapped ground states. Regarding the clustering condition, it has been proven that the ground state in the finite-dimensional gapped system shows an exponential decay for separable observables [37, 38]. Hence, it is natural to expect that the canonical distribution exhibits the clustering property at an extremely low temperature. However, a counterexample also exists where the condition (9) breaks down for a system with a gapped ground state (see Sec. IV in Ref. [29]).
The eigenstate thermalization inferred from the theorem 2 is special compared with the typical ETH for the finite temperature regime. In a one-dimensional system, the clustering property for the ground state results in the area law [39]. Hence, the low-lying eigenstate in the present version is expected to exhibit the area law. Meanwhile, the ETH for finite temperatures indicates the volume law. In this sense, the present version of the eigenstate thermalization should be regarded as an extreme case of the ETH.

Furthermore, we should discuss the outcome if we consider systems that exhibit the many-body localization phenomenon [40]. In this case, we should notice that our temperature range is as small as $\beta^* \propto \log n$. Although the one-dimensional systems exhibit the clustering property in general, it is applicable only for $\beta = O(1)$. In systems with many-body localization, the canonical state $p_\beta$ does not appear to satisfy the clustering property at sufficiently small temperatures. We discuss this point in the supplemental material [25]. Hence, the absence of thermalization in systems with many-body localization is consistent with Theorem 2.

Summary and perspective. — We herein addressed the role of the clustering property on the ensemble equivalence and the eigenstate thermalization in low-energy regime. Two primary results are discussed herein Theorems 1 and 2.

The theorem 1 shows that a subexponentially small energy width is sufficient for realizing the ensemble equivalence. We also gave the best general upper bound on the system-size dependence of the weak version of the ETH. Although the ensemble equivalence is concerned with local observables as defined in (2), the theorem 1 can also provide a quantitative description of equivalence between the reduced density matrices of the microcanonical and canonical ensembles (see the supplemental material [25]). This improves the original argument by Brázdová and Cramer [15].

The theorem 2 provides the first rigorous proof of eigenstate thermalization realized in low-energy eigenstates for system class having the clustering property. This explicitly shows that the clustering property can be a critical condition for the thermalization. As a special property of this energy regime, eigenstate thermalization can occur even in integrable systems. We should note that we do not consider any dynamics of thermal relaxation but focus on the static property of one eigenstate. One can anticipate a different relaxation dynamics between integrable and nonintegrable systems [41]. Also, our theorem does not exhibit inconsistency to the absence of thermalization in systems with many-body localization.

At the end of this paper, we list several open problems relevant to the present study. Finding the explicit conditions for the eigenstate thermalization in the high-temperature regime remains the most important future challenge, although it appears to be an extremely difficult problem as nonintegrability must be explicitly taken into account [42, 43]. Another intriguing future work is to extend the present results to long-range interacting systems. Concerning the first theorem, it appears to be possible provided that a high-temperature regime is considered [44]. To derive the strong ETH for low-lying eigenstates, we need an alternative assumption to the clustering of the canonical state that ensures the concentration bound. Thus far, such a concentration bound has been ensured for gapped ground states in long-range interacting systems [45, 46]. Hence, it would be natural to expect the concentration bound of canonical states in long-range interacting systems at extremely low temperatures.

Although we have demonstrated that the clustering property is crucial for eigenstate thermalization, an explicit system class exhibiting the clustering property is unclear. As demonstrated with a specific model herein, a wide class of gapped systems appears to exhibit the clustering property, although a clear argument on this does not exist, to our knowledge [47]. As one candidate, one may consider a weakly perturbed classical lattice system: $H = \sum_{i=1}^{n} \sigma_i^z + \lambda H_{\text{int}}$, where $H_{\text{int}}$ is an arbitrary quantum Hamiltonian. It has been proven by Yarotsky [48] that the Hamiltonian is always gapped and away from a critical point provided that $\lambda$ is sufficiently small. We conjecture that if $\lambda$ is smaller than some constant threshold, the system satisfies the clustering property at arbitrary temperatures and the strong ETH holds universally for low-energy states.

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If we consider a general value for the energy of the ground state, the same relation can be derived by shifting the eigenenergy to $E - E_0$.

More precisely, $\log Z_\beta \sim \alpha n^\beta$ ($\alpha < 1/2$) is sufficient for convergence in the right-hand side.

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For $N_{\epsilon,1} \sim n$ we assume $\beta^* = c^* \log n$ satisfying $c^* > c$. Subsequently, we have $\beta^* = \sum_n e^{-\beta^* E} \leq 1 + \sum_{j>1} (n-c)^j$, which is finite even for the thermodynamic limit. Recall that the energy of the ground state is set to zero. Note that in the high-energy regime, the bound (9) is too loose to describe the true system-size dependence of $N_{\epsilon,1}$, and hence this computation overestimates the amplitude of $Z$ (nevertheless, it is still of $O(1)$).

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Under the periodic boundary condition, $\epsilon_k$ is exactly given by $\epsilon_k = (\cos(2\pi k/n) - h)^2 + 1/2(\sin(2\pi k/n))^2)^{1/2}$. This solution also gives the approximate value of $\epsilon_k$ under the open boundary condition.

Let us define $\tilde{\epsilon}$ as such $2\epsilon_k \geq \tilde{\epsilon}$ for all $1 \leq k \leq n$. Subsequently, the total number of eigenstates whose energy is smaller than $m \tilde{\epsilon}$ is less than $\sum_{q \leq \tilde{\epsilon}} (\tilde{\epsilon}^n)$, and hence $N_{\epsilon,1} \leq n^{-1/2}$.

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[47] Even if the condition (9) is satisfied and the system exhibits a gapped ground state, clustering may be violated for $\beta = O(\log(n))$. Let us consider the Ising model with extremely weak magnetic fields as

$$H = \sum_{i=1}^{n} (\sigma^z_i \sigma^z_{i+1} - \sigma^z_i / n)$$

for example. In this system, the condition (9) is satisfied and the Hamiltonian contains the all-up state as its unique ground state and the all-down state as its first excited state with the spectral gap of 2. However, for a sufficiently low temperature $\beta = O(\log(n))$, the canonical state $\rho^{\text{can}}$ does not satisfy the clustering. Here, the first excited state $|E_1\rangle$ is macroscopically distinct from $|E_0\rangle$ and yields

$$\frac{1}{2} |\langle E_1 | \mathcal{M}_z | E_1 \rangle - \langle E_0 | \mathcal{M}_z | E_0 \rangle| = 2.$$

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**Supplementary Material for**

“Ensemble equivalence and eigenstate thermalization from clustering of correlation”

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**I. SETUP**

**A. Notations and definitions**

We iterate several definitions that are presented in the primary text. The Hamiltonian that we considered consists of $n$ local terms:

$$H = \sum_{i=1}^{n} H_i, \quad \|H_i\| \leq 1.$$  \hspace{1cm} (S.1)

The local Hamiltonian $H_i$ contains spin operators that act nontrivially on spins $j$ with the distance $\text{dist}(i,j) \leq \ell_0$.

The canonical and microcanonical distributions are defined as

$$\rho_\beta := \frac{e^{-\beta H}}{Z_\beta},$$  \hspace{1cm} (S.2)

$$\rho_{U,\Delta} := \frac{1}{N_{U,\Delta}} \sum_{E \in [U-\Delta, U]} |E\rangle\langle E|,$$  \hspace{1cm} (S.3)

where

$$N_{U,\Delta} := \text{tr} \left[ \sum_{E \in [U-\Delta, U]} |E\rangle\langle E| \right].$$  \hspace{1cm} (S.4)

For an arbitrary operator $O$, the canonical and microcanonical averages are expressed as follows, respectively:

$$\langle O \rangle_\beta := \text{tr}(\rho_\beta O),$$  \hspace{1cm} (S.5)

$$\langle O \rangle_{U,\Delta} := \text{tr}(\rho_{U,\Delta} O).$$  \hspace{1cm} (S.6)

Next, we focus on the following operator:

$$\Omega = \sum_{i=1}^{n} \Omega_i, \quad \|\Omega_i\| \leq 1,$$  \hspace{1cm} (S.7)

where $\Omega_i$ is composed of spin operators that act on spins $j$ with the distance $\text{dist}(i,j) \leq \ell$.

In our theory, we assume the clustering property for $\rho_\beta$, which is defined as follows:

**Definition 2.** Let $A_X, B_Y$ be arbitrary operators with a unit norm (i.e., $\|A_X\| = \|B_Y\| = 1$) supported on subsets $X$ and $Y$, respectively. We say that a density matrix $\rho$ satisfies the $(r, \xi)$-clustering if

$$|\text{tr}(\rho A_X B_Y) - \text{tr}(\rho A_X)\text{tr}(\rho B_Y)| \leq e^{-\text{dist}(X,Y)/\xi}$$

for $\text{dist}(X,Y) \geq r$, where $r$ and $\xi$ are fixed constants.
B. Concentration inequality

As the core of the proof of our theorems, we utilize the following concentration inequality that is resulted from the \((r, \xi)-\text{clustering}\). We start with the following lemma, whose proof is shown in Section VII. This lemma is essentially the same as that in Ref. [24].

**Lemma 1.** Let \(\rho\) be an arbitrary density matrix that satisfies the \((r, \xi)-\text{clustering}\) (Def. 2). Subsequently, for an arbitrary even integer \(m\), the \(m\)-th moment of the operator \(\Omega\) is bounded from above by

\[
\text{tr}\left[ (\Omega - \langle \Omega \rangle_\rho)^m \right] \leq 8\alpha n m (3^d)^{m/2} + 3\alpha [8\alpha n m^{d+1} (3^d/2)^{d}]^{m/2} =: 3\xi [\tilde{c}_1 n m^{d+1}/(2e)]^{m/2} + [\tilde{c}_2 m^{d+1}/(2e)]^{m/2}
\]

with \(\langle \cdots \rangle_\rho := \text{tr}(\rho \cdots)\) and

\[
\tilde{c}_1 := 16\alpha (3^d/2)^d \quad \text{and} \quad \tilde{c}_2 := 3^d (16\alpha),
\]

where \(\alpha\) is a geometric parameter defined in Ineq. (S.63) of Section VII, and we assume \(\ell \geq r\). If \(\ell \leq r\), the parameter \(\ell\) in (S.8) is replaced by \(r\).

We define the probability density to observe the value \(x\) for the observable \(\Omega\) in terms of the density matrix \(\rho\)

\[
P_\rho(x) := \text{tr}[\rho \delta(x - \Omega)] ,
\]

where \(\delta(\cdots)\) is the Dirac delta function. We relate the inequality (S.8) to the concentration bound for this distribution. For the given positive value \(x_0\), the following relation for the cumulative distribution is satisfied:

\[
P_\rho(\|x - (\Omega)_\rho\| \geq x_0) := \int_{\|x - (\Omega)_\rho\| \geq x_0} P_\rho(x) dx = P_\rho(\|x - (\Omega)_\rho\|^m \geq x_0^m) \leq \text{tr}\left[ (\Omega - \langle \Omega \rangle_\rho)^m \right] \leq 3\xi \left( \frac{\tilde{c}_1 n m^{d+1}}{2ex_0^{d+1}} \right)^{m/2} + \left( \frac{\tilde{c}_2 m^{d+1}}{2ex_0^{d+1}} \right)^{m/2} ,
\]

where \(m\) is a positive integer. We use the Markov inequality for the second line, and the inequality (S.8) for the third line. We subsequently choose \(m/2 \in \mathbb{Z}\) as

\[
m/2 = \left\lfloor \min \left\{ \left( \frac{x_0^2}{\tilde{c}_1 n} \right)^{1/(d+1)}, \frac{x_0^2}{\tilde{c}_2 m^{d+1}} \right\} \right\rfloor ,
\]

where \([\cdots]\) is the floor function. This choice ensures \(\frac{\tilde{c}_1 n m^{d+1}}{2ex_0^{d+1}} \leq 1/e\) and \(\frac{\tilde{c}_2 m^{d+1}}{2ex_0^{d+1}} \leq 1/e\); hence, the upper bound (S.11) reduces to

\[
P_\rho(\|x - (\Omega)_\rho\| \geq x_0) \leq (e + 3\xi) \max \left( e^{-[\tilde{c}_1 n/(\tilde{c}_1 n)]^{1/(d+1)}}, e^{-x_0^2/(\tilde{c}_2 m^{d+1})} \right) .
\]

Note that the cumulative distribution must be less than 1. Combining this with the inequality above, we obtain the following relation:

\[
P_\rho(\|x - (\Omega)_\rho\| \geq x_0) \leq \min \left( 1, (e + 3\xi) \max \left( e^{-[\tilde{c}_1 n/(\tilde{c}_1 n)]^{1/(d+1)}}, e^{-x_0^2/(\tilde{c}_2 m^{d+1})} \right) \right) .
\]

C. Useful formula

For the calculations in the following sections, the following lemma is useful.

**Lemma 2.** Let \(p(x)\) be an arbitrary probability distribution whose cumulative distribution is bounded from above:

\[
P(|x - a| \geq x_0) := \int_{|x - a| \geq x_0} p(x) dx \leq \min(1, e^{-x_0^2/\sigma + x_1}), \quad \gamma > 0, \sigma > 0, \ x_0 > 0 .
\]

Subsequently, for an arbitrary \(k \in \mathbb{N}\), we obtain

\[
\int_{-\infty}^{\infty} |x - a|^k p(x) dx \leq (2\sigma x_1)^{k/\gamma} + \frac{k}{\gamma} (2\sigma)^{k/\gamma} \Gamma(k/\gamma)
\]

with \(\Gamma(\cdots)\) as the gamma function.
We first define \( \tilde{x} := (2\sigma x_1)^{1/\gamma} \), which is the solution of \(-\tilde{x}^\gamma / \sigma + x_1 = -\tilde{x}^\gamma / (2\sigma)\). Subsequently, \(-x_0^\gamma / \sigma + x_1 \leq -x_0^\gamma / (2\sigma)\) for \(x_0 \geq \tilde{x}\); that is, \(P(|x - a| \geq x_0) \leq e^{-x_0^\gamma / (2\sigma)}\) for \(x_0 \geq \tilde{x}\). Using this, we obtain the following relation:

\[
\int_{-\infty}^{\tilde{x}} |x - a|^k p(x)dx = \int_{-\infty}^{\tilde{x}} |x|^k p(x + a)dx \leq \tilde{x}^k \int_{-\tilde{x}}^{\tilde{x}} p(x + a)dx + \int_{x \geq \tilde{x}} x^k [p(x + a) + p(-x + a)]dx \\
\leq \tilde{x}^k - \int_{\tilde{x}}^{\infty} x^k \frac{d}{dx} \left[ \int_{|x'| - a \geq x} p(x')dx' \right] dx.
\] (S.17)

The second term reduces to

\[
-\int_{\tilde{x}}^{\infty} x^k \frac{d}{dx} \left[ \int_{|x'| - a \geq x} p(x')dx' \right] dx = -\tilde{x}^k P(|x - a| \geq \tilde{x}) + \int_{\tilde{x}}^{\infty} kx^{k-1} \left[ \int_{|x'| - a \geq x} p(x')dx' \right] dx \\
\leq \int_{0}^{\infty} kx^{k-1} e^{-x^\gamma / (2\sigma)} dx = \frac{k}{\gamma} (2\sigma)^{k/\gamma} \Gamma(k/\gamma),
\] (S.18)

where we use the partial integration in the first equation. By combining the two inequalities (S.17) and (S.18), we obtain the inequality (S.16). This completes the proof. \(\square\)

II. PROOF OF THEOREM 1.

In this section, we prove the following inequality (S.21) which implies that almost all the eigenstates in the energy shell \((U - \Delta, U]\) have the same expectation value of \((\Omega)\). Then, the inequality (1) is derived as the corollary.

Here, following Ref. [16], we relate the energy \(U\) to the inverse temperature \(\beta\) as follows:

\[
U = \nu^* \Delta, \quad \nu^* := \arg\max_{\nu \in \mathbb{Z}} \left( e^{-\beta \nu \Delta} N_{\nu, \Delta} \right).
\] (S.19)

We define a probability distribution \(P_{U, \Delta}(x)\) such that

\[
P_{U, \Delta}(x) = \frac{1}{N_{U, \Delta}} \sum_{E \in (U - \Delta, U]} \delta(x - \langle E | \Omega | E \rangle),
\] (S.20)

where \(\delta\) is the Dirac delta function. Using Lemma 1, we obtain the following proposition (the proof is presented in the two subsequent subsections):

**Proposition 3.** Let \(P_{U, \Delta}(|x - \langle \Omega \rangle| \geq x_0) (x_0 > 0)\) be the cumulative probability distribution of the distribution \(P_{U, \Delta}(x)\). Subsequently, if the canonical distribution with the corresponding inverse temperature \(\rho_{\beta}\) exhibits the \((r, \xi)\)-clustering property, we have

\[
P_{U, \Delta}(|x - \langle \Omega \rangle| \geq x_0) \leq \min \left[ 1, C_{\Delta} \max \left( e^{-|x_0^\gamma / (\tilde{e}_1 n)|^{1/(d+1)}}, e^{-x_0^\gamma / (\tilde{e}_2 e^\ell n)} \right) \right],
\] (S.21)

where \(C_{\Delta} := 2e^{\beta \Delta} (e + 3e) [2 + (C_1 \Delta^{-1} \sqrt{n})] \) with \(C_1\) a constant that depends on \(d, \alpha, \xi\) and \(\ell_0\).

Theorem 1 is a direct result from this proposition. To show Theorem 1, we evaluate the upper bound of

\[
|\langle \Omega | U - \langle \Omega \rangle| = \int_{-\infty}^{\infty} (x - \langle \Omega \rangle)P_{U, \Delta}(x)dx \leq \int_{-\infty}^{\infty} |x - \langle \Omega \rangle|P_{U, \Delta}(x)dx.
\] (S.22)

Hence, we apply Lemma 2 with \(k = 1\). From Ineq. (S.21), we identify the parameter sets in Lemma 2 as follows:

\[
a = \langle \Omega \rangle, \quad \{ \gamma, \sigma, \nu \} = \{ 2/(d + 1), (\tilde{e}_1 n)^{d+1}, \log C_{\Delta} \} \quad \text{and} \quad \{ 2, \tilde{e}_2 e^\ell n, \log C_{\Delta} \}.
\] (S.23)

We subsequently obtain

\[
|\langle \Omega | U, \Delta - \langle \Omega | \Delta| \leq \max(\tilde{A}_1, \tilde{A}_2),
\] (S.24)

where

\[
\tilde{A}_1 := \sqrt{c_1 n} (2 \log C_{\Delta})^{d+1} + 2^{(d-1)/2}(d + 1)\sqrt{c_1 n} \Gamma[(d + 1)/2],
\]

\[
\tilde{A}_2 := 2\tilde{e}_2 e^\ell n \log C_{\Delta} + \frac{1}{2} \sqrt{2\pi} \tilde{e}_2 e^\ell n.
\] (S.25)

Here, we use \(\Gamma(1/2) = \sqrt{\pi}\). Because \(C_{\Delta} = O(\sqrt{n})\), the first terms in (S.25) are dominant. We thus obtain the primary inequality in Theorem 1. This completes the proof of Theorem 1.
A. Proof of Proposition 3.

Let \( m \) be a positive even integer. Subsequently, we define the \( m \)th order moment of the observable

\[
M_{U,\Delta}(m) := \int_{-\infty}^{\infty} (x - \langle \Omega \rangle_{\beta})^m P_{U,\Delta}(x) dx.
\]

We note the following relation:

\[
M_{U,\Delta}(m) = \frac{1}{N_{U,\Delta}} \sum_{E \in (U-\Delta, U]} \langle E | (\Omega - \langle \Omega \rangle_{\beta})^m | E \rangle
\]

\[
\leq \frac{1}{N_{U,\Delta}} \sum_{E \in (U-\Delta, U]} \langle E | (\Omega - \langle \Omega \rangle_{\beta})^m | E \rangle = \langle (\Omega - \langle \Omega \rangle_{\beta})^m \rangle_{U,\Delta},
\]

where we used the following relation that is valid for any state \( |\psi\rangle \) from the convexity of the function \( x^m \) with even \( m \)

\[
\langle \psi | (\Omega - \langle \Omega \rangle_{\beta})^m | \psi \rangle \leq \langle \psi | (\Omega - \langle \Omega \rangle_{\beta})^m | \psi \rangle.
\]

We next use the following relation for arbitrary non-negative operators \( \tilde{O} \), which is discussed in Ref. [16] (We also provide the proof in the next subsection)

\[
\frac{\langle \tilde{O} \rangle_{U,\Delta}}{\langle \tilde{O} \rangle_{\beta}} \leq 2e^{\beta \Delta} \left[ 2 + (C_1 \sqrt{n}/\Delta) \right].
\]

Applying the non-negative operator \( \tilde{O} = (\Omega - \langle \Omega \rangle_{\beta})^m \) to this inequality, we obtain the following relation:

\[
M_{U,\Delta}(m) \leq \langle (\Omega - \langle \Omega \rangle_{\beta})^m \rangle_{U,\Delta} \leq 2e^{\beta \Delta} \left[ 2 + (C_1 \sqrt{n}/\Delta) \right] \langle (\Omega - \langle \Omega \rangle_{\beta})^m \rangle_{\beta}.
\]

By combining the inequality above with Markov’s inequality, we obtain

\[
P_{U,\Delta}(|x - \langle \Omega \rangle_{\beta}| \geq x_0) = P_{U,\Delta}(x - \langle \Omega \rangle_{\beta})^m \geq x_0^m)
\]

\[
\leq \frac{M_{U,\Delta}(m)}{x_0^m} \leq 2e^{\beta \Delta} \left[ 2 + (C_1 \sqrt{n}/\Delta) \right] \frac{\langle (\Omega - \langle \Omega \rangle_{\beta})^m \rangle_{\beta}}{x_0^m}.
\]

From Lemma 1, the moment \( \langle (\Omega - \langle \Omega \rangle_{\beta})^m \rangle_{\beta} \) satisfies the inequality (S.8). Hence, the inequality (S.21) can be derived by choosing \( m \) as in Eq. (S.12) such that inequality (S.14) holds. This completes the proof of Proposition 3.

\[ \square \]

B. Proof of the inequality (S.29)

We follow the proof in Ref. [16]. We start with the following inequality:

\[
\langle \tilde{O} \rangle_{U,\Delta} = \frac{1}{N_{U,\Delta}} \sum_{E \in (U-\Delta, U]} \langle E | \tilde{O} | E \rangle
\]

\[
\leq e^{\beta U} \frac{1}{N_{U,\Delta}} \sum_{E \in (U-\Delta, U]} e^{-\beta E} \langle E | \tilde{O} | E \rangle
\]

\[
\leq \frac{Z_{\beta} e^{\beta U}}{N_{U,\Delta}} \sum_{E \in (-\infty, \infty]} e^{-\beta E} \langle E | \tilde{O} | E \rangle = \left( Z_{\beta} e^{\beta U} / N_{U,\Delta} \right) \langle \tilde{O} \rangle_{\beta}.
\]

To bound \( (Z_{\beta} e^{\beta U} / N_{U,\Delta}) \) from above, we consider that the concentration inequality (S.14) can be applied to the Hamiltonian \( H \) because the Hamiltonian satisfies the criterion of \( \Omega \), (S.7) by setting \( \ell = \ell_0 \). By applying \( \Omega = H \) in the probability distribution (S.10), the concentration is bound for the distribution of the canonical distribution. This implies that the finite distribution is exponentially dominated by the regime around the average. Hence, the regime \( \zeta_{\beta} \) exists that satisfies

\[
\text{tr} \left[ \sum_{E \in \zeta_{\beta}} \frac{e^{-\beta E}}{Z_{\beta}} |E\rangle \langle E| \right] \geq 1/2,
\]

\[
\zeta_{\beta} := \left( \langle H \rangle_{\beta} - C_1 \sqrt{n}/2, \langle H \rangle_{\beta} + C_1 \sqrt{n}/2 \right).
\]
where \( C_1 \) depends only on \( d, \xi, \) and \( \ell_0 \). Let us define the following:

\[
\hat{Z} := \text{tr} \left[ \sum_{E \in \zeta_{\beta}} e^{-\beta E} |E\rangle \langle E| \right] \geq Z_{\beta}/2. \tag{S.35}
\]

Subsequently, using a slightly extended regime \( \zeta_{\beta} := \langle (H)_{\beta} - \Delta - C_1 \sqrt{n}/2 , (H)_{\beta} + \Delta + C_1 \sqrt{n}/2 \rangle \), the quantity \( \hat{Z} \) is bounded from above as follows:

\[
\hat{Z} \leq \sum_{\nu \in \mathbb{Z}^2, \Delta \in \zeta_{\beta}} N_{\nu, \Delta} e^{-\beta \Delta (\nu - 1)},
\]

\[
\leq e^\beta \Delta \left[ 2 + (C_1 \sqrt{n}/\Delta) \right] \max_{\nu \in \mathbb{Z}} (N_{\nu, \Delta} e^{-\beta \nu} \Delta)
\]

\[
= e^\beta \Delta \left[ 2 + (C_1 \sqrt{n}/\Delta) \right] N_{\nu, \Delta} e^{-\beta \nu \Delta} \tag{S.36}
\]

\[
= e^\beta \Delta \left[ 2 + (C_1 \sqrt{n}/\Delta) \right] N_{U, \Delta} e^{-\beta U},
\]

where we use the definition of \( U \) in Eq. (S.19). We note \( Z_{\beta} \leq 2\hat{Z} \) as well as the inequalities (S.36) and (S.32) and subsequently arrive at the following relation:

\[
\frac{\langle \hat{O} \rangle_{U, \Delta}}{\langle \hat{O} \rangle_{\beta}} \leq \frac{2\hat{Z} e^{\beta U}}{N_{U, \Delta}} \leq 2e^\beta \Delta \left[ 2 + (C_1 \sqrt{n}/\Delta) \right]. \tag{S.37}
\]

This completes the proof. \( \square \)

### III. WEAK ETH FROM THEOREM 1

From the definition of (S.20), Proposition 3 provides the probability such that a randomly chosen eigenstate \(|E_j\rangle\) from the energy shell satisfies

\[
\frac{1}{n} |\langle E_j | \Omega | E_j \rangle - \langle \Omega \rangle_{U, \Delta}^{\text{mc}}| \leq n^{-\epsilon} \quad (0 < \epsilon < 1/2). \tag{S.38}
\]

Because this probability subexponentially converges to 1 as \( 1 - \exp \left[ -O \left( \frac{n^{1/2}}{n^{1/3}} \right) \right] \), we have \( \langle E_j | \Omega | E_j \rangle / n \approx \langle \Omega \rangle_{U, \Delta}^{\text{mc}} / n \) with a probability of almost 1 for a sufficiently large \( n \).

For a more quantitative discussion, we calculate the variance in the energy shell:

\[
\frac{1}{N_{U, \Delta}} \sum_{E_j \in (U^{-\Delta}, U]} \left( \langle E_j | \Omega | E_j \rangle \right)^2 - \left( \frac{1}{N_{U, \Delta}} \sum_{E_j \in (U^{-\Delta}, U]} \langle E_j | \Omega | E_j \rangle \right)^2, \tag{S.39}
\]

which is equivalent to \( M_{U, \Delta}(2) - [M_{U, \Delta}(1)]^2 \). Recall that the function \( M_{U, \Delta}(m) \) has been defined in Eq. (S.26). Our task is to calculate

\[
M_{U, \Delta}(2) - [M_{U, \Delta}(1)]^2 = \int_{-\infty}^{\infty} x^2 P_{U, \Delta}(x) dx - \left( \int_{-\infty}^{\infty} x P_{U, \Delta}(x) dx \right)^2 \leq \int_{-\infty}^{\infty} x^2 P_{U, \Delta}(x) dx, \tag{S.40}
\]

where we set \( \langle \Omega \rangle_{\beta} = 0 \). Because of the inequality (S.21), we can utilize Lemma 2 by choosing the parameters \((\gamma, \sigma, x_1)\) in Eq. (S.23). From the inequality (S.16) with \( k = 2 \), a straightforward calculation yields

\[
\int_{-\infty}^{\infty} x^2 P_{U, \Delta}(x) dx \leq \max(\tilde{A}_1, \tilde{A}_2) \tag{S.41}
\]

with

\[
\tilde{A}_1 := \tilde{c}_1 n (2 \log C_{\Delta})^{d+1} + 2^{d+1} \tilde{c}_1 n (d+1)!,
\]

\[
\tilde{A}_2 := 2 \tilde{c}_2 \ell^d n \log C_{\Delta} + 2 \tilde{c}_2 \ell^d n. \tag{S.42}
\]

Therefore, provided that \( \Delta = 1 / \text{poly}(n) \), this estimation provides the upper bound of the variance of \( \Omega / n \) by \( O(\log^{d+1}(n)/n) \).
IV. PROOF OF THEOREM 2.

In this section, we prove Theorem 2. The proof is almost the same as that of Theorem 1. We start by defining the probability distribution to observe the value $x$ for the given observable $E$:

$$P_E(x) = \text{tr} \left[ |E\rangle\langle E| \delta(x - \Omega) \right]. \quad (S.43)$$

Subsequently, we consider the cumulative distribution $P_E(|x - \langle \Omega \rangle_{\beta^*}| \geq x_0)$ where, at this stage, the inverse temperature $\beta^*$ is arbitrary. From Markov’s inequality with a positive even integer $m$, we have the following relation:

$$P_E(|x - \langle \Omega \rangle_{\beta^*}| \geq x_0) = P_E((x - \langle \Omega \rangle_{\beta^*})^m \geq x_0^m) \leq \frac{\langle E\rangle \langle \Omega - \langle \Omega \rangle_{\beta^*} \rangle^m}{x_0^m}. \quad (S.44)$$

Below, we bound $\langle E \rangle (\Omega - \langle \Omega \rangle_{\beta^*})^m |E\rangle$ from above using $(\langle \Omega - \langle \Omega \rangle_{\beta^*} \rangle^m)_{\beta^*}$. For notational convenience, we define $E_{\beta^*}$ through $Z_{\beta^*} = e^{-\beta^* E_{\beta^*}}$. Note that the operator $(\Omega - \langle \Omega \rangle_{\beta^*})^m$ is a non-negative operator; hence, we can obtain the following relation:

$$\langle E \rangle (\Omega - \langle \Omega \rangle_{\beta^*})^m |E\rangle \leq Z_{\beta^*} e^{\beta^* E} \sum_{E' \in (-\infty,\infty)} e^{-\beta^* E'} (E') (\Omega - \langle \Omega \rangle_{\beta^*})^m |E'\rangle = e^{\beta^* (E - E_{\beta^*})} (\langle \Omega - \langle \Omega \rangle_{\beta^*} \rangle^m)_{\beta^*}. \quad (S.45)$$

Combining inequality (S.44) with this, the following relation is obtained:

$$P_E(|x - \langle \Omega \rangle_{\beta^*}| \geq x_0) \leq e^{\beta^* (E - E_{\beta^*})} \frac{\langle \Omega - \langle \Omega \rangle_{\beta^*} \rangle^m}{x_0^m}. \quad (S.46)$$

From the assumption of the $(r, \xi)$-clustering for the density matrix $\rho_{\beta^*}$, the $m$-th moment $(\langle x - \langle \Omega \rangle_{\beta^*} \rangle^m)_{\beta^*}$ obeys the inequality (S.8) from Lemma 1. Hence, we have

$$P_E(|x - \langle \Omega \rangle_{\beta^*}| \geq x_0) \leq e^{\beta^* (E - E_{\beta^*})} \left[ 3e \left( \bar{c}_2 \frac{m+1}{2} \right)^{m/2} + \left( \frac{\bar{c}_1 m}{2x_0^2} \right)^{m/2} \right]. \quad (S.47)$$

By choosing $m$ as in Eq. (S.12), we arrive at the concentration bound as

$$P_E(|x - \langle \Omega \rangle_{\beta^*}| \geq x_0) \leq \min \left\{ 1, e^{\beta^* (E - E_{\beta^*})} (e + 3e\xi) \max \left( e^{-|x_0^2/(\bar{c}_1 n)|^{1/(d+1)}}, e^{-x_0^2/(\bar{c}_1 n)} \right) \right\}. \quad (S.48)$$

Having obtained the concentration inequality, we evaluate the integration bound:

$$\langle |E\rangle | E - \langle \Omega \rangle_{\beta^*} \rangle = \int_{-\infty}^{\infty} |x - \langle \Omega \rangle_{\beta^*} | P_E(x) dx \leq \int_{-\infty}^{\infty} |x - \langle \Omega \rangle_{\beta^*} | P_E(x) dx. \quad (S.49)$$

For evaluating the most right expression in (S.49), we use Lemma 2 with $k = 1$. From the inequality given in (S.48), the parameter sets in Lemma 2 are identified as

$$a = \langle \Omega \rangle_{\beta^*} ,$$

$$\{ \gamma, \sigma, x \} = \{ 2/(d + 1), (\bar{c}_2 n)^{1/d+1}, \beta^* (E - E_{\beta^*}) + \log(e + 3e\xi) \} \quad \text{and} \quad \{ 2, \bar{c}_2 \ell^d n, \beta^* (E - E_{\beta^*}) + \log(e + 3e\xi) \}.$$

We subsequently obtain the following from Ineq (S.16):

$$\langle |E\rangle | E - \langle \Omega \rangle_{\beta^*} \rangle \leq \max(\tilde{B}_1, \tilde{B}_2), \quad (S.50)$$

where

$$\tilde{B}_1 := \sqrt[4]{\bar{c}_1 n \left[ 2\beta^* (E - E_{\beta^*}) + 2 \log(e + 3e\xi) \right]^{1/2} + 2(d-1/2)(d+1) \sqrt{\bar{c}_1 n} [(d + 1)/2] } ,$$

$$\tilde{B}_2 := \sqrt{2\bar{c}_2 \ell^d n \left[ 2\beta^* (E - E_{\beta^*}) + 2 \log(e + 3e\xi) \right] + 1/2 \sqrt{2\bar{c}_2 \ell^d n} }. \quad (S.51)$$

Therefore, the upper bound (S.49) reduces to

$$\frac{1}{n} \langle |E\rangle | E - \langle \Omega \rangle_{\beta^*} \rangle \leq \frac{1}{\sqrt{n}} \max \left( (\bar{c}_1 [\beta^* (E - E_{\beta^*})])^{(d+1)/2}, (\bar{c}_2 [\ell^d \beta^* (E - E_{\beta^*})])^{1/2} \right). \quad (S.52)$$
where $c_1', c_2'$ are constants that only depend on $d$, $\xi$, and $\alpha$. Note that $\vert\langle E\vert \Omega \rangle \vert = \vert \langle E\vert \Omega \rangle - \langle \Omega \vert \beta^\ast \vert \rangle$ for $\langle \Omega \vert \beta^\ast \vert \rangle = 0$. This completes the proof of Theorem 2. □

We remark that the inequality (S.52) also holds for the ground state:

$$
\frac{1}{n} \vert \langle E_0 \vert \Omega \rangle - \langle \Omega \vert \beta^\ast \vert \rangle \vert \leq \frac{1}{\sqrt{n}} \max \left( c_1' [\beta^\ast (E - E_0)]^{(d+1)/2}, c_2' [\rho E]^{1/2} \right),
$$

where $|E_0\rangle$ is the ground state. Recall that we set the ground energy equal to zero. By combining the inequalities (S.52) and (S.53) with the triangle inequality, we have

$$
\frac{1}{n} \vert \langle E \vert \Omega \rangle - \langle E_0 \vert \Omega \rangle \vert \leq \frac{1}{\sqrt{n}} \max \left( c_1' [\beta^\ast (E - E_0)]^{(d+1)/2}, c_2' [\rho E]^{1/2} \right).
$$

When the ground states exhibit a $D$-fold degeneracy, we denote the ground states by $\{ |E_j\rangle \}_{j=0}^{D-1}$ (i.e., $H|E_j\rangle = 0$ for $j \leq D - 1$) and consider

$$
\langle \Omega \rangle_\infty = \frac{1}{D} \sum_{j=0}^{D-1} \langle E_j \vert \Omega \rangle.
$$

We subsequently obtain

$$
\vert \langle \Omega \rangle_\infty - \langle \Omega \vert \beta^\ast \vert \rangle \vert = \frac{1}{D} \left| \sum_{j=0}^{D-1} \langle E_j \vert \Omega \rangle - \langle \Omega \vert \beta^\ast \vert \rangle \right| \leq \frac{1}{D} \sum_{j=0}^{D-1} \vert \langle E_j \vert \Omega \rangle - \langle \Omega \vert \beta^\ast \vert \rangle \vert.
$$

Therefore, we can derive the same inequality as (S.54) for the degenerate ground states.

V. CORRELATION LENGTH VS. INVERSE TEMPERATURE IN MANY-BODY LOCALIZED SYSTEMS

We herein discuss that in one-dimensional disordered systems, the clustering condition can break down at sufficiently low temperatures. For such disordered systems, we consider many-body localized systems, where thermalization do not occur. Hence, we consider the $xy$ model with random magnetic fields:

$$
H = \sum_{i=1}^{n} (3/4) \sigma_i^x \sigma_{i+1}^x + (1/4) \sigma_i^y \sigma_{i+1}^y + \sum_{i=1}^{n} h_i \sigma_i^z,
$$

where each of $\{ h_i \}_{i=1}^{n}$ is chosen randomly from a uniform distribution in $[-1, 1]$. This system can be mapped onto a bilinear fermionic system; hence, the system cannot be regarded as a many-body localized system but as a system exhibiting the Anderson localization. However, we expect to extract the essential property even with this model. This model allows us to consider a large system by which an accurate correlation length can be computed.

We where we discuss that in one-dimensional disordered systems, the clustering condition can break down at sufficiently low temperatures. We consider the mutual information $I_{ij}(\rho_\beta)$ between the sites $i$ and $j$ is defined as $I_{ij}(\rho_\beta)$ for $1 \leq \beta \leq 20$. In Fig. 2 (a), we calculate the $\beta$-dependence of the correlation length $\xi(\beta)$. Furthermore, we present the distance dependence of the mutual information $I_{ij}(\rho_\beta)$ for $\beta = 3$ (red plots), $\beta = 7$ (blue plots), $\beta = 13$ (purple plots) in Fig. 1 (b). From this plot, the correlation length diverges as $\beta$ increases and the clustering property breaks down at sufficiently low temperatures.

VI. REDUCED DENSITY MATRICES OF $\rho_{U,\Delta}$ AND $\rho_\beta$ AND THEOREM 1

To compare the result from Theorem 1 with the previous one by Bråndao and Cramer [15], we estimate the trace distance between the reduced density matrices of the canonical and micro-canonical states. Let $\{ B_s \}_{s=1}^{n_x}$ be the set of all $d$-dimensional $\ell \times \ell \times \cdots \times \ell$ hypercubes (see Fig. 3), where we assume that the total number of hypercubes $n_\ell$ is $n/\ell^d$ (i.e., $n_\ell := n/\ell^d$). We now denote the reduced density matrices within the hypercubes $\{ B_s \}_{s=1}^{n_x}$ by $\{ (\rho_\beta)_{B_s} \}_{s=1}^{n_x}$ and $\{ (\rho_{U,\Delta})_{B_s} \}_{s=1}^{n_x}$. From theorem 1, we can prove

$$
\frac{1}{n_\ell} \sum_{s=1}^{n_x} \Vert (\rho_{U,\Delta})_{B_s} - (\rho_\beta)_{B_s} \Vert_1 \leq \max \left[ c_1 \ell^{-\frac{d}{2}} \log \frac{d+1}{\sqrt{\pi}}, c_2 \sqrt{\log \left( \frac{\sqrt{\pi}}{\ell} \right)} \right],
$$

(S.58)
where \( \| \cdots \|_1 \) denotes the trace norm (see below for the derivation). If we assume the translation invariance of the Hamiltonian (3), all the reduced density matrices \( \{ \rho_{B_s} \}_{s=1}^n \), each of which contains \( \ell \times \ell \) spins (\( \ell = 4 \) in the picture above), do not depend on the index \( s \). Hence, for an arbitrary hypercube \( B \), the norm difference between \( \| \rho_{B} \|_B \) and \( \| (\rho_{B};\Delta) \|_B \) is smaller than \( O(1/\sqrt{n}) \). From the inequality (S.58), provided that \( \ell^d = O(n^{1-\epsilon}) \) (\( \epsilon > 0 \)) and \( \Delta = 1/poly(n) \), the reduced density matrices between the canonical and the microcanonical ensembles are indistinguishable in the limit of \( n \to \infty \), where the size dependence of the error behaves as \( O(1/\sqrt{n}) = O(n^{-\epsilon/2}) \) with a logarithmic correction \( poly[\log(n)] \).

The upper bound of (S.58) qualitatively improves the results of previous studies [8–11, 15, 16]. In Refs [8–11], the thermodynamic limit \( n \to \infty \) has been considered, and the energy width \( \Delta \) and block size \( \ell \) are assumed to be independent of the system size \( n \). In Ref [15], the finite-size effect has been considered for the first time, where the LHS of (S.58) has been bounded from above by \( C \max(\sqrt{\ell d(d+1)/n}, n^{-1/(2d+2)}) \) with \( C = poly[\log(n)] \) under the assumptions of the clustering and \( \Delta = O(\log_2 n) \). Subsequently, the block size \( \ell^d \) can be as large as \( \ell^d = n^{1/(d+2)} \) (\( \epsilon > 0 \)). In Ref. [16], this upper bound for the LHS of (S.58) has been improved to \( \sqrt{\Delta^{-1}} \ell^d/n^{1/2} \) under some additional assumptions. Then, the ensemble equivalence holds for \( \ell^d = \Delta \cdot n^{1/2-\epsilon} \) (\( \epsilon > 0 \)).

**A. Proof of the inequality (S.58)**

We first consider that for an arbitrary hypercube \( B_s \), there exists an operator \( O_{B_s} \) with \( \| O_{B_s} \| = 1 \) such that

\[
\| (\rho_{\nu,\Delta})_{B_s} - (\rho_{B_s})_{B_s} \|_1 = \text{tr} [ O_{B_s} ((\rho_{\nu,\Delta})_{B_s} - (\rho_{B_s})_{B_s}) ].
\]

We subsequently choose \( \Omega = \sum_{i=1}^{n} \Omega_i \) as

\[
\Omega_i = O_{B_s} \quad \text{for } i \in B_s,
\]

FIG. 2. (color online) Numerical demonstrations. The first figure (a) shows \( \beta \)-dependence of the correlation length \( \xi(\beta) \) in the canonical state \( \rho_{\beta} \) for one sample of the random Hamiltonian (S.57). The correlation length \( \xi(\beta) \) is calculated from the mutual information between the spin pairs of \( (r, n - r + 1)_{r=1}^{n/2} \) with \( n = 100 \). The second figure (b) shows the distance dependence of the mutual information \( I_{i,j}(\rho_{\beta}) \) for \( \beta = 3 \) (red plots), \( \beta = 7 \) (blue plots), \( \beta = 13 \) (purple plots).

FIG. 3. (color online). Schematics of the setup in Ineq. (S.58) on a two-dimensional square lattice. We decompose the lattice to \( n_{\ell} \) subsets \( \{B_s\}_{s=1}^{n_{\ell}} \), each of which contains \( \ell \times \ell \) spins (\( \ell = 4 \) in the picture above). We focus on the reduced density matrices with respect to \( \{B_s\}_{s=1}^{n_{\ell}} \), and estimate the norm difference in Ineq. (S.58) between the canonical and the microcanonical states.
which yields

\[
\frac{1}{n}|\langle \Omega \rangle_{\ell, \Delta} - \langle \Omega \rangle_\beta| = \frac{\ell^d}{n} \sum_{s=1}^{n_\ell} |\langle O_{B_s} \rangle_{\ell, \Delta} - \langle O_{B_s} \rangle_\beta| = \frac{1}{n\ell} \sum_{s=1}^{n_\ell} \| (\rho_{\ell, \Delta} B_s - (\rho_\beta B_s)\|_1,
\]

(S.61)

where we use the assumption of \( n_\ell = n/\ell^d \). By combining the inequality (S.61) with Theorem 1, we obtain the inequality (S.58).

VII. CONCENTRATION BOUND FROM THE CLUSTERING OF CORRELATION

We herein show the proof of Lemma 1 that reduces to the concentration bound (S.14). The proof that we address herein is essentially the same as that of Ref. [24] but is more general and simplified. To account for the lattice geometry, we consider a generic graph \( G = (V, E) \) with \(|V| = n\), where each of the spin sits on the vertex. For two arbitrary subsets \( X, Y \subset V \), we define the distance \( \text{dist}(X, Y) \) as the minimum path length from \( X \) to \( Y \) on the graph. For an arbitrary vertex \( i \in V \), we define the set of \( X_i^{(s)} \in V \) (\( s \in \mathbb{N} \)) as

\[
X_i^{(s)} := \{ j \in V | \text{dist}(j, i) \leq s \}.
\]

(S.62)

Each of the local terms \( \{ \Omega_i \}_{i \in V} \) in Eq. (S.7) is supported on the subset \( X_i^{(\ell)} \). We introduce a geometric parameter \( \alpha \) that depends on the lattice structure as

\[
|X_i^{(s)}| \leq \alpha s^d,
\]

(S.63)

where \( d \) was defined as the spatial dimension of the lattice.

A. Proof of Lemma 1

We define \( \delta \Omega := \Omega - \langle \Omega \rangle_\rho \) for \( \forall i \in V \) that yields \( \langle \delta \Omega \rangle_\rho = 0 \). We calculate the upper bound of \( \langle (\Omega - \langle \Omega \rangle_\rho)^m \rangle_\rho \), where \( m \) is a positive even integer. Next, we decompose

\[
\langle (\Omega - \langle \Omega \rangle_\rho)^m \rangle_\rho = \sum_{i_1, i_2, \ldots, i_m \in V} \langle \delta \Omega_{i_1} \delta \Omega_{i_2} \ldots \delta \Omega_{i_m} \rangle_\rho.
\]

(S.64)

We subsequently define \( \ell_{i_1, \ldots, i_m} \) as

\[
\ell_{i_1, \ldots, i_m} := \max_{1 \leq q \leq m} [\text{dist}(i_q, \{ i_r \}_{r \neq q})].
\]

(S.65)

That is, the most spatially isolated vertex in \( \{ i_1, \ldots, i_m \} \) is separated from the other vertices by a distance \( \ell_{i_1, \ldots, i_m} \).

If \( \ell_{i_1, \ldots, i_m} = \tilde{l} \), there exists \( i_q \in \{ i_1, \ldots, i_m \} \) such that \( \text{dist}(i_q, \{ i_r \}_{r \neq q}) = \tilde{l} \). Because each of the \( \delta \Omega_i \) is supported on the subset \( X_i^{(\ell)} \) from the assumption (S.7), the two operators \( \delta \Omega_{i_q} \) and \( \delta \Omega_{i_1} \cdots \delta \Omega_{i_{q-1}} \delta \Omega_{i_{q+1}} \cdots \delta \Omega_{i_m} \) are separated at least by the distance \( \tilde{l} - 2\ell \). Hence, for \( \tilde{l} \geq 2\ell + r \), the \( \langle r, \xi \rangle \)-clustering condition yields

\[
|\langle \delta \Omega_{i_1} \delta \Omega_{i_2} \ldots \delta \Omega_{i_m} \rangle_\rho - \langle \delta \Omega_{i_1} \rangle_\rho \langle \delta \Omega_{i_2} \cdots \delta \Omega_{i_{q-1}} \delta \Omega_{i_{q+1}} \cdots \delta \Omega_{i_m} \rangle_\rho | \leq 2^m e^{-(l - 2\ell)/\xi},
\]

(S.66)

where we use \( \| \delta \Omega_i \| \leq 2 \) from \( \| \Omega \| \leq 1 \) for \( \forall i \in V \).

We define \( C_{l} (C_{\leq l}) \) as the set of string \( \{ i_1, \ldots, i_m \} \) such that \( \ell_{i_1, \ldots, i_m} = \tilde{l} (\ell_{i_1, \ldots, i_m} \leq \tilde{l}) \). Here, we take the element order in the string into account. For instance, we count \( (i_1, i_2) \) and \( (i_2, i_1) \) as a different string if \( i_1 \neq i_2 \). We
To count the total number of strings in the set \( \mathcal{C} \). Herein, we use the inequality (S.66) in the first inequality as well as the relation of the core vertices within the distance  \( \tilde{l} \). FIG. 4. (color online). Schematics of the core vertices (red dots) and the surrounding vertices (black dots). Around each of the core vertices within the distance  \( \tilde{l} \) (blue shaded region), there exists at least one surrounding vertex. Any string \( \{i_1, \ldots, i_m\} \in \mathcal{C}_{\leq \tilde{l}} \) can be decomposed into \( u \) core vertices and \((m-u)\) surrounding vertices with  \( u \leq m/2 \).

Mathematically, for a core vertex \( \tilde{X} \), there exists \( \tilde{i} \in \{i_1, \ldots, i_m\} \setminus \{i_1, \ldots, i_u\} \) such that

\[
\text{dist}(i_1, \tilde{i}) \leq \tilde{l} \quad \text{or} \quad \tilde{i} \in X_{i_1}^{(l)}
\]

with  \( X_{i_1}^{(l)} \) defined in Eq. (S.62). This constraint implies that the number of core vertices is smaller than  \( m/2 \) (i.e., \( u \leq m/2 \)). We note that any string in  \( \mathcal{C}_{\leq \tilde{l}} \) can be described by the formalism above. Thus, our task is to count all the possible arrangements of 1) the core vertices, 2) the surrounding vertices for  \( u = 1, 2, \ldots, m/2 \), and 3) the order of elements in the string. For a fixed  \( u \), it is bounded from above as follows:

1. The number of possible locations of the core vertices is clearly smaller than  \( n^u \).

2. After the locations of the core vertices are determined, there are at the most  \(|X_{i_1}^{(l)} \cup X_{i_2}^{(l)} \cup \cdots \cup X_{i_u}^{(l)}| \leq u(\tilde{l}^u) \) methods of positioning, at which each of the surrounding vertices can be placed. In total, the number of possible arrangements of the surrounding vertices is smaller than  \( u(\tilde{l}^u)^{m-u} \).

3. We next consider the string order. Inside each set of the core and surrounding vertices, the order is already considered by the two estimations above. Hence, we must consider the order of the types of vertices (i.e., “core” and “surrounding”). The number of this combination is  \( \binom{m}{u} \).

Herein, we use the inequality (S.66) in the first inequality as well as the relation \( \|\delta \Omega_i\| \leq 2 \). Furthermore, in the second last inequality, we use \( e^{-\tilde{l}(2\tilde{l})/\xi} \leq e^{-\tilde{l}/(3\xi)} \) for  \( \tilde{l} \geq 3\xi \). At the last inequality, we use a trivial relation where \( \mathcal{C}_{\leq \tilde{l}} \) is a larger set than \( \mathcal{C}_l \).

To count the total number of strings in the set \( \mathcal{C}_{\leq \tilde{l}} \), we follow the strategy below. We first choose \( u \) “core” vertices \( \{i_1, \ldots, i_u\} \) from  \( n \) vertices. We next assign the other \((m-u)\) vertices. We refer to the \((m-u)\) vertices \( \{i_1, \ldots, i_m\} \setminus \{i_1, \ldots, i_u\} \) as the “surrounding” vertices. Each of the core vertices contains at least one surrounding vertex within the distance  \( \tilde{l} \) around it (otherwise, the distance \( \ell_{i_1, \ldots, i_m} \) exceeds  \( \tilde{l} \). See the schematics in Fig. 4).

Mathematically, for a core vertex  \( i_q \), there exists  \( \tilde{i} \in \{i_1, \ldots, i_m\} \setminus \{i_1, \ldots, i_u\} \) such that

\[
\text{dist}(i_q, \tilde{i}) \leq \tilde{l} \quad \text{or} \quad \tilde{i} \in X_{i_q}^{(\ell)}
\]
We thus obtain
\[
\sum_{\{i_1, i_2, \ldots, i_m\} \in C_{\leq \ell}} 1 \leq \sum_{u=1}^{m/2} \binom{m}{u} n^u [u(\alpha \tilde{d})]^{m-u} \leq [mn(\alpha \tilde{d})/2]^{m/2} \sum_{u=1}^{m/2} \binom{m}{u} \\
\leq 2^m [mn(\alpha \tilde{d})/2]^{m/2} \leq [2mn(\alpha \tilde{d})]^{m/2}. \tag{S.69}
\]

By combining the inequality (S.69) with (S.67),
\[
\langle [\Omega]^m \rangle \rho \leq [8mn(3\ell)^d]^{m/2} + \sum_{l=3\ell+1}^{\infty} [8mn(\alpha \tilde{d})]^{m/2} e^{-l/(3\ell)} \\
\leq [8\alpha mn(3\ell)^d]^{m/2} + 3\xi [8\alpha mn^{d+1} (3\xi d/2)^d]^{m/2}, \tag{S.70}
\]
where the second inequality is from
\[
\sum_{l=3\ell+1}^{\infty} [8mn(\alpha \tilde{d})]^{m/2} e^{-l/(3\ell)} \leq (8\alpha mn)^{m/2} \int_{0}^{\infty} x^{dm/2} e^{-x/(3\ell)} \, dx \\
= (8\alpha mn)^{m/2} (3\xi)^{dm/2+1} (dm/2)! \leq 3\xi [8\alpha mn^{d+1} (3\xi d/2)^d]^{m/2}. \tag{S.71}
\]
Note that we have \(s! \leq s^s\) for an arbitrary integer \(s\). This completes the proof of Lemma 1. \(\square\)