Is microcanonical ensemble stable?

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Abstract

No, in a rigorous sense specified below.

1 Introduction

For the purpose of this work, it suffices to work with a chain of n spins (qu$d$its), each of which has local dimension $d = \Theta(1)$. We are given a local Hamiltonian $H = \sum_{j=1}^{n-1} H_j$ with open boundary conditions, where $\|H_j\| = O(1)$ acts on the spins j and $j+1$ (nearest-neighbor interaction). Since the standard bra-ket notation can be cumbersome, in most but not all cases quantum states and their inner products are simply denoted by $\psi, \phi, \dots$ and $\langle\psi, \phi\rangle$, respectively, cf. $\||\psi\rangle - |\phi\rangle\|$ versus $\|\psi - \phi\|$. Let $\psi_1, \psi_2, \dots, \psi_{d^n}$ be the eigenstates of H with the corresponding eigenvalues $E_1 \le E_2 \le \cdots \le E_{d^n}$ in non-descending order. The projector onto the energy window $[E - \delta, E + \delta]$ is given by

$$P(E, \delta) = \sum_{j:|E_j - E| \le \delta} |\psi_j\rangle\langle\psi_j|. \tag{1}$$

A microcanonical ensemble is a fundamental concept in statistical mechanics. Throughout this paper, we only consider the physical situation that the bandwidth is (at most) a constant.

Definition 1 (microcanonical ensemble)**.** An (exact) microcanonical ensemble of energy E and bandwidth $2\Delta_e = O(1)$ is the set

$$EXT = \{\psi : \psi = P(E, \Delta_e)\psi\}. \tag{2}$$

The state in practice may well only be approximately rather than exactly in a microcanonical ensemble. A state is in an approximate microcanonical ensemble if the population "leakage" outside a distance (in the spectrum) from the target energy is exponentially small in the distance.

Definition 2 (approximate microcanonical ensemble)**.** An approximate microcanonical ensemble of energy E and bandwidth $2\Delta_a = O(1)$ is the set

$$APX = \{\phi : |\langle\phi, P(E, x)\phi\rangle| \ge 1 - O(e^{-x/\Delta_a}), \forall x \ge 0\}. \tag{3}$$

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The stability of a microcanonical ensemble can be phrased as follows. Suppose a microcanonical ensemble has a universal physical property in the mathematical sense of an inequality satisfied by all states in EXT. Is this inequality valid (possibly up to small corrections) for all states in APX? If not, the physical property of the microcanonical ensemble is not robust against perturbations.

One might tend to believe that a microcanonical ensemble is stable due to a continuity argument. Given $\phi \in APX$, let $\psi = P(E, \Delta_e)\phi / \|P(E, \Delta_e)\phi\|$ so that $\psi \in EXT$ and $|\langle \psi, \phi \rangle| \geq 1 - O(e^{-\Delta_e/\Delta_a})$. For $\Delta_a \ll \Delta_e = O(1)$, the states ψ, ϕ are close to each other, and thus believed to behave similarly. The pitfall of this hand-waving argument is that ψ, ϕ differ only by a small constant, which has the potential of affecting the physics significantly.[1] Therefore, the continuity argument (if not combined with more sophisticated reasonings) does not immediately lead to the stability of a microcanonical ensemble.

We show that a microcanonical ensemble is unstable from an entanglement point of view.

Definition 3 (entanglement entropy)**.** The Renyi entanglement entropy $R_\alpha (0 < \alpha < 1)$ of a bipartite (pure) quantum state $\rho_{AB} = |\psi\rangle\langle\psi|$ is defined as

$$R_\alpha(\psi) = (1-\alpha)^{-1} \log \operatorname{tr} \rho_A^\alpha, \quad \rho_A = \operatorname{tr}_B \rho_{AB}, \tag{4}$$

where ρ_A is the reduced density matrix. The von Neumann entanglement entropy is defined as

$$S(\psi) = -\operatorname{tr}(\rho_A \log \rho_A) = \lim_{\alpha \to 1^-} R_\alpha(\psi). \tag{5}$$

Remark. For fixed ψ, the Renyi entanglement entropy R_α is a non-increasing function of α.

We consider the evolution of entanglement entropy across a particular cut.

Definition 4 (dynamical entanglement scaling exponent)**.** Suppose the state ψ_0 at time $t = 0$ has bond dimension D_0 across the cut. Let z be a nonnegative number such that

$$R_\alpha(e^{-iHt}\psi_0) \leq \log D_0 + O(t^z \operatorname{poly}\log t), \ \forall t. \tag{6}$$

Remark. On the right-hand side, the first term is an upper bound on the entanglement of the initial state. Note that D_0 is allowed to grow (even exponentially, e.g., $D_0 = d^{n/100}$) with the system size. The second term, which involves polylogarithmic corrections due to a technical reason, characterizes the growth of entanglement.

Traditional Lieb-Robinson techniques imply a universal bound $z \leq 1$ for arbitrary initial states. This bound can (cannot) be improved for states in an exact (approximate) microcanonical ensemble.

Theorem 1. *For any initial state $\psi_0 \in EXT$, we have $z \leq 1/2$, and this bound is tight.*

Proposition 1. *There is a Hamiltonian H_{XX} and an initial state $\phi_0 \in APX$ such that $z = 1$.*

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[1]For example, a generic state in a small-constant neighborhood of a product state has volume law for entanglement. The stability of area law for entanglement can be proved, but only if in the presence of additional structure.

2 Proof of Theorem 1

We go beyond traditional Lieb-Robinson techniques using the idea of polynomial approximation. For the dynamics in a microcanonical ensemble, consider the Taylor expansion

$$e^{-iHt}\psi_0 = \sum_{k=0}^{+\infty} \frac{(-iHt)^k}{k!}\psi_0 \approx \sum_{k=0}^{g} \frac{(-iHt)^k}{k!}\psi_0, \tag{7}$$

where $E = 0$ is assumed without loss of generality. The truncation error is upper bounded by

$$\sum_{k=g+1}^{+\infty} \left\| \frac{(-iHt)^k}{k!}\psi_0 \right\| = \sum_{k=g+1}^{+\infty} \left\| \frac{(-iHt)^k}{k!}P(0,\Delta_e)\psi_0 \right\| \le \sum_{k=g+1}^{+\infty} \frac{(\Delta_e t)^k}{k!} \approx \frac{(e\Delta_e t)^g}{g^g}, \tag{8}$$

which is super-exponentially small in g for $g \ge 3\Delta_e t$. Let $\tilde{O}(x) := O(x \operatorname{poly}\log x)$ hide a polylogarithmic factor. A polynomial interpolation argument leads to the following result.

Lemma 1 ([1], Lemma 4.2)**.** *Suppose ψ_0 has bond dimension D_0 across a particular cut. The bond dimension of $p(H)\psi_0$ across the cut is $\le D_0 e^{\tilde{O}(\sqrt{g})}$, where p is an arbitrary polynomial of degree g.*

Combining Lemma 1 with the error estimate (8), a straightforward calculation shows

$$R_\alpha(e^{-iHt}\psi_0) \le \log D_0 + \tilde{O}(\sqrt{\Delta_e t} + 1/\alpha). \tag{9}$$

Therefore, $z \le 1/2$. To prove the tightness of this bound on z, it suffices to construct an example that violates the bound $z \le 1/2 - \delta$ for any $\delta > 0$.

Proposition 2 ([3])**.** *Let H_{Is} be the Hamiltonian of the critical transverse-field Ising chain with length n, and ψ_0 be a product state that respects the Z_2 symmetry of H_{Is}. The entanglement entropy $S(e^{-iH_{\mathrm{Is}}t}\psi_0)$ across the middle cut saturates to $\Omega(n)$ in time $t = O(n)$.*

The Hamiltonian $H'_{\mathrm{Is}} = H_{\mathrm{Is}}/n$ has bandwidth $O(1)$. Hence, any state, including ψ_0, is in a microcanonical ensemble (with respect to H'_{Is}). The entanglement entropy $S(e^{-iH'_{\mathrm{Is}}t}\psi_0)$ saturates to $\Omega(n)$ in time $t = O(n^2)$. This violates the bound $z \le 1/2 - \delta$.

Remark. To approximate the propagator with polynomials, we used the "naive" Taylor expansion, which is known to be non-optimal. The optimal approach is to expand e^{-iHt} in the basis of the Chebyshev polynomials of the first kind. Unfortunately, this only improves the parameters hided in $\tilde{O}(\cdots)$. Also, the bound in Lemma 1 is tight up to polylogarithmic corrections due to the tightness of the bound $z \le 1/2$.

3 Proof of Proposition 1

Consider the XX chain of length $2n$ with a defect in the middle:

$$H_{XX} = (1-\lambda)(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y) + \sqrt{1-\lambda^2}(\sigma_n^z - \sigma_{n+1}^z) - \sum_{j=1}^{2n-1}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right),\ 0 \le \lambda \le 1, \tag{10}$$

where $\sigma_j^x, \sigma_j^y, \sigma_j^z$ are the Pauli matrices at the site j. Let $\phi_0 = |\Uparrow\rangle \otimes |\Downarrow\rangle$ with $|\Uparrow\rangle = |\uparrow\rangle^{\otimes n}$ and $|\Downarrow\rangle = |\downarrow\rangle^{\otimes n}$. The entanglement entropy across the middle cut grows linearly with time only in the presence of a detect $\lambda \ne 1$.

Proposition 3 ([4]). *In the thermodynamic limit, we have*

$$S(e^{-iHt}\phi_0) = h(\lambda^2)t/(4\pi) + O(\log t), \quad h(x) := -x\ln x - (1-x)\ln(1-x). \tag{11}$$

Proposition 4. *The state ϕ_0 is in an approximate microcanonical ensemble with $E = 2\sqrt{1-\lambda^2}$ and $\Delta_a = 20$.*

Proof. We decompose H_{XX} into three parts: $H_{XX} = H_L + H_\partial + H_R$, where H_L, H_R include the terms acting only on the left or right half of the chain, and $H_\partial = -\lambda(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y)$ is the term across the middle cut. Note that H_L, H_R are decoupled from each other. For the domain wall state $\phi_0 = |\Uparrow\rangle \otimes |\Downarrow\rangle$, it is easy to see that $|\Uparrow\rangle$ or $|\Downarrow\rangle$ is an eigenstate of H_L or H_R with energy $\sqrt{1-\lambda^2}$. The proof is completed by applying Theorem 2.3 in Ref. [2]. □

References

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