Why and when does statistical mechanics work for isolated quantum systems? Eigenstate Thermalization Hypothesis

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For an isolated system in classical statistical mechanics, the local Hamiltonian can be determined from classical microstates in this system. Does statistical mechanics also work for isolated quantum systems in the sense that we could have access to their full Hamiltonian through an quantum mechanical analogy? Garrison and Grover proposed that the Eigenstate Thermalization Hypothesis (ETH) implies that a single eigenstate encodes the full Hamiltonian in their paper. [1] To check the validity of ETH, they introduced the notion of "equithermal" (Class I) and "non-equithermal" (Class II) operators, and discussed why and when ETH is satisfied for each class.

INTRODUCTION

It's known to us that the ground states of quantum many-body systems contain information about their excitations, since ground states of local Hamiltonian satisfies the area law of entanglement entropy as discussed in lecture. In this paper, we instead go from the ground state to an excited eigenstate with a finite energy density $\lim_{V\to\infty} E/V \neq 0$, to avoid the exception of eigenstates with zero energy density that continue to satisfy the area law, and consider the information encoded in this single eigenstate.

Srednicki and Deutsch's work on the study of a finite energy density state both lead to suggestion of the "Eigenstate Thermalization Hypothesis" (ETH), which demands that the thermalization occurs at the level of each individual eigenstate.[2] [3] If ETH holds true,

$$\langle\psi|O|\psi\rangle = \frac{tr(Oe^{-\beta H})}{tr(e^{-\beta H})} \tag{0.1}$$

follows, which implies the precise equality between the equal-time correlators of an operator O with respect to a finite energy density eigenstate $|\psi\rangle$ and those from a thermal ensemble in the thermodynamic limit. We choose β so that Eq(0.1) holds true when O equals to the Hamiltonian H, and thus we use $|\psi\rangle_\beta$ for an eigenstate with energy density corresponding to temperature β^{-1}.

This paper gives conjecture and numerical evidence that Eq(1) holds for the following cases. When the subsystem A has volume $V_A/V \to 0$ as $V \to \infty$, it holds for all operators within A. In the more general case of a subsystem A with $0 < V_A/V < f^* \sim O(1)$, it holds for all operators not explicitly involving energy conservation. In particular for $V_A < V/2$, it's shown that it holds for a large class of operator as well.

The case where Eq(0.1) is satisfied for all operators in a subsystem A is equivalent to

$$\rho_A(|\psi\rangle_\beta) = \rho_{A,th}(\beta) \tag{0.2}$$

where $\rho_{A,th}(\beta) = \frac{tr_{\bar{A}}(e^{-\beta H})}{tr(e^{-\beta H})}$, and $\rho_A(|\psi\rangle_\beta) = \mathrm{tr}_{\bar{A}} |\psi\rangle_\beta\, {}_\beta\langle\psi|$. One implication of Eq(0.2) is that the thermodynamical properties of a system at any temperature β^{-1} can be calculated using a single eigenstate. An approximate form of ETH compared to Eq(0.2) is given by

$$\rho_A(|\psi\rangle_\beta) \approx \frac{e^{-\beta H_A}}{tr_A(e^{-\beta H_A})} \tag{0.3}$$

Both Eq(0.2) and Eq(0.3) give the same results for all bulk quantities and correlation functions of operators with support only far from the boundary. The validity of Eq(0.2) and Eq(0.3) is checked in this paper as well.

CONJECTURES AND NUMERICAL RESULTS

Basics of Statistical Mechanics

Start with an isolated system described by classical statistical mechanics. Access to all classical microstates C_A in a small energy window is sufficient for us to determine the underlying local Hamiltonian.

$$P(C_A) = \frac{e^{-\beta E(C_A)}}{\sum_{\{C_A\}} e^{-\beta E(C_A)}} \tag{0.4}$$

Inverse of Eq(0.4) gives the Hamiltonian for subsystem A, and any thermodynamic property at any temperature can be calculated given $E(C_A)$.

How do we go from here to the isolated quantum systems? We will argue that the quantum mechanical analog of Eq(0.4) is given by Eq(0.2),(0.3) through comparing the operators and their canonical expectation values. Based on the conjecture proposed in later sections, we want to check precisely the extent to which the quantities, von Neumann entropy(Class I) and Renyi entropy(Class II) for example, match between a single eigenstate and the canonical ensemble using evidence from the numerical results.

Preparation

To discuss the conditions under which Eq(0.2), Eq(0.3) is valid, the separation of operators in a given Hilbert space into "Equithermal operators" (Class I) and "Non-equithermal operators" (Class II) will be useful. When the reduced density matrix takes the thermal form as given in Eq(0.3), only the eigenstates of H_A at an energy density corresponding to the inverse temperature β contribute to the expectation value of equithermal operators as $V \to \infty$. All the other operators without this property goes into Class II. The extra significance of having ETH to hold for Class II operator is that one is allowed to access the properties of the Hamiltonian at a temperature different than β^{-1}.

Consider the relationship between Eq(0.1) and Eq(0.2), Eq(0.3). Eq(0.1) can be rewritten as

$$\mathrm{tr}_A(\rho_A O) = \frac{\mathrm{tr}_A(O \mathrm{tr}_{\bar{A}}(e^{-\beta H}))}{\mathrm{tr}(e^{-\beta H})} \tag{0.5}$$

If Eq(0.5) holds true for all operators in a subsystem A, then we can show that the expansion of $\rho_A(|\psi\rangle_\beta)$ and $\rho_{A,th}(\beta)$ in terms of complete set of operators in A are equivalent element-by-element by choosing O properly, which directly leads to Eq(0.2). This equality implies that a single eigenstate gives us access to properties of the Hamiltonian at any temperature.

ETH with $V_A \ll V$

In the case when $V_A \ll V$, ETH for Class I operators corresponds to the traditional definition of ETH, where all such operators match their values in the canonical ensemble. Remarkably, this paper extends the validity of ETH in this limit to all Class II operators.

The numerical results presented in this paper substantiate the conjecture that ETH as given by Eq(0.1) is valid for all Class I and Class II operators in the case $V_A \ll V$ as $V \to \infty$. We also expect all the results to hold true for the case where $f \equiv V_A/V \to 0$ as $V_A, V \to \infty$. It follows that ETH as specified by Eq(0.2) also holds when $V_A \ll V$. Thus a single eigenstate of finite energy density encodes information on properties of the system at all temperatures.

Numerical results on the entanglement spectrum of individual eigenstates and the corresponding Schmidt states help with testing the validity of Eq(0.2) and Eq(0.3). Comparing the four different quantities as specified in Fig 1 presents the agreements among $\rho_A(|\psi\rangle_\beta)$, $\rho_{A,th}(\beta)$, the actual Hamiltonian H_A and its expectation value. It follows that the Schmidt eigenvalues and eigenvectors match with that of the thermal density matrix. Directly calculating the overlaps between the eigenvectors of the reduced density matrix $\rho_A(|\psi\rangle_\beta)$ and that of the thermal density matrix $\rho_{A,th}(\beta)$ as in Fig 2 also leads to agreement. Both results strongly support the validity of Eq(0.2) and Eq(0.3).

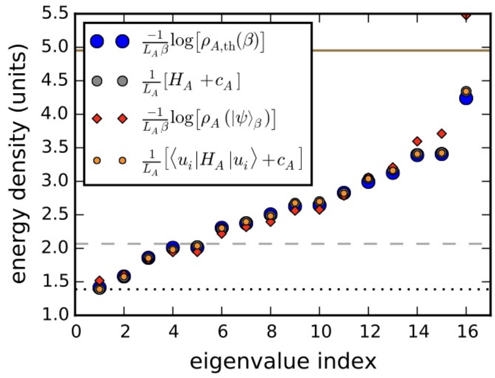

FIG. 1: Comparison of four quantities defined in the inset for an $L_A = 4$ subsystem at $L = 21$, $\beta = 0.3$ from [1].

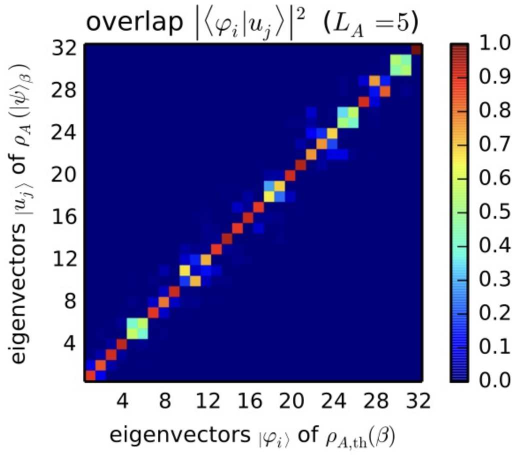

FIG. 2: Direct calculation of overlaps between the Schmidt eigenvectors and eigenvectors of the canonical density matrix, for an $L_A = 5$ subsystem at $L = 21$, $\beta = 0.3$.[1]

To quantify the extent to which Eq(0.2) is valid, we define the trace norm distance as

$$\| \rho_A(|\psi\rangle_\beta) - \rho_{A,th}(\beta) \|_1 \equiv \frac{1}{2}\mathrm{tr}(\sqrt{(\rho_A(|\psi\rangle_\beta) - \rho_{A,th}(\beta))^2}) \tag{0.6}$$

Based on the results in [4], the trace norm distance should go to zero as $1/L$ if ETH holds for all operators in subsystem A. The results in Fig 3 verify that the trace norm distance is tending towards zero at least linearly with $1/L$ as expected.

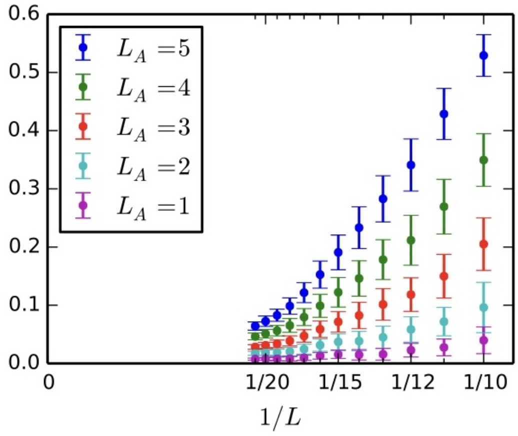

FIG. 3: The mean and standard deviation of the trace norm distance in the range $0.28 < \beta < 0.32$ for L up to 21 and L_A up to 5.[1]

ETH with finite ratio V_A/V

Now consider the validity of ETH for Class I operators in the fixed-ratio limit where $0 < f < \frac{1}{2}$ is finite. Some known results from the study of conformal field theories (CFTs) indicates that Eq(0.1) might hold for operators in Class I operators as long as $V_A < V/2$ with $V_A, V \to \infty$. One evidence comes from [5], where the closeness between the time dependent reduced density matrix $\rho_A(t)$ of a system evolved with a CFT Hamiltonian from a low entanglement state and the thermal density matrix $\rho_{A,th}$ is exponentially close to unity for $V_A/2 < t < V_{\bar{A}}/2$. This evidence doesn't apply to Class II operators since the measure of closeness only received contribution from eigenstates at temperature β^{-1} in the thermodynamic limit according to its definition. Another evidence comes from [6] [7] concerning comparison between the entanglement entropy of pure eigenstates in large central charge CFTs and the thermal entropy in the same limit.

However, the well-known counterexample of energy variance operator leads to another restriction for ETH to hold for Class I operators in the finite ratio case. Based on the subsystem energy variance mismatch between the reduced density matrix and canonical ensemble by a factor of $(1 - f)$, we expect that all Class I operators not related to energy conservation should satisfy ETH as in Eq(0.1).

The top panel in Fig 4 shows the mismatch of energy variance between a single eigenstate and the canonical ensemble, and the bottom panel shows the agreement of a different Class I operator J_A between the two systems in comparison. This numerical result strongly suggests that all Class I operators not related to energy conservation should satisfy ETH as in Eq(0.1) even with finite ratio V_A/V.

Moreover, given that the difference in subsystem energy variance occurs only in the finite ratio case, we can calculate the lower bound on trace normal distance for a modified bounded energy variance operator in the thermodynamic limit. As shown in Fig 5, the trace norm distance rapidly approaches its theoretical minimum bound, potentially providing the result in thermodynamic limit.

Similarly, we do not expect ETH to hold for all Class II operators when f is finite. In addition, there exists a physical constraint in this limit on the energy density range for the spectrum of $|\psi\rangle_\beta$ to match that of $\rho_{A,th}(\beta)$. Start with considering an arbitrary Hamiltonian of hard-core bosons with particle number conservation at infinite temperature, we find out a necessary condition for the wavefunction $|\psi\rangle_{\beta=0}$ to encode properties of the system at all fillings. We carried on this derivation to systems with (only) energy conservation, and obtained a necessary condition for ETH to hold for all Class II operators. The Schmidt decomposition of an eigenstate $|\psi\rangle_\beta$ with eigenvalue E is

$$|\psi\rangle_\beta = \sum_i \sqrt{\lambda_i}\, |u_i\rangle \otimes |v_i\rangle \qquad (0.7)$$

Notice that ETH requires: $|u_i\rangle$'s are approximate eigenstates of H_A and Schmidt coefficients $\lambda_i \propto e^{-\beta\langle u_i|H_A|u_i\rangle} = e^{-\beta E_A}$. For the requirements to be satisfied, the constraint necessary for ETH to hold for all Class II operators is

$$f \le f^* \equiv \min[\frac{e}{e_{max}}, 1 - \frac{e}{e_{max}}] \qquad (0.8)$$

in the case $e > e_{max}/2$ where $e = E/V$.

From the numerical result as shown in Fig 6, we observe that significant deviation in the Schmidt eigenvalue spectrum from their ETH prediction begins where this constraint breaks down, i.e. beyond the critical energy density $e^* = e/f$.

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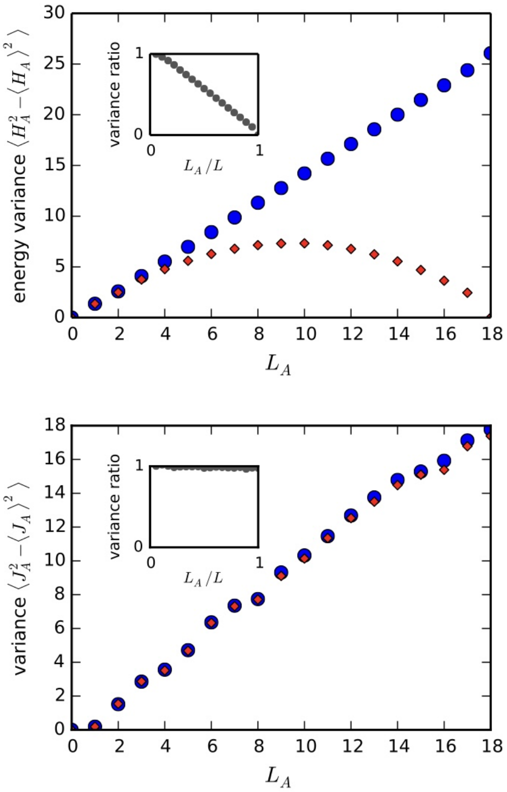

FIG. 4: Top panel gives the subsystem energy variance, and bottom panel gives the variance of an operator $J_A \equiv \sum_{i=1}^{L_A}(h_x^i \sigma_i^x h_z^i \sigma_i^z) + \sum_{i=1}^{L_A-1} J_z^i \sigma_i^z \sigma_{i+1}^z$ with respect to subsystem size L_A for the canonical ensemble(blue) and a single eigenstate $|\psi\rangle_\beta$(red) at $L = 18$ and $\beta = 0.3$. In particular the inset gives the ratio between the two quantities.[1]

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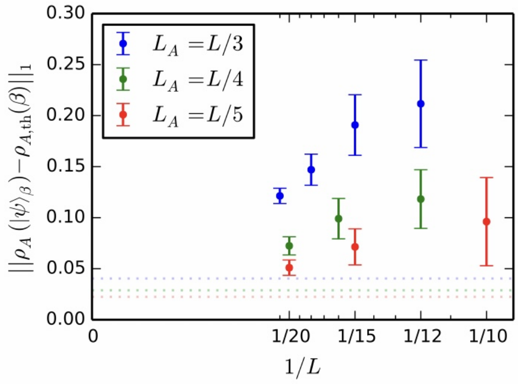

FIG. 5: The mean and standard deviation of the trace norm distance between the canonical density matrix and reduced density matrix for fixed ratio L_A/L and $0.28 < \beta < 0.32$. The horizontal lines are the theoretical minimum each trace norm distance can take.[1]

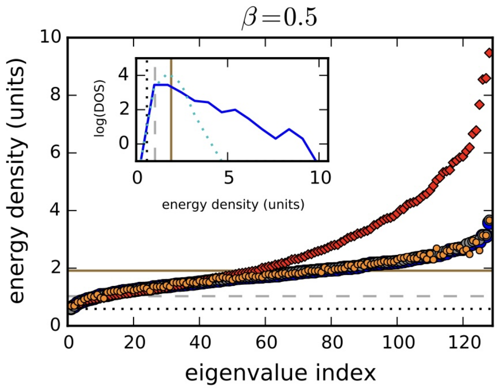

FIG. 6: Comparison of the four quantities defined in the inset of Fig 1 for eigenstates of an $L = 21$ system with $L_A = 7$ at $\beta = 0.5$. The inset plots the log of the density of states versus the energy density for both a single eigenstate(blue curve) and the canonical ensemble(cyan dot).[1]