Does a single eigenstate encode the full Hamiltonian?

James R. Garrison\textsuperscript{1} and Tarun Grover\textsuperscript{2}

\textsuperscript{1}Department of Physics, University of California, Santa Barbara, California 93106, USA  
\textsuperscript{2}Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA

The Eigenstate Thermalization Hypothesis (ETH) posits that the reduced density matrix for a subsystem corresponding to an excited eigenstate is “thermal”. Here we expound on this hypothesis by asking: for which class of operators, local or non-local, is ETH satisfied? We show that this question is directly related to a seemingly unrelated question: is the Hamiltonian of a system encoded within a single eigenstate? We formulate a strong form of ETH where in the thermodynamic limit, the reduced density matrix of a subsystem corresponding to a pure, finite energy density eigenstate asymptotically becomes equal to the thermal reduced density matrix, as long as certain conditions on the ratio of the subsystem size to the total system size are satisfied. This allows one to access the properties of the underlying Hamiltonian at arbitrary energy densities/temperatures using just a single eigenstate. We provide support for our conjecture by performing an exact diagonalization study of a non-integrable 1D lattice quantum model with only energy conservation. For this particular model, we provide evidence that the aforementioned strong form of ETH holds up to finite size corrections, which enables us to extract the free energy density and correlators of operators at various temperatures using a single eigenstate. We also study a particle number conserving model at infinite temperature which also substantiates our conjecture.

PACS numbers:

I. Introduction

II. General Considerations
\quad A. Determining Hamiltonian from Microstates in Classical Statistical Mechanics  
\quad B. Two Classes of Operators  
\quad C. ETH: Class I Vs Class II Operators  \quad 1. ETH for Class I operators  \quad 2. ETH for Class II operators  
\quad D. Summary

III. A warmup: von Neumann and Renyi Entropy of Eigenstates at Infinite T

IV. Model Hamiltonian with only Energy Conservation

V. von Neumann and Renyi Entropy of Eigenstates at Finite T
\quad A. ETH Prediction for von Neumann and Renyi Entropy  
\quad B. Numerical Results for von Neumann and Renyi Entropies

VI. Entanglement Hamiltonian Vs Actual Hamiltonian

VII. Trace norm distance between reduced and canonical density matrices

VIII. An application: Equal-time correlators as a function of temperature from a single eigenstate

IX. Summary and Discussion

References

I. INTRODUCTION

Given a local Hamiltonian, what information about the system is encoded in a single eigenstate? If the eigenstate happens to be a ground state of the Hamiltonian, tremendous amount of progress can be made on this question for Lorentz invariant systems, especially conformal field theories (CFTs) and for topological phases. For example, one can read off the central charge of a CFT from the ground state entanglement entropy, while for topological phases, essentially all ‘topological data’ such as braiding statistics of anyons can be extracted from the degenerate ground states. In this paper we argue that a single finite energy density eigenstate of an ergodic quantum many-body Hamiltonian is sufficient to determine the properties of the system at all temperatures.

It is not very surprising that the ground states of quantum many-body systems contain some information about their excitations. This is because an entanglement cut often mimics an actual physical cut through the system, thus exposing the underlying excitations along the entangling boundary. The same intuition is tied to the fact that the ground state entanglement satisfies a “boundary law” of entanglement entropy, that is, the von Neumann entanglement entropy $S_1 = -\text{tr}_A (\rho_A \log(\rho_A))$ of the ground state corresponding to a subsystem $A$ scales with the size of the boundary of subsystem $A$.

How does the nature of information encoded evolve as one goes from the ground state to an excited eigenstate?
Typically, there always exist eigenstates with energy $E$ just above the ground state which continue to satisfy an area law of entanglement. These are the eigenstates which have a zero energy density, i.e. $\lim_{V \to \infty} \frac{E - E_0}{V} = 0$ where $E_0$ is the ground state energy and $V$ is the total volume of the system. These eigenstates can often be interpreted as the action of a sum of local operators acting on the ground state; for example, in a system with spontaneous symmetry breaking one can construct an eigenstate consisting of a few magnons by a superposition of spin-flips acting on the ground state. Furthermore, the level spacing between two contiguous low-lying excitations scales as $\delta E \sim 1/L^\alpha$ where $\alpha > 0$ depends on dimensionality and the phase of matter under consideration. In this paper, we will instead be concerned with excited eigenstates that have a finite energy density, i.e. $\lim_{V \to \infty} \frac{E - E_0}{V} \neq 0$. For notational convenience, we will set $E_0 = 0$ for the remainder of this paper.

As argued by Srednicki,[13] a typical finite energy density state (i.e. a typical state in the Hilbert space that satisfies $\langle \psi | H | \psi \rangle = V e$ where $e$ is the energy density) when time-evolved with the Hamiltonian $H$ for sufficient time is expected to lead to predictions dictated by the basic tenets of equilibrium statistical mechanics, if the system thermalizes. Such an expectation leads to the “Eigenstate Thermalization Hypothesis” (ETH)[13,15] which stipulates that the thermalization occurs at the level of each individual eigenstate. An alternative approach by Deutsch[14] which is based on perturbing an integrable system by a small integrability breaking term, leads to the same suggestion. If ETH holds true, then in the thermodynamic limit the equal-time correlators of an operator with respect to a finite energy density eigenstate $|\psi\rangle$ are precisely equal to those derived from a thermal ensemble, i.e.

$$\langle \psi | O | \psi \rangle = \frac{\text{tr} \left( O e^{-\beta H} \right)}{\text{tr} \left( e^{-\beta H} \right)}$$

where $\beta$ is chosen such that the Eqn. 1 holds true when $O = H$, the Hamiltonian. Henceforth we will use the notation $|\psi\rangle_{\beta}$ to denote an eigenstate whose energy density corresponds to temperature $\beta^{-1}$. A notable exception to ETH is a many-body localized system in the context of strongly disordered interacting quantum systems[16,17] which fails to thermalize and does not satisfy Eqn. 1. The possibility[18,19] or impossibility[20,21] of the violation of ETH without disorder has also been discussed recently.

In this paper, we restrict ourselves to systems where ETH, as defined by Eqn. 1 holds. However, Eqn. 1 alone is incomplete unless one also specifies the class of operators for which it holds. For example, one simple non-local operator for which Eqn. 1 breaks down is the projection operator $|\psi\rangle \langle \psi|$ onto the eigenstate $|\psi\rangle$ that enters Eqn. 1; the left hand side of Eqn. 1 yields unity for this operator, while the right hand side is exponentially small in the volume, a clear disagreement. On that note, it is often mentioned that in systems where Eqn. 1 does hold, it does so only for “few body” operators[22,23] where, to our knowledge, the precise meaning of few-body operator has not been clarified. In this paper, we conjecture and provide numerical evidence that Eqn. 1 holds for all operators within a subsystem $A$, where the volume $V_A$ of subsystem $A$ can be arbitrarily large as long as it satisfies $V_A < f^* V$, where $f^* \neq 0$ $(< 1/2)$ is an $O(1)$ number, to be defined later. In fact, we will make the case that for a large class of non-local operators, as well as all local operators (which we define as the operators whose support does not scale with the subsystem size $V_A$), the condition $V_A < V/2$ suffices. On that note, we should mention that the questions such as which Hamiltonians (and which operators) satisfy ETH is now entering the realm of experimental physics (see e.g. Ref.[24] due to advances in high resolution imaging techniques[25].

The satisfaction of Eqn. 1 for all operators in a subsystem $A$ is equivalent to the statement that the reduced density matrix $\rho_A(|\psi\rangle_{\beta}) = \text{tr}_A |\psi\rangle_{\beta} \langle \psi |$ corresponding to an eigenstate $|\psi\rangle_{\beta}$ is given by

$$\rho_A(|\psi\rangle_{\beta}) = \rho_A,_{\text{th}}(\beta)$$

(2a)

where

$$\rho_A,_{\text{th}}(\beta) = \frac{\text{tr}_\beta(e^{-\beta H})}{\text{tr}(e^{-\beta H})},$$

$A$ being the complement of $A$. Note that the trace in the denominator is over the whole Hilbert space. When $V_A$ is held constant, the equality in Eqn. 2a means the density matrices become elementwise equal in any basis as $V \to \infty$. When the ratio $V_A/V$ is held constant, however, the number of matrix elements increases exponentially as $V \to \infty$. In this case we consider the validity of Eqn. 2a in terms of the trace norm distance of the density matrices on either side raised to any power—a point which is further explained in Sec. VII.

One immediate consequence of Eqn. 2a is that the thermodynamical properties of a system at arbitrary temperatures can be calculated using a single eigenstate. For example, Eqn. 2a implies that to the leading order, the Renyi entropies $S_\alpha (\equiv - \frac{1}{\alpha - 1} \log [\text{tr}_A (\rho_A^{\alpha})])$ for an eigenstate $|\psi\rangle_{\beta}$ corresponding to a subsystem $A$ with $V_A < V/2$ are given by

$$S_\alpha = \frac{\alpha}{\alpha - 1} V_A \beta (f(\alpha \beta) - f(\beta)),$$

(3)

where $f(\beta)$ is the free energy density at temperature $\beta^{-1}$. The result for $V_A > V/2$ follows from the constraint $S_A = S_{\overline{A}}$. The above equation allows one to access the free energy density $f$ at an arbitrary temperature by varying $\alpha$. Note that Eqn. 3 holds only to the leading order because Renyi entropies $S_\alpha$ receive additional subleading contributions due to the conical singularity induced at the boundary of subsystem $\overline{A}$[26]. In the limit
\( \alpha \to 1 \), one recovers the equality between the von Neumann entanglement entropy \( S_1 \) and the thermal entropy \( S_\text{th} = V_A s_{\text{th}}(\beta) \) where \( s_{\text{th}}(\beta) \) is the thermal entropy density at temperature \( \beta^{-1} \), a result which was argued to hold in Ref.\textsuperscript{22} for the special case of two weakly coupled ergodic systems. We emphasize that these results cannot be derived from Eqn.\textsuperscript{1} alone were it to hold only for local operators, since entanglement entropies do not correspond to the expectation value of any local operator. We also note that Refs.\textsuperscript{23,24} simulated the thermal Renyi entropy \( S_\alpha \) (starting with the expression on the right hand side of Eqn.\textsuperscript{2a}) using Quantum Monte Carlo to access the properties of the system at temperature \( (\alpha \beta)^{-1} \). Of course, Quantum Monte Carlo methods are not well suited to verifying ETH since they cannot access properties of a single eigenstate (the left hand side of Eqn.\textsuperscript{2a}).

We will also discuss an approximate, but more intuitive form of ETH, given by

\[
\rho_A(\psi_\beta) \approx \frac{e^{-\beta H_A}}{\text{Tr}_A(e^{-\beta H_A})} \tag{2b}
\]

where \( H_A \) is the projection of the original Hamiltonian onto subsystem \( A \). This form is approximate compared to Eqn.\textsuperscript{2a} because generically, it does not capture the correlations near the boundary correctly due to the somewhat arbitrary truncation scheme used to obtain \( H_A \). Nevertheless, equations\textsuperscript{2a} and\textsuperscript{2b} both yield the same results for all bulk quantities such as the Renyi entropy densities, as well as correlation functions of operators that have support only far from the boundary.

A central task of this paper is to check the validity of Eqns.\textsuperscript{2a} and\textsuperscript{2b} and their consequences for model non-integrable systems. As already mentioned, we will argue that ETH allows one to calculate thermodynamical quantities as well as correlators at all temperatures/energy densities using only a single eigenstate. We will demonstrate this explicitly by studying a quantum 1D model numerically.

As mentioned above, we find evidence that Eqn.\textsuperscript{2a} holds even when \( V_A/V \) is held constant with \( V_A/V \) less than some number \( f^* > 0 \). In particular, as we discuss later, our results strongly indicate that \( f < 1/2 \) is sufficient to guarantee equivalence between the von Neumann entropy density of a pure eigenstate, and the thermal entropy density at the corresponding temperature. This is in contrast to Ref.\textsuperscript{22} where it was argued that such an equivalence holds only in the limit \( f^* \to 0 \). Recently\textsuperscript{22,23} the requirement \( f^* \to 0 \) was substantiated using analytical and large scale numerical calculations for free fermions, an integrable system. Our results indicate that the \( f^* \to 0 \) requirement is likely a consequence of the integrable nature of the models in Refs.\textsuperscript{22,23}.

The paper is organized as follows. Sec.\textsuperscript{1} discusses general considerations for the validity of ETH, and introduces a division of all operators in a given subsystem into two distinct classes, which have different requirements for ETH to hold. Sec.\textsuperscript{11} illustrates some general features of ETH by studying the entanglement entropies of a hardcore boson model with global particle number conservation for infinite temperature eigenstates. Sec.\textsuperscript{1V} introduces the model we study in the remainder of the paper, the transverse field Ising model with longitudinal field. Sec.\textsuperscript{1V} focuses on the entanglement entropies at finite temperature. Sec.\textsuperscript{1VII} provides a close look into the entanglement Hamiltonian, focusing on its spectrum and Schmidt vectors. Sec.\textsuperscript{1VII} studies the validity of Eqn.\textsuperscript{2a} in the thermodynamic limit by considering the trace norm distance of both sides. Sec.\textsuperscript{1VIII} provides an application, by using the reduced density matrix from a single eigenstate to predict correlators at all (finite) temperatures. Sec.\textsuperscript{IX} summarizes our results and provides thoughts for future discussion.

\section{General Considerations}

\subsection{Determining Hamiltonian from Microstates in Classical Statistical Mechanics}

Suppose, for an isolated system described by classical statistical mechanics in a total volume \( V \), we are given access to all classical microstates in a small energy window \([E, E + \Delta E]\), where \( \Delta E \sim \sqrt{V} \) is on the order of the energy fluctuations in the total system were the system coupled to a thermal bath, and thus all microstates correspond to the same energy density. We pose the question: does this information suffice to determine the underlying Hamiltonian, assuming that the Hamiltonian is local? The answer is indeed yes, following the standard procedure of obtaining canonical ensemble from a microcanonical ensemble. In particular, let us make a fictitious division of the system into \( A \) and \( \overline{A} \) such that \( V_A \ll V \), and count the number of times a particular configuration \( C_A \) appears in subsystem \( A \). This determines the probability distribution for finding a given configuration, \( P(C_A) \). If all microstates are equally likely, then\textsuperscript{1V}

\[
P(C_A) = \frac{e^{-\beta E(C_A)}}{\sum(C_A) e^{-\beta E(C_A)}} \tag{4}
\]

where \( E(C_A) \) is the energy in subsystem \( A \). One may now invert this equation to obtain the energy \( E(C_A) = -\frac{1}{\beta} \log(P(C_A)) \), up to an irrelevant constant shift of energy. In a classical statistical mechanical system \( E(C_A) \) is the Hamiltonian for subsystem \( A \). In particular, knowing \( E(C_A) \), one may now calculate any thermodynamic property at any temperature. Here it is crucial to note that Eqn.\textsuperscript{4} does not assume that the energy density \( E(C_A)/V_A \) equals the energy density \( E/V \) of the microstates being sampled.

As discussed in the introduction, we will provide evidence that the quantum mechanical analog of Eqn.\textsuperscript{4} is given by Eqns.\textsuperscript{2a,2b}. We now proceed to discuss the conditions under which Eqns.\textsuperscript{2a,2b} are valid.
B. Two Classes of Operators

For reasons soon to be discussed, we find it useful to separate operators in a given Hilbert space into two classes:

Class I ("Equithermal Operators"): If the reduced density matrix takes the thermal form (i.e. the right hand side of Eqn. 2b), then in the limit $V_A \rightarrow \infty$, the expectation value of equithermal operators receives contribution only from eigenstates of $H_A$ at energy density corresponding to the temperature $\beta^{-1}$. One might have thought that this is true for all operators, however, there exist operators such as $e^{-n\beta H_A}$, whose expectation value includes contribution from eigenstates of $H_A$ at energy density $(n + 1)\beta^{-1}$ in addition to the temperature $\beta^{-1}$. Clearly, local operators fall into this class, as do sums of local operators. Several non-local operators, including the von Neumann entropy $S_A$, also fall into this class.

Class II ("Non-equithermal Operators"): We dub all operators not in Class I as "non-equithermal operators", or Class II operators. All Renyi entropies $S_\alpha$ (for $\alpha \neq 1$) fall into this class.

C. ETH: Class I Vs Class II Operators

Let us first consider the relationship between Eqn. 1 and Eqns. 2a, 2b. Eqn. 1 may be rewritten as,

$$\text{tr}_A(\rho_A O) = \frac{\text{tr}_A \left( O \text{tr}_A \left( e^{-\beta H_A} \right) \right)}{\text{tr} \left( e^{-\beta H_A} \right)}$$  \hspace{1cm} (5)

If this equation holds for all operators in a subsystem $A$, hermitian as well as non-hermitian, then one obtains Eqn. 2a $\rho_A(\psi_\beta) = \rho_{A,\text{th}}(\beta)$. This is because one may expand both the $\rho_A$ and $\rho_{A,\text{th}}$ in terms of the complete set of operators in subsystem $A$, and by choosing appropriate $O$ prove that they are equal to each other element-by-element. One of the most important consequences of this equality is that it allows one to extract properties of the Hamiltonian at arbitrary temperatures using a single eigenstate, which is one of the central points of this paper.

1. ETH for Class I operators

In contrast to classical statistical mechanics, we expect that quantum mechanically, one does not require the constraint $V_A \ll V_\mathcal{T}$ for ETH to hold for Class I operators. Indeed, as discussed below, several known results point to the conclusion that Eqn. 1 holds for all operators in Class I, as long as $V_A < V_\mathcal{T}$ with both $V_A, V_\mathcal{T} \rightarrow \infty$. Therefore, the number of operators that satisfy ETH scales exponentially not only with the subsystem size $V_A$, but also with total system size $V$ (in contrast to just "few-body" operators).

The strongest evidence for the sufficiency of the condition $V_A < V_\mathcal{T}$ so that Eqn. 1 holds for Class I operators comes from the study of quantum quenches in conformal field theories (CFTs). As shown in Ref. 10, the temperature-dependent reduced density matrix $\rho_A(t)$ of a system initially prepared in a low-entanglement state, and evolved with a CFT Hamiltonian, approaches the thermal density matrix, as long as $V_A < V/2$, with $V_A, V \rightarrow \infty$. Ref. 10 characterized the closeness between $\rho_A(t)$ and the thermal density matrix $\rho_{A,\text{th}}$ (Eqn. 2a) in terms of the operator overlap $I(t) = \frac{\text{tr}(\rho_A(t)\rho_{A,\text{th}})}{\text{tr}(\rho_A^2(t))\text{tr}(\rho_{A,\text{th}}^2)}$, which is exponentially close to unity for $V_A/2 < t < V_\mathcal{T}/2$. It is important to note that in the thermodynamic limit, $I$ only gets contribution from eigenstates at temperature $\beta^{-1}$, so this only guarantees that operators in Class I will satisfy Eqn. 1.

Recently studied large central charge theories also support the same conclusion17. In particular, Refs. 17, 10 studied the entanglement entropy of pure states in finite temperature conformal field theories with large central charge. In the limit $V_A, V \gg 1/T$, while keeping $V_A/V$ fixed, it was found that the entanglement entropy becomes equal to the thermal entropy at all non-zero temperatures as long as $V_A < V_\mathcal{T}$.

Lastly, another piece of evidence for the sufficiency of the condition $V_A < V_\mathcal{T}$ comes from studying random states, which mimic the behavior of an eigenstate at infinite temperature (i.e. $|\psi_\beta=0\rangle$). The entanglement entropy for a random state is given by52,53

$$S = -\log \left( |\mathcal{H}_A|^{-1} + |\mathcal{H}_\mathcal{T}|^{-1} - |\mathcal{H}|^{-1} \right)$$  \hspace{1cm} (6)

where $|\mathcal{H}_A|, |\mathcal{H}_\mathcal{T}|, |\mathcal{H}|$ are the sizes of the Hilbert spaces of subsystems $A$, $\mathcal{A}$ and the total system ($= A \cup \mathcal{A}$) respectively. Thus, as soon as $V_A < V_\mathcal{T}$, one obtains $S = -\log(|\mathcal{H}_A|)$, which is indeed the thermal entropy for subsystem $A$ at infinite temperature.

The above results support the notion that for ETH to hold for Class I operators, it is sufficient (and necessary) that the ratio of the Hilbert space sizes of subsystem $A$ to $|\mathcal{H}_{\mathcal{T}}|$, goes to zero in the thermodynamic limit. Our results are in agreement with, and substantiate this conclusion.

2. ETH for Class II operators

The extra ingredient introduced by Class II operators is that if ETH holds for them, then taking such an operator's expectation value with respect to a state $|\psi_\beta\rangle$ allows one to access the properties of the Hamiltonian at a temperature different than $\beta^{-1}$. For example, the Renyi entropy $S_\alpha$ corresponding to $\rho_A(|\psi_\beta\rangle)$ satisfies $S_\alpha = \frac{\alpha-1}{\alpha} V_A \beta (f(\alpha \beta) - f(\beta))$, thus allowing one to access the free energy density at temperature $(\alpha \beta)^{-1}$. 
Figure 1: Entanglement entropies $S_1$ through $S_4$ for a model with no conservation law (left panel, given by Eqn. 27 at $L = 21$), and a model with particle number conservation (right panel, given by Eqns. 21 at $L = 27$ with filling $N = 6$). We use the parameters mentioned in the text to place each model at a nonintegrable point. In each case we consider eigenstates in the $k = 1$ sector, with subsystem size $L_A = 4$. The grey vertical line denotes infinite temperature (point of maximum $S_1$), and the black circles mark the theoretical predictions for the entanglement entropies there. The brown markers denote the theoretical values of the entropies in the limit $L_A, L \to \infty$ while $L_A/L \to 0$, as given by Eqns. 25 and 26. Notice that the Renyi entropies all match at infinite temperature if and only if there are no additional conservation laws besides energy.

Figure 2: Eigenvalue spectrum of the reduced density matrix of an infinite temperature eigenstate, $\rho_A(\langle \psi \rangle_{\beta=0})$ for the hardcore boson model Eqn. 24 with $L = 27$, $L_A = 4$, and filling $N = 6$. The red lines plot the theoretical value of each eigenvalue in the thermodynamic limit, determined from the filling $N_A$ of the sector in which it lies.

For a given ratio $V_A/V$ with both $V_A, V \to \infty$, there is a physical constraint on the range of energy densities for which the spectrum of $|\psi\rangle_\beta$ in principle can match that of $\rho_{\text{A,th}}(\beta)$. To appreciate this, let us consider a slightly different problem—an arbitrary Hamiltonian of hardcore bosons with particle number conservation, at infinite temperature. We will consider an explicit example of such a system in the next section. Since the total particle number operator $\hat{N}$ commutes with the Hamiltonian and satisfies the equation $\hat{N} = \hat{N}_A + \hat{N}_B$, the reduced density matrix $\rho_A$ for a wavefunction $|\psi\rangle_{\beta=0}$ is block diagonal in the number of particles $N_A$ in subsystem A. Furthermore, if ETH holds (as given by a generalization of Eqns. 2a and 2b), then the Schmidt decomposition is given by

$$|\psi\rangle_{\beta=0} = \sum_{N_A=0}^N \sqrt{\lambda_{N_A}} \sum_i |u_i\rangle_{N_A} \otimes |v_i\rangle_{N-N_A}$$  \hspace{1cm} (7)

where $\lambda_{N_A}$ are the Schmidt coefficients in the sector $N_A$, and $|u_i\rangle_{N_A}, |v_i\rangle_{N-N_A}$ are the corresponding eigenvectors. The label $i$ captures fluctuations of particles within a fixed sector $N_A$. Note that there is no index $i$ on $\lambda_{N_A}$ because we are at infinite temperature and all Schmidt states within a sector $N_A$ are equally likely.

The decomposition in Eqn. 7 allows one to calculate properties of subsystem $A$ at infinite temperature even away from filling $N/V$ since the reduced density matrix $\rho_A$ will contain sectors with various densities $N_A/V_A$. However, there is both an upper limit and a lower limit on the density in subsystem $A$, since

$$\max [N - (V - V_A), 0] \leq N_A \leq \min [N, V_A]$$  \hspace{1cm} (8)

And thus the particle density $N_A/V_A$ in subsystem $A$ satisfies

$$\max [1 - (1 - n)/f, 0] \leq \frac{N_A}{V_A} \leq \min [n/f, 1]$$  \hspace{1cm} (9)
where \( n = N/V \) is the overall particle density and \( f = V_4/V \). Thus, a necessary condition for the wavefunction in Eqn. [7] to encode properties of the system at all fillings is

\[
f \leq \min \{n, 1 - n\} \tag{10}
\]

The above discussion, with some modifications, carries to systems with (only) energy conservation, at an arbitrary temperature. The Schmidt decomposition of an eigenstate \( |\psi\rangle \beta \) with eigenvalue \( E \) may now be written as:

\[
|\psi\rangle \beta = \sum_i \sqrt{\lambda_i} |u_i\rangle \otimes |v_i\rangle \tag{11}
\]

The physical content of ETH, as approximated in Eqn. [25], is that \( \lambda_i \propto e^{-E A_i} \), where \( E A_i \) is the \( i \)th energy eigenvalue of \( H_A \) (the projection of the Hamiltonian to subsystem \( A \)) while \( |u_i\rangle \) is the corresponding eigenstate of \( H_A \). Denoting the ground state energy to be zero, one naively expects that \( \langle u_i | H_A | u_i \rangle \leq E \forall |u_i\rangle \) since the energy density in the subsystem \( \overline{A} \) cannot be less than the ground state energy density. However, this argument has a loophole since in contrast to the particle number operator \( \hat{N} \), the total Hamiltonian is not separable into subsystems \( A \) and \( \overline{A} \): \( H = H_A + H_{\overline{A}} + H_{A\overline{A}} \), which actually allows \( \langle u_i | H_A | u_i \rangle \) to exceed \( E \) as we will see in Sec. VI below. To understand the constraint on \( \langle u_i | H_A | u_i \rangle \) precisely, let us derive an expression which encapsulates the classical notion that the sum of energies in subsystems \( A \) and \( \overline{A} \) equals \( E \).

We first note:

\[
\langle v_0 | \otimes \langle v_0 | H | \psi \rangle \beta = E \langle v_0 | \otimes \langle v_0 | \psi \rangle \beta \tag{12}
\]

\[
\langle u_0 | \otimes \langle v_0 | H | \psi \rangle \beta = E \langle u_0 | \otimes \langle v_0 | \psi \rangle \beta \tag{13}
\]

The above expression can be re-evaluated using the decomposition \( H = H_A + H_{\overline{A}} + H_{A\overline{A}} \):

\[
\langle u_0 | \otimes \langle v_0 | H | \psi \rangle \beta = \langle u_0 | \otimes \langle v_0 | H_A + H_{\overline{A}} + H_{A\overline{A}} | \psi \rangle \beta
\]

\[
= \sqrt{\lambda_0} \langle u_0 | \otimes \langle v_0 | H_A | u_0 \rangle + \sqrt{\lambda_0} \langle v_0 | H_{\overline{A}} | v_0 \rangle + \sum_j \sqrt{\lambda_j} \langle u_0 | \otimes \langle v_0 | H_{A\overline{A}} | u_j \rangle \otimes | v_j \rangle \tag{14}
\]

Equating the two ways to calculate the same expression, one finds:

\[
\langle v_0 | H_{A\overline{A}} | v_0 \rangle + \sum_j \sqrt{\lambda_j} \langle u_0 | \otimes \langle v_0 | H_{A\overline{A}} | u_j \rangle \otimes | v_j \rangle = E - \langle u_0 | H_A | u_0 \rangle \tag{15}
\]

Due to the variational principle for the ground state, \( \langle v_0 | H_{\overline{A}} | v_0 \rangle \geq -c f^{d-1} \) where \( c \) is a constant (recall that in our convention, the ground state energy for the full Hamiltonian is set to zero). Since both \( E \) and \( \langle u_0 | H_A | u_0 \rangle \) scale as \( L^d \), the only way for \( E - \langle u_0 | H_A | u_0 \rangle \) to exceed \( E \) is that the second term on the left hand side of Eqn. [16] viz. \( E_{\text{boundary}} \) is negative and scales as \( L^d \). When that happens, ETH no longer holds, as we now argue on general grounds, and will also demonstrate numerically for a lattice Hamiltonian in Sec. VI. To see this, we reiterate that ETH requires that (i) \( |u_j\rangle \)'s are approximate eigenstates of \( H_A \), and (ii) \( \lambda_j \propto e^{-E A_j} \). Firstly, when \( \langle u_0 | H_A | u_0 \rangle < E \) so that ETH could in principle hold, the \( E_{\text{boundary}} \) term can be neglected because the ‘diagonal term’ in \( E_{\text{boundary}} \) (i.e. the term corresponding to \( j = 0 \)) scales as the boundary \( (\propto L^{d-1}) \) and is thus subleading, while the off diagonal terms scale as \( e^{-L^d} \) and thus vanish in the thermodynamic limit (recall that \( V_A > V_{\overline{A}} \)). On the other hand, when \( \langle u_0 | H_A | u_0 \rangle > E \), the \( |u_0\rangle \)'s now correspond to states of zero energy density, and the aforementioned argument for neglecting off-diagonal terms is no longer valid. So, let us assume that \( \langle u_0 | H_A | u_0 \rangle > E \) and each \( |u_0\rangle \) continues to be an eigenstate of \( H_A \). Thus, one requires that

\[
\int \text{d}e' \sqrt{\frac{\lambda(e')}{\lambda(e)}} M(e, e') e^{S(e')} \propto g(e)/L^{d-1}, \tag{17}
\]

where we have taken the continuum limit and \( \lambda(e) \) denotes the Schmidt eigenvalue corresponding to an eigenvector \( |u\rangle \) at energy density \( e \), while \( M(e, e') = \langle u(e) | \otimes \langle v(e) | H_{A\overline{A}} | u(e') \rangle \otimes | v(e') \rangle \) and \( g(e) = e - \langle u(e) | H_A | u(e) \rangle / L^d \). It is obvious from Eqn. [17] that \( \lambda(e) \propto e^{-E A_e} = e^{-\beta E L^d} \) is no longer the solution. In fact, the only way for the integral on the left hand side of Eqn. [17] not to have any exponential dependence on \( L \) (as required by the right hand side) is that the integrand itself does not have such dependence, i.e.

\[
\frac{\lambda(e)}{\lambda(e)} \propto \frac{1}{M(e, e')} e^{-S(e')}. \tag{18}
\]

This implies a breakdown of ETH when \( \langle u_0 | H_A | u_0 \rangle > E \).

The above discussion implies that for a given wavefunction and bipartition, the maximum energy density that is potentially accessible in a subsystem \( A \), such that the corresponding Schmidt weight satisfies ETH is,

\[
e^* = \min(E/V_A, e_{\text{max}}) = \min(e/f, e_{\text{max}}) \tag{18}
\]

where \( e = E/V \) is the energy density corresponding to the wavefunction and \( e_{\text{max}} \) is the maximum energy density for the Hamiltonian \( H \) (recall that \( e_{\text{max}} \) can be finite for lattice-regularized quantum systems, e.g. for models of fermions or spins/hardcore bosons). Above, we have assumed that \( e < e_{\text{max}}/2 \). In the case when \( e > e_{\text{max}}/2 \), the range of available energies is instead bounded from below by max \([0, e_{\text{max}}(1 - 1/f) - e/f]\). If our goal is to capture the fluctuations in the system for all energy den-
sities so that all Class II operators satisfy ETH, we obtain an analog of Eqn. \ref{eq:10} for the energy: \( E/V_A \geq \epsilon_{\text{max}} \), and, \( (\epsilon_{\text{max}} V - E)/V_A \geq \epsilon_{\text{max}} \). Expressed in terms of the fraction \( V_A/V \), and the energy density of the eigenstate \( \epsilon = E/V \), this constraint is,

\[
f \leq \min \left[ \frac{\epsilon}{\epsilon_{\text{max}}}, 1 - \frac{\epsilon}{\epsilon_{\text{max}}} \right]
\]  

(19)

D. Summary

Let us summarize the discussion in this section.

1. ETH holds for local as well as non-local Class I operators as long as \( V_A < V_\gamma \). This implies that ETH is not restricted only to few-body operators (as can be seen in the limit \( V_A, V \rightarrow \infty \)). It also follows that the number of operators that satisfy ETH actually grows exponentially with the total system size \( V \).

2. Determining the full Hamiltonian from a single eigenstate is equivalent to the satisfaction of Eqn. \ref{eq:1} for both Class I and Class II operators. A necessary condition for this to be possible is the constraint \( \ref{eq:19} \), which in the presence of additional symmetries will be supplemented by constraints such as Eqn. \ref{eq:20}.

Our numerical results described in the following sections strongly suggest that the constraint, Eqn. \ref{eq:19} is not only necessary, but sufficient as well. Therefore, one should be able to extract information about the full Hamiltonian at arbitrary energy densities/temperatures using a single eigenstate as long as these constraints are satisfied.

Note that even if the constraint (Eqn. \ref{eq:19}) is not satisfied, the above arguments combined with our results in the subsequent sections indicate that a single eigenstate still encodes the properties of the Hamiltonian within the energy density window defined by \( \epsilon^* \) in Eqn. \ref{eq:18}. We will elaborate on this further while discussing the numerical results in Sec. \ref{sec:7}.

III. A WARMUP: VON NEUMANN AND RENYI ENTROPY OF EIGENSTATES AT INFINITE \( T \)

By definition, the thermal entropy reaches a maximum at infinite temperature. Together with Eqn. \ref{eq:22}, this implies that when ETH holds, eigenstates at “infinite temperature” are ones where the entanglement entropy is at its maximum. Consider a 1D transverse field Ising model with longitudinal field, \( H = \sum_{i=1}^L (\sigma_i^z \sigma_{i+1}^z + h_x \sigma_i^x + h_z \sigma_i^z) \). Here the von Neumann entropy \( S_1 \) takes its maximum possible value when the eigenvalues of the reduced density matrix are all equivalent to one another. Thus, from counting the basis size of the reduced Hilbert space, we expect for infinite temperature eigenstates that each eigenvalue of the reduced density matrix will approach \( 2^{-L^A} \) in the thermodynamic limit. From this, it follows that the Renyi entropies at infinite temperature satisfy

\[
S_\alpha = L^A \log 2,
\]  

(20)

that is, they are independent of Renyi index \( \alpha \). The left panel of Fig. \ref{fig:1} shows how the entropies \( S_1 \) through \( S_4 \) together match this predicted value at the infinite temperature point for a \( L = 21 \) system with periodic boundary conditions and subsystem size \( L_A = 4 \). In general, as \( L \rightarrow \infty \) the \( T = \infty \) entropy density is given by \( S_\alpha/L_A = \log 2 \).

Now let us instead consider a model with an additional conservation law, namely particle number conservation. Consider a 1D chain of hardcore bosons

\[
H = -\sum_i \left( t b_i^\dagger b_{i+1} + t' b_i^\dagger b_{i+2} + \text{H.c.} \right) + \sum_i \left( V n_i n_{i+1} + V' n_i n_{i+2} \right)
\]  

(21)

where \( n_i = b_i^\dagger b_i \). We focus on this system with periodic boundary conditions at the non-integrable point \( t = V = 1 \) and \( t' = V' = 0.96 \). This model was previously studied and shown to exhibit ETH in Refs. \ref{ref:13}.

Due to particle number conservation, the reduced density matrix from any pure state is block diagonal, with each block corresponding to some filling number \( N_A \) of the subsystem \( A \). The block of the reduced density matrix \( \rho_A^{(N_A)} \) corresponding to filling \( N_A \) is a \( d_{N_A} \times d_{N_A} \) matrix, where \( d_{N_A} = \binom{L_A}{N_A} \). At infinite temperature, the eigenvalues of \( \rho_A \) must be equal to one another within a given block, but the eigenvalues in different blocks will be different: they are in fact proportional to \( \binom{L-L_A}{N-N_A} \), the number of microstates consistent with such a configuration in subsystem \( A \). Taking into account that \( \text{tr}(\rho_A) = 1 \), one finds that each of the \( d_{N_A} = \binom{L_A}{N_A} \) eigenvalues of \( \rho_A^{(N_A)} \) are given by \( \lambda_{N_A} = \binom{L-L_A}{N_N-N_A}/\binom{L}{N_N} \). The spectrum of \( \rho_A \) we find for a single eigenstate is in agreement with that of the thermal reduced density matrix \( \rho_A^{(\beta = 0)} \) studied in Ref.\ref{ref:10}, consistent with ETH.

With this, the von Neumann entropy at infinite temperature becomes

\[
S_1 = -\sum_{N_A} d_{N_A} \lambda_{N_A} \log \lambda_{N_A}
\]  

(22)

and the Renyi entropies are given by

\[
S_\alpha = -\frac{1}{\alpha - 1} \log \left( \sum_{N_A} d_{N_A} \lambda_{N_A}^\alpha \right),
\]  

(23)

where the sums over \( N_A \) are restricted to subsystem particle fillings \( N_A \) that satisfy the constraint in Eqn. \ref{eq:8}.

Because the eigenvalues are non-uniform, the Renyi entropies \( S_\alpha \) at infinite temperature depend on the Renyi index \( \alpha \), in contrast to an energy-only conserving model.
able, even with the small system sizes we can access, the states are volume-law and are thus likely to satisfy ETH. The $\beta = 1.0$ eigenstate, on the other hand, is clearly not linear, and is too close to the ground state at this system size to exhibit ETH.

The right panel of Fig. 1 shows how the actual values of $S_1$ through $S_4$ match those predicted by the above counting argument.

For comparison, we also calculate $S_\alpha$ analytically in the thermodynamic limit. For simplicity, we consider the limits, $L, N, L_A \to \infty$ such that $n = N/L$ is held constant, while $L_A/L \to 0$. In these limits, one can evaluate the expressions in Eqn. 23 using Stirling’s approximation $\log(x!)/x \approx \log(x) - x$. One finds that in the limits considered, $S_\alpha$ receives contribution only from $N_A$ given by

$$N_A^* = \frac{L_A}{1 + \left(\frac{1}{\alpha} - 1\right)^{n}}$$

Thus, $S_\alpha$ probes the system at a filling $N_A^*/L_A = \frac{1}{1 + \left(\frac{1}{\alpha} - 1\right)^{n}}$, which is different than the actual filling $n$, unless $\alpha = 1$ (which corresponds to the von Neumann entanglement entropy). This also immediately leads to expressions for Renyi and von Neumann entanglement entropies in the thermodynamic limit:

$$S_\alpha/L_A = -\frac{1}{\alpha - 1} \log [n^\alpha + (1 - n)^\alpha]$$

and

$$S_1/L_A = -[n \log(n) + (1 - n) \log(1 - n)]$$.

We plot these values in Fig. 1 for comparison. Remarkably, even with the small system sizes we can access, the difference between the exact finite size result (obtained by counting over all sectors) and the result valid in the thermodynamic limit is quite small.

IV. MODEL HAMILTONIAN WITH ONLY ENERGY CONSERVATION

To develop some understanding of the questions posed in the introduction, we study a finite 1D quantum spin-$1/2$ chain with the following Hamiltonian:

$$H = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + h_x \sigma_i^z + h_z \sigma_i^z\right)$$

We set $h_x = 0.9045$ and $h_z = 0.8090$ such that the model is far away from any integrable point, and is expected to satisfy ETH in the sense of Eqn. 1 as shown in Ref. 29. We use periodic boundary conditions throughout.

We diagonalized the Hamiltonian in Eqn. 27 for system sizes up to $L = 21$, obtaining all eigenvalues and eigenstates. As hinted earlier, to each eigenstate we assigned a temperature $\beta^{-1}$ by finding the value $\beta$ for which the energy expectation value in the canonical ensemble matches the energy of the eigenstate:

$$\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\text{tr}(H e^{-\beta H})}{\text{tr}(e^{-\beta H})}.$$  (28)

By definition, $\beta = +\infty$ for the ground state and $\beta = -\infty$ for the highest excited state. In practice, the range of available $\beta$ values on a finite size system is much smaller. With $L = 21$, for instance, the first excited state has $\beta \approx 4.0$, and the second-to-highest excited state has $\beta \approx -0.6$ (as determined from Eqn. 28). It follows that eigenstates outside the range $4.0 \lesssim \beta \gtrsim -0.6$ will not appear fully thermal due to the large thermal correlation length expected at low temperatures. (This can be seen for instance in Fig. 3 where the finite size corrections to the linear scaling of the entanglement entropy become more prominent as temperature decreases.) Another thing to consider is that the infinite temperature eigenstate $|\psi\rangle_{\beta=0}$ is completely random and contains no information about the Hamiltonian. In a finite size system, states near infinite temperature will also contain little information about the Hamiltonian and will therefore be unable to predict properties of the system at other energy densities. As a result of these finite size considerations, we typically study values of $\beta$ between 0.2 and 0.5 in the remainder of this paper.
V. VON NEUMANN AND RENYI ENTROPY OF EIGENSTATES AT FINITE $T$

A. ETH Prediction for von Neumann and Renyi Entropy

Let us consider the Renyi Entropy $S_\alpha = -\frac{1}{\alpha - 1} \log \left( \text{tr} \rho_\alpha^A (|\psi\rangle_\beta) \right)$ corresponding to an eigenstate $|\psi\rangle_\beta$ at inverse temperature $\beta$. Assuming that ETH, as encoded in Eqn. 2a holds, $S_\alpha$ may be reexpressed as:

$$S_\alpha = -\frac{1}{\alpha - 1} \log \left( \frac{Z(A, \alpha, \beta)}{Z(1, \beta)^{\alpha}} \right)$$  \hspace{1cm} (29)

where $Z(A, \alpha, \beta)$ is the partition function of the system on an $\alpha$-sheeted Riemann surface, such that subsystem $A$ has an effective temperature $(\alpha \beta)^{-1}$ while subsystem $A$ has an effective temperature $\beta^{-1}$. $Z(1, \beta)$ is the regular partition function of the system. Therefore, keeping terms only to the leading order in the subsystem size, the above expression leads to Eqn. 3 advertised in the Introduction,

$$S_\alpha = -\frac{1}{\alpha - 1} \log \left( \frac{e^{-\alpha \beta V_A f(\alpha \beta) - \alpha \beta V_f(\beta)}}{e^{-\alpha \beta V_A f(\beta) - \alpha \beta V_f(\beta)}} \right)$$ \hspace{1cm} (30)

$$\frac{\alpha}{\alpha - 1} V_A \beta \left( f(\alpha \beta) - f(\beta) \right)$$ \hspace{1cm} (31)

where $f$ is the free energy density. Therefore, the wavefunction at temperature $\beta^{-1}$ can be used to calculate the free energy at temperature $(\alpha \beta)^{-1}$. Indeed, the same result also follows using the approximate form in Eqn. 2b.

Taking the limit $\alpha \to 1$ leads to the conclusion that the von Neumann entanglement entropy $S_1$ satisfies

$$S_1 = V_A s_{th}(\beta)$$ \hspace{1cm} (32)
where \( s_{\text{th}}(\beta) = S_1(\rho_{A,\text{th}}(\beta))/L_A \) is the thermal entropy density at temperature \( \beta^{-1} \).

**B. Numerical Results for von Neumann and Renyi Entropies**

Fig. 5 shows the scaling of von Neumann entropy \( S_1 \) as a function of subsystem size \( L_A \) for the eigenstates \( |\psi\rangle_{\beta} \) of our model (Eqn. 27). As discussed in Sec. II C 1, since \( S_1 \) is the expectation value of a Class I operator in our nomenclature, we expect Eqn. 22 to hold as long as \( V_A < V_A^{\tau} \), in the limit \( V_A, V_A^{\tau} \to \infty \). This implies that in the thermodynamic limit, the function \( S_1(V_A) \) is expected to form an inverted triangle shape, similar to the behavior of a random pure state (Eqn. 6). However, in a finite total system at any non-infinite temperature, \( S_1 \) is an analytic function of the ratio \( V_A/V \) with a negative sign for \( \frac{d^2 S_1}{dV_A^2} \), as shown in Fig. 3 (note that the sign of the curvature is fixed by the strong subadditivity of entanglement). However, even in finite system, the volume law does hold to a good accuracy when \( V_A \lesssim V/2 \), and the finite size scaling, discussed below, indicates that the inverted triangle shape is recovered in the thermodynamic limit.

Fig. 4 shows the comparison of \( S_1, S_2, S_3, \) and \( S_4 \) calculated for each individual eigenstate for a subsystem size \( L_A = 4 \) in a \( L = 21 \) system, with their ETH predicted canonical counterparts, Eqns. 32 and 3. We use two different canonical counterparts corresponding to Eqns. 2a and 2b, the latter version being susceptible to boundary errors, which nevertheless are expected to vanish as \( V_A, V_A^{\tau} \to \infty \). The agreement for each entropy is remarkable. It is worth re-iterating that the Renyi entropies for an eigenstate \( |\psi\rangle_{\beta} \) encode the free energy densities at temperatures different than \( \beta^{-1} \) (Eqn. 3), and these results provide an instance of non-local Class II operators satisfying ETH. The condition (19) does not come into play while calculating \( S_n \) because the energy density corresponding to temperature \( (\alpha\beta)^{-1} \) is lower than the critical energy density (Eqn. 15), up to which the entanglement spectrum matches the actual spectrum of the Hamiltonian. We will discuss this in detail in the next section. Also note that as \( \alpha \) becomes larger, finite size effects become more pronounced because \( S_n \) probes the system at lower temperatures \( (\alpha\beta)^{-1} \).
We also studied finite-size scaling of the von Neumann entropy and Renyi entropies by keeping $L_A$ constant and varying the total system size. The top panel of Fig. 5 shows the deviation $\Delta S_1/L_A$ for eigenstates in a range of temperatures. The difference $\Delta S_1/L_A$ seemingly goes to zero faster than any inverse power of $L$, and is consistent with an exponential dependence $\Delta S_1/L_A \sim e^{-L}$, or at the very least, a power-law decay $\Delta S_1/L_A \sim 1/L^2$ with $x \gg 1$ (although we should caution that inferring the precise asymptotic finite size scaling behavior using exact diagonalization studies is an inherently difficult task). The bottom panel shows a similar plot for the deviation of Renyi entropy $S_2$ from its ETH predicted value, Eq. 3. The finite size scaling of $\Delta S_2$ is relatively difficult because unlike $S_1$, $S_2$ shows oscillations as a function of $L_A$ (see e.g. 10, 13). Despite this, $\Delta S_2$ is less than a few percent of $S_2$ itself.

Fig. 5 plots the entropy deviation $\Delta S_1/L_A$ for constant ratio $L_A/L$ at all available system sizes. Although it is difficult to do a detailed scaling analysis with so few points, the data strongly suggests that $\Delta S_1/L_A$ vanishes in the thermodynamic limit. A further, and perhaps more robust indication of this result follows from the discussion in the next section where we provide evidence that the energy constraint in Eqs. 18 and 19 is sufficient for the satisfaction of Eqn. 2a. We also substantiate this conclusion by utilizing the notion of trace norm distance in Sec. VII.

VI. ENTANGLEMENT HAMILTONIAN VS ACTUAL HAMILTONIAN

We now probe in detail the entanglement spectra of individual eigenstates as well as the corresponding Schmidt states. As discussed in Sec. II C 2, a necessary condition for a full agreement between the entanglement spectrum of the reduced density matrix $\rho_A(|\psi\rangle_\beta)$ of a single eigenstate and the thermal reduced density matrix (Eq 2a) is the constraint in Eqn. 19 on the energy density of the state $|\psi\rangle_\beta$. Remarkably, we find that not only is this condition necessary but sufficient as well. Furthermore, when this condition is not satisfied, the entanglement spectra still matches with the actual spectra up to the critical energy density $e^* = e/f$ in Eqn. 18 where $e$ is the energy density of the state $|\psi\rangle_\beta$ and $f = V_A/V$. This is the reason that the Renyi entropies discussed in the previous section show an agreement with their canonical counterparts even when $L_A/L$ is kept constant.

Specifically, we compare four different quantities, as shown in Fig. 7 which test the validity of Eqs 2a and 2b. The agreement of the spectra of $\frac{1}{\beta} \log[\rho_A(|\psi\rangle_\beta)]$ with that of $\frac{1}{\beta} \log[\rho_{A,th}(\beta)]$ as well as with the actual Hamiltonian $H_A$ in region $A$ implies that essentially, the Schmidt eigenvalues $\lambda_i$ satisfy $\lambda_i \propto e^{-\beta E_{A,i}}$ where $E_{A,i}$ are the eigenvalues of $H_A$. Similarly, the agreement with the expectation value $\langle u_i | H_A | u_i \rangle$ shows that the Schmidt eigenvectors $|u_i\rangle$ have the same character as the eigenvectors of the thermal density matrix.

To probe the Schmidt eigenvectors further, we directly calculated the overlaps between the eigenvectors of the reduced density matrix $\rho_A(|\psi\rangle_\beta)$ and the eigenvectors of the thermal density matrix $\rho_{A,th}(\beta)$ (see Fig. 8). Again, we find excellent agreement.

Next, we discuss how the energy constraint Eqn. 19 comes into play as the energy density of an eigenstate is varied for fixed ratio $f = V_A/V$. Fig. 9 shows the comparison of spectra of the aforementioned four different quantities for several different energy densities of the reference state $|\psi\rangle_\beta$ with $f = 1/3$, at four different values of $\beta$. At this value of $f$, the energy constraint Eqn. 19 is violated, and therefore we expect that the entanglement spectrum should deviate from the actual spectrum of the Hamiltonian at least beyond the critical energy density $e^* = e/f$. We find for each value of $\beta$ that the deviation starts to occur essentially right at this critical energy density, below which the agreement continues to hold.

![Figure 7: Comparison of the four quantities defined in the inset for an $L_A = 4$ subsystem at $L = 21$ and $\beta = 0.3$. Each of the quantity has been normalized so that the $y$-axis has units of energy density. The blue markers show the spectra of the canonical (i.e. thermal) reduced density matrix while the red diamond markers correspond to the eigenvalues of a reduced density matrix $\rho_A(|\psi\rangle_\beta)$ for a single eigenstate at temperature $\beta$. The grey markers show the eigenvalues of $H_A$ with a shift $c_A \equiv \frac{1}{2} \log Z_A = \frac{1}{2} \log [\rho_{A,th}(\beta)]$ so that it can be directly compared with $\frac{1}{\beta} \log[\rho_A(|\psi\rangle_\beta)]$ in accordance with Eq 2b (note also that the combination $H_A + c_A$ is independent of the shift of the spectra of $H_A$ by an arbitrary uniform constant). Finally, the orange markers represent the expectation value of $H_A$, again with a shift $c_A$, with respect to the Schmidt eigenvector $|u_i\rangle$ of $\rho_A(|\psi\rangle_\beta)$. In each case, the eigenvalues/eigenvectors are ordered from smallest to largest energy density. The horizontal lines plot the energy density $e$ (dashed, grey) and the critical energy density $e^* = \frac{1}{\beta} e_A$ (solid, brown) of the original eigenstate $|\psi\rangle_\beta$, with respect to the ground state energy density of $H_A + c_A$ (dotted, black).](image-url)
Surprisingly, even though the entanglement spectrum does not match the actual spectrum beyond the energy density $e^*$, the expectation values $\langle u_i | H_A | u_i \rangle / L_A$ continue to match the energy eigenvalues of the actual Hamiltonian! To understand this phenomenon better, we analyze the different terms in Eqn. 16. As argued in Sec. IIC2, the only way the energy density $E$ of the eigenstate is, if the $E_{\text{boundary}}$ term,

$$E_{\text{boundary}} \equiv \sum_j \sqrt{\frac{\lambda_j}{\lambda_0}} \langle u_{i0} | \otimes (v_{i0} | H_A | u_j \rangle \otimes | v_j \rangle, \quad (33)$$

scales with the total system size. We find that this is indeed the case, as shown in Fig. 10. In agreement with the general considerations in Sec IIC2, Schmidt eigenvalues deviate from their ETH predicted value beyond $e^*$ (Fig. 9) and become considerably smaller.

VII. TRACE NORM DISTANCE BETWEEN REDUCED AND CANONICAL DENSITY MATRICES

To quantify the extent to which Eqn. 2a is valid, we measure the trace norm distance $||\rho_A (|\psi\rangle) - \rho_{A,\text{th}} (|\beta\rangle)||_1$ between the reduced and canonical density matrices at various system sizes. The trace norm distance, defined as

$$||\rho_A (|\psi\rangle) - \rho_{A,\text{th}} (|\beta\rangle)||_1 \equiv \frac{1}{2} \text{tr} \left[ \sqrt{(\rho_A (|\psi\rangle) - \rho_{A,\text{th}} (|\beta\rangle))^2} \right] \quad (34)$$

places an upper bound on the probability difference that could result from any quantum measurement on the two density matrices. As such, it provides an excellent measure of how distinguishable the two density matrices are. If the trace norm distance between two finite sized density matrices is zero, they are equal to each other element.
We first consider scaling of the trace norm distance with system size $L$ while the subsystem size $L_A$ is kept constant; that is, in the thermodynamic limit we will assume that $L_A \ll L$. If ETH holds for all operators in subsystem A, then the results of Ref.\cite{15} imply that the trace norm distance should go to zero as $1/L$. The suggestion that the trace norm distance between pure state and thermal reduced density matrix with fixed subsystem size would tend to zero was also made in Ref.\cite{58}. We restrict ourselves to states in a $\beta$ range given by $0.28 < \beta < 0.32$. In the left panel of Fig.\cite{11} we plot the trace norm distance of every eigenstate in this $\beta$ range at $L_A = 5$ for a few select system sizes. For each system size, the distribution of the trace norm distance is nearly constant throughout the given $\beta$ range. The right panel then takes this data for each pair of $L$ and $L_A$ and plots the mean and standard deviation of the trace norm distance against $1/L$. The trace norm distance is tending toward zero at least linearly with $1/L$, perhaps even faster.

Next we consider the stronger form of ETH that we propose, namely that the reduced and canonical density matrices are equivalent when keeping the ratio $L_A/L$ $(<\frac{1}{2})$ fixed as $L_A, L \to \infty$. Fig.\cite{12} plots the scaling of the trace norm distance in this case with $1/L$. Although there are few points available for each ratio, the trend is clearly toward zero as $L$ increases, and a linear extrapolation suggests that the trace norm distance does indeed go to zero in the thermodynamic limit. Remark-
ably, the definition of the trace norm distance does not require that the operators used to distinguish between the reduced and canonical density matrices be “local” in any sense. As such, these numerics strongly suggest that given a single eigenstate, all possible operators in sub-system A will assume their canonical expectation values in the thermodynamic limit, even though sub-system A is of infinite spatial extent.

At this point it is crucial to emphasize that in the limit when $L_A/L$ is kept fixed while both $L_A, L \to \infty$, the trace norm distance $\|\rho_A(\psi_\beta) - \rho_{A,th}(\beta)\|_1$ can go to zero even if the reduced density matrix does not contain information about temperatures away from $\beta^{-1}$. This is because in the thermodynamic limit, energy densities away from $\beta^{-1}$ do not contribute to the trace norm distance, as one can evaluate any measurable operator in the saddle point approximation, which becomes exact in the thermodynamic limit. In other words, no conceivable quantum measurement could determine whether the information in the two density matrices away from temperature $\beta^{-1}$ are equivalent. A more direct test is necessary to determine whether the reduced density matrix contains information about temperatures away from the original eigenstate’s energy density.

To test this strongest form of ETH, which is already strongly suggested by results in Figs. [7][8] and [9], we use the trace norm distance of modified density matrices to determine whether a single eigenstate at temperature $1/\beta$ can predict the bulk properties of the canonical ensemble at a different temperature $1/\beta'$. Specifically, we consider the trace norm distance

Figure 10: Decomposition of the energy density corresponding to an eigenstate amongst the three terms in Eqn. 16 for $\beta = 0.2$ (left panel) and $\beta = 0.5$ (right panel) at $L = 18$ and $L_A = 6$. The dotted magenta line marks the ground state of $H_T$. As in Fig. [7], the solid brown line denotes the critical energy density $e^*$ for sub-system $A$.

Figure 11: Trace norm distance between the canonical density matrix $\rho_{A,th}(\beta)$ and the reduced density matrix $\rho_A(\psi_\beta)$ for all eigenstates $\psi_\beta$ in the range $0.28 < \beta < 0.32$. The left panel plots the trace norm distance for all such eigenstates with system sizes $L = 12, 15$, and $20$, and subsystem size $L_A = 5$. The right panel plots the mean and standard deviation of the trace norm distance in this $\beta$ range for values of $L$ up to 21 and $L_A$ up to 5.
where \( \rho_A^{(n)} = \rho_A^{(n)} / \text{tr}_A(\rho_A^{(n)}) \). Raising a thermal density matrix to the \( n \)th power adjusts its saddle point so that it is dominated by properties at temperature \( (n\beta)^{-1} \) and thus if this trace norm distance vanishes as \( L \to \infty \), Eqn. 2a holds for properties at temperature \( (n\beta)^{-1} \). (For \( n = 1 \), this comparison reduces to the case discussed in the paragraph above.) In Fig. 13 we plot the trace norm distance between these density matrices for \( n = 1/2 \) (left panels) and \( n = 3/2 \) (right panels). For these values of \( n \), the energy density corresponding to the shifted saddle point lies within the window given by Eqn. 18. Remarkably, as \( L \) increases, the trace norm distance decreases, both when holding \( L_A \) fixed (top panels) and when keeping the ratio \( L_A/L \) fixed (bottom panels). For \( n \neq 1 \), \( \rho_A^{(n)}(\beta) \) corresponds to a thermal density matrix with a conical singularity\(^{20}\) In line with the reasoning behind Eqn. 2b we expect that \( \rho_A^{(n)}(\beta) \approx e^{-\beta H_A} \), from which it follows that \( \rho_A^{(n)}(\beta) \approx \rho_A^{(n)}(\beta_0) \). This means that all correlators with support away from the boundary are equal to each other for these density matrices. The Renyi entropies will also be correct. Together with the results in Sec. VI this builds the case that the reduced density matrix taken from a single eigenstate can predict equal time correlators at all energy densities that lie within the window given by Eqn. 18. We study this point further in the next section.

**VIII. AN APPLICATION: EQUAL-TIME CORRELATORS AS A FUNCTION OF TEMPERATURE FROM A SINGLE EIGENSTATE**

In the previous sections we provided evidence that a single eigenstate encodes the full Hamiltonian as long as the constraints in Eqn. 19 are satisfied. As an application of this result, we now calculate correlation functions at arbitrary temperatures using a single eigenstate \( |\psi\rangle_\beta \). The basic idea is similar to the relation between the Renyi entropies and the free energy densities (Eqn. 3).

In particular, consider the correlation function,

\[
\langle O(x)O(y) \rangle_{\beta,n} = \frac{\text{tr}_A(\rho_A^{(n)}(|\psi\rangle_\beta O(x)O(y))}{\text{tr}_A(\rho_A^{(n)}(|\psi\rangle_\beta))}
\]

where \( x, y \) are located in subsystem \( A \), away from the boundary. Using Eqs. 2a, 2b to the leading order in the subsystem size, \( \langle O(x)O(y) \rangle_{\beta,n} \) equals the expectation value of the operator \( O(x)O(y) \) at a temperature \( (n\beta)^{-1} \).

Fig. 14 shows the expectation values of local operators within subsystem \( A \) as a function of \( \beta \), as predicted from a single eigenstate at inverse temperature \( \beta_0 \) (indicated by a yellow dot on the red curve). We choose operators that are as far away from the subsystem boundary as possible, and choose the bipartition size and \( \beta_0 \) so that the energy constraint Eqn. 19 is satisfied for \( |\psi\rangle_{\beta_0} \). Even though the agreement with the canonical ensemble is not perfect, the qualitative trends and the numerical values match incredibly well, given the modest total system sizes to which we are restricted. These predicted correlators also undoubtedly suffer from corrections expected due to the conical singularity at the boundary of \( A \) in Eqn. 36.

**IX. SUMMARY AND DISCUSSION**

In this paper, we analyzed the structure of reduced density matrices corresponding to the eigenstates of generic, non-integrable quantum systems. We argued that given an eigenstate \( |\psi\rangle_\beta \) with energy density \( e \) and a corresponding temperature \( \beta^{-1} \), the reduced density matrix for a subsystem \( A \) is given by

\[
\rho_A(|\psi\rangle_\beta) = \rho_{A,\text{th}}(\beta)
\]

where

\[
\rho_{A,\text{th}}(\beta) = \frac{\text{tr}_A(e^{-\beta H_A})}{\text{tr}(e^{-\beta H_A})}
\]

if the condition \( f \leq \min \left[ \frac{e}{e_{\max}}, 1 - \frac{e}{e_{\max}} \right] \) is satisfied, where \( e_{\max} \) is the maximum energy density for the given
Figure 13: Scaling with $1/L$ of the trace norm distance $||\tilde{\rho}_{A}^{(2/n)}(|\psi\rangle_\beta) - \tilde{\rho}_{A,th}^{(2/n)}(\beta)||_1$ as $L_A/L$, for $n = 1/2$ (top left), $n = 2/3$ (top right), $n = 3/4$ (bottom left), and $n = 3/2$ (bottom right). The grey lines indicate linear fits for each ratio $L_A/L$. The fit is done by following the same procedure as in Fig. 12.

Hamiltonian and $f = V_A/V$ is the ratio of the subsystem size to the total system size. This means that for a fixed eigenstate $|\psi\rangle_\beta$, one can always extract the properties of the corresponding Hamiltonian at arbitrary energy densities by choosing sufficiently small $f$. Similarly, for a fixed bipartition ratio $f (< 1/2)$, if the above condition on $f$ is not satisfied, one can still access the properties of the underlying Hamiltonian for a range of energy densities in the interval described in Eqn. 18.

We also introduced the notion of “equithermal” (Class I) and “non-equithermal” (Class II) operators. In a canonical ensemble at temperature $T$, the expectation value of Class I operators depends only on the properties of the underlying Hamiltonian at temperature $T$, while the same is not true for Class II operators. Our results strongly suggest that Class I operators, local or non-local, satisfy Eqn. 1 as long as $V_A < V/2$. On the other hand, all Class II operators, local or non-local, satisfy Eqn. 1 as long as the energy densities they receive contribution from lies in the range of energy densities mentioned in the previous paragraph.

In the paper we only considered contiguous subsystems. It seems reasonable to conjecture that Eqn. 2a continues to hold as long as the support of operator $O$ can be chosen to lie in a subsystem which is not necessarily contiguous and whose volume satisfies $V_A/V \leq \min \left[ \frac{e}{e_{\max}}, 1 - \frac{e}{e_{\max}} \right]$. This encompasses the expectation values of local operators such as $\langle O(x)O(0) \rangle$, where $O(x)$ is localized at point $x$ and $|x|$ can be greater than $L/2$ (where $L$ is the linear dimension of the total system).

In a lattice-regularized quantum field theory with lattice cutoff $a$, the scaling limit corresponds to $a \rightarrow 0$, which implies $e_{\max} \rightarrow \infty$. Therefore, for a continuum quantum field theory, our results imply that in the limit $f \rightarrow 0$ the reduced density matrix takes the thermal form (Eqn. 2a), allowing one to obtain properties of the Hamil-
Figure 14: Equal time correlators for an $L = 21$ system plotted against inverse temperature $\beta$. The blue dots denote the expectation value with respect to each eigenstate, the dashed cyan curve plots the expectation value in the canonical ensemble, and the red curve plots the expectation value predicted from a single eigenstate at $\beta_0 = 0.3$ (yellow dot) by raising the $L_A = 4$ density matrix to the power $\beta/\beta_0$ and rescaling it to have unit trace. However, in line with the discussion above, the Renyi entropies $S_\alpha$ corresponding to a wavefunctional at temperature $T$ will continue to follow Eqn. 3 as long as $e(T/\alpha) < e/f$, where $f \equiv V_A/V$ and $e(T)$ is the energy density at temperature $T$. For example, this implies that in a conformal field theory in $d$ spatial dimensions, where $e \propto T^{d+1}$, one should see a deviation from the ETH predicted value when $\alpha < f^{d+1}$. It will be interesting if such a ‘phase transition’ can be detected using the methods developed in Refs. 47,49.

We note the uncanny resemblance between the Schmidt decomposition of an individual finite energy density eigenstate (Eqn. 11) and the ‘thermofield double’ state $|\psi\rangle_{TD,\beta}$ defined as $|\psi\rangle_{TD,\beta} = \sum_{E_A} e^{-\beta E_A/2}|E_A\rangle \otimes |E_A\rangle$ where $Z_A(\beta) = \sum_{E_A} e^{-\beta E_A}$. Coventionally, $|\psi\rangle_{TD,\beta}$ is thought of as a wavefunction for two copies of a system (denoted by an absence or presence of a bar over the eigenvectors), where each copy has the same set of eigenvectors $\{ |E_A\rangle \equiv |\overline{E_A}\rangle \}$ and the corresponding eigenvalues $\{ E_A \}$. Within thermofield double formalism, the reduced density matrix for one copy of the system equals the thermal density matrix $\rho_A = e^{-\beta E_A}/Z_A(\beta)$. Eigenstate thermalization, as defined in this paper, provides a new viewpoint on the thermofield double formalism wherein $|\psi\rangle_{TD,\beta}$ can be reinterpreted as a finite energy density eigenstate $|\psi\rangle_\beta$ of a Hamiltonian, and the two copies correspond to the subsystems obtained by equal bipartition of the total system. There is one problem however with this identification. As discussed in our paper, the reduced density matrix for an equal bipartition of a subsystem is expected to be thermal only up to an energy density $e/f = 2e$, where $e$ is the energy density corresponding to the eigenstate $|\psi\rangle_\beta$. Nevertheless, the reinterpretation of the thermofield double state as a Schmidt decomposition
of a finite energy density eigenstate is a valid description at least for all equithermal (= Class I) operators since they explore the equality between the true state and thermal reduced density matrix only at the energy density corresponding to the eigenstate.

Let us mention some of the practical implications of our results. Firstly, the fact that a single eigenstate encodes properties of the full Hamiltonian could potentially be a useful numerical tool. For example, one could imagine targeting a finite energy density eigenstate of a Hamiltonian \( H \) by variationally minimizing the energy of the Hamiltonian \( (H - E)^2 \) with respect to trial wavefunctions. The techniques in this paper would then allow one to access thermal properties of the Hamiltonian without directly calculating the partition function, which could be extremely helpful for Hamiltonians that suffer from the sign problem.

Secondly, owing to the recent progress in single atom imaging techniques in cold atomic systems\(^{15}\), one can now access non-local operators experimentally\(^{17,37}\). This potentially allows one to check some of our predictions pertaining to the violation of ETH in cold atomic systems. For example, one can perform a quantum quench on a low entanglement state which would at sufficiently long times lead to a thermal state in the same sense as Eqn. 2a. In such a state, one can then employ high resolution imaging to measure string or membrane operators that span more than half the system size to detect violation of ETH. A more ambitious goal, beyond current experimental techniques, would be to measure Renyi entropies for fractional indices, as this would allow one to access the critical energy density \( e^* \) in Eqn. 18.

We conclude by posing a few questions and future directions.

In the paper we extracted equal-time correlators at different temperatures using a single eigenstate. It will be interesting to see if a similar method also works for unequal time correlators at arbitrary temperatures. The main difference is that this requires calculating expressions such as Eqn. 37 at an imaginary exponent, and estimating the effects due to the conical singularity in this case requires further study.

Presumably, all our discussion carries over to time-evolved product states as well since such states are expected to also have thermal behavior at long times in the same sense as a single finite energy density eigenstate. If so, does the time scale for thermalization for a given operator (i.e. the time it takes for the expectation value of the operator to become equal to its canonical expectation value) depend on whether the operator is Class I (equithermal) or Class II (non-equithermal)?

Another question concerns the subleading corrections to the entanglement entropy. One expects that there always exist subleading area-law contributions to the entanglement entropy (either von Neumann or Renyi) of a single eigenstate. Are these contributions also captured correctly in the entanglement entropies calculated via a thermal reduced density matrix? Perhaps a more interesting question is whether the mutual information of two disjoint intervals (which cancels out both the volume law contribution and the area law contribution) takes the same value for a single eigenstate and its canonical counterpart.

Finally, we studied the particle number conserving model only at the infinite temperature. It will be worthwhile to extend this discussion to finite temperatures. Do all our conclusions continue to hold when energy is not the only conserved quantity? Presumably, at least in the limit \( f \to 0 \), the reduced density matrix for a single eigenstate takes the form

\[
\rho_A = \frac{\text{tr}(e^{-\beta H - \Sigma_i \mu_i O_i})}{\text{tr}(e^{-\beta H})}
\]

where \( O_i \) are the operators corresponding to the conserved quantities (e.g. particle number) and \( \mu_i \) are the corresponding chemical potentials. But does this form continue to hold even when \( f < 1/2 \) is an order unity number, analogous to the case of the energy-only conserving model? A natural extension of this question is to consider integrable systems which have an infinite number of conservation laws. Finally, in the opposite limit, it also seems interesting to study the structure of the reduced density matrix for systems with no conservation laws (e.g. Floquet systems or arbitrary time-dependent Hamiltonians) along lines similar to this paper.

We are grateful to Leon Balents, Matthew Fisher, Tom Hartman, Patrick Hayden, Anatoli Polkovnikov, Marcos Rigol, Lea Santos, Brian Swingle and especially Xiao-liang Qi for conversations about this work. This research was supported in part by the National Science Foundation, under Grant No. DMR-14-04230 (JRG), by the Caltech Institute of Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation (JRG), and by the Gordon and Betty Moore Foundations’ EPiQS Initiative through Grant GBMF4304 (TG). This research was also supported in part by the National Science Foundation under Grant No. NSF PHY11-25915. We also acknowledge support from the Center for Scientific Computing at the CNSI and MRL; an NSF MRSEC (DMR-1121053) and NSF CNS-0960316.

---

1. J. J. Bisognano and E. H. Wichmann, J. Math. Phys. 17, 303 (1976); J. J. Bisognano and E. H. Wichmann, J. Math. Phys. 16, 985 (1975).
2. Leonard Susskind, An Introduction To Black Holes, Information And The String Theory Revolution: The Holographic Universe, World Scientific Publishing Company (2004).
3. C. Holzhey, F. Larsen and F. Wilczek, Nucl. Phys. B 424, 443 (1994).
4. C. G. Callan and F. Wilczek, Phys. Lett. B 333, 55 (1994).
