Does a Single Eigenstate of a Hamiltonian Encode the Critical Behaviour of its Finite-Temperature Phase Transition?

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Recent work on the subject of isolated quantum thermalization has suggested that an individual energy eigenstate of a non-integrable quantum system may encode a significant amount of information about that system’s Hamiltonian. We provide a theoretical argument, along with supporting numerics, that this information includes the critical behaviour of a system with a second-order, finite-temperature phase transition.

I. INTRODUCTION

The eigenstate thermalization hypothesis (ETH) $^{1–5}$ has recently been the subject of a large body of experimental and theoretical work $^{6–21}$. ETH can explain how an isolated, quantum many-body system in an initial pure state can come to thermal equilibrium (as determined by measurements of a specified set of observables) in finite time, and is thus fundamental to understanding the validity of conventional quantum statistical mechanics as an accurate description of the long-time behavior of quantum systems; for a review, see $^{22}$. ETH is expected to hold in systems without disorder that are sufficiently far from integrability (including effective integrability caused by many-body localization in disordered systems), for observables that are sufficiently simple functions of the fundamental degrees of freedom.

While the key statements of ETH have been cast in several forms by various authors, in this work we will be interested in what we will refer to as the strong version of ETH $^{20}$, which concerns the entanglement behaviour of individual energy eigenstates in a non-integrable quantum system. This strong version of ETH is the statement that within one individual energy eigenstate of a non-integrable quantum system, the reduced density matrix (RDM) of a sufficiently small subsystem will resemble that of a thermal one. More precisely, the RDM on a subsystem $A$, constructed from an eigenstate $|\psi\rangle$ of the full quantum system, will be approximately given by

$$\rho_A^{\psi} \sim \frac{e^{-\hat{H}_A/T_\psi}}{Z(\hat{H}_A, T_\psi)} \; ; \; Z(\hat{H}_A, T_\psi) = \text{Tr} \left[ e^{-\hat{H}_A/T_\psi} \right]$$  \hspace{1cm} (1)

where $T_\psi$ is the “temperature” of the thermal eigenstate $|\psi\rangle$, and $\hat{H}_A$ is the Hamiltonian of the subsystem $A$. The heuristic interpretation of this statement is that even in a pure energy eigenstate, the full system acts as a thermal reservoir for its small subsystems, thermalizing them through the quantum entanglement between the subsystem and the larger thermal reservoir.

Previous authors have made precise the exact definitions of $T_\psi$ and $\hat{H}_A$ which are necessary for the above statement to hold, and have also elucidated the conditions under which it should be expected to hold, and how well $^{20,23}$. Here we will not be focused with these details, as they have been thoroughly addressed previously.

We will, however, be concerned with an interesting corollary to equation 1 mentioned already in $^{20}$. Given a thermal density matrix for a system at one temperature, it is always possible to compute the density matrix at another temperature, by simply raising the density matrix to a power and re-normalizing it, since

$$\left( \frac{e^{-\hat{H}/T_1}}{Z(\hat{H}, T_1)} \right)^{T_2/T_1} = \frac{e^{-\hat{H}/T_2}}{Z(\hat{H}, T_2)} \left[ Z(\hat{H}, T_1) \right]^{T_1/T_2}. \hspace{1cm} (2)$$

Thus, in principle, the RDM of a small subsystem, extracted from a thermal eigenstate of a much larger non-integrable quantum system, should possess information about the thermal behaviour of this subsystem across a range of temperature scales, to the extent that equation 1 is a valid approximation. This claim has in fact been investigated thoroughly by previous authors, and has been verified to be true under appropriate circumstances, outlined in $^{20}$.

Here we will focus on what this information reveals about the behaviour of a quantum, non-integrable system with a second-order phase transition at finite temperature. Previous work $^{24,26}$ has suggested that ETH should also be expected to hold in such systems, and in fact signatures of ETH and quantum chaos have indeed been found to exist even in the broken symmetry phase of such a system. In the present paper, we will argue that if such a system with a finite-temperature phase transition satisfies the strong version of ETH, then individual energy eigenstates of this system can diagnose the existence of this phase transition, and will also contain quantitative information about its critical behaviour, without any knowledge of the original Hamiltonian itself. Below, we outline a procedure by which one could arrive at this information from such an energy eigenstate.
II. THE EXTRACTION PROCEDURE

Consider a non-integrable quantum system, with some Hamiltonian \( \hat{H} \), which may or may not be known to us. We suspect that this system may possess a second-order phase transition at finite temperature, with corresponding order parameter \( Q \), and we wish to diagnose this fact from the information contained in one individual eigenstate of this Hamiltonian. We will assume that a reasonable notion of “subsystem” can be defined in our system. We will also assume that the system, while finite, is sufficiently “large,” such that subsystems can be defined which are themselves “large,” yet still much smaller than the full system. For example, in a spin system consisting of \( N \) spins, we imagine that \( N \) is large enough such that we can define subsystems of \( n \) spins, with \( 1 << n << N \).

We now consider a single energy eigenstate \( |\psi\rangle \) of this quantum system. Under the assumption that this eigenstate is thermal, with some characteristic temperature \( T_\psi \), the RDMs constructed on a sufficiently small subsystem should be appropriately thermal, in the sense described by equation [1]. Based upon the arguments outlined in [20], we should be able to probe the thermal density matrix of such a subsystem across a wide range of temperatures,

\[
\tilde{\rho}_A (T) \equiv (\rho_A)^{1/T} \sim (e^{-\hat{H}_A/T_\psi})^{1/T} = e^{-\hat{H}_A/T}, \tag{3}
\]

where we have defined\n
\[
\hat{H}_A \equiv \hat{H}_A/T_\psi \tag{4}
\]

to be the “scaled,” dimensionless subsystem Hamiltonian, and \( \tilde{\rho}_A (T) \) its canonical density matrix at temperature \( T \). Without knowledge of the original Hamiltonian, it is not possible to determine this \( T_\psi \), and thus the absolute temperature scale of our predictions, but this information will not be necessary for our purposes; we will simply assume that such a \( T_\psi \) exists, and thus make thermal predictions regarding the scaled Hamiltonian. Such an overall scale factor will not affect any predictions regarding the critical exponents of such a Hamiltonian.

With such a thermal density matrix at an arbitrary temperature, the thermal expectation value of any observable \( O_A \) which lives on this subsystem can be computed at this temperature,

\[
\langle O_A \rangle = \text{Tr}[\tilde{\rho}_A O_A]. \tag{5}
\]

In particular, the observable in question could be the order parameter of the system, its associated susceptibility, or any relevant correlation functions. Since this procedure could be repeated for various subsystems of different sizes, it should be possible to perform a finite-size scaling analysis of these quantities as a function of temperature, thus allowing for the quantitative extraction of various critical exponents [27].

Any such finite-size scaling analysis will of course be limited by the size of the system \( N \), but if we anticipate that equation [4] holds for arbitrarily large system sizes, then one can always extract these critical exponents to the desired accuracy by considering sufficiently large \( N \). Thus, as we approach the thermodynamic limit, the information about the critical point extracted from a single eigenstate can be made arbitrarily accurate, and it is in this limit in which a single eigenstate will encode the full information regarding the critical point of the original Hamiltonian.

To see how this procedure could work in somewhat more detail, we provide a specific example involving a system of \( N \) Ising spins defined on a lattice, and examine the order parameter which is the total magnetization in the z-direction,

\[
Q = M_z \equiv \sum_i \sigma_i^z. \tag{6}
\]

This order parameter would be the relevant one for systems possessing an Ising transition. As a result of the Ising symmetry, any finite system will always possess

\[
\langle M_z \rangle = 0, \tag{7}
\]

and so a more useful metric for studying the critical behaviour of this model is given by the Binder cumulant of the order parameter,

\[
U \equiv 1 - \frac{\langle M_z^4 \rangle}{3\langle M_z^2 \rangle^2}. \tag{8}
\]

At low temperatures, in a system with an Ising transition, the Binder cumulant approaches a value of \( 2/3 \), up to corrections which scale as \( 1/N \), while at high temperatures it approaches a value of zero, again up to corrections which scale as \( 1/N \). In the large system size limit, the transition between these two Binder cumulant values is sharp, transitioning between the two limiting cases at the critical temperature of the model, \( T_c \). When the Binder cumulant is plotted as a function of temperature for different finite system sizes, the crossing point of these curves provides a good estimate for the critical temperature, \( T_c \) [28].

If we now imagine starting from one eigenstate of this system, computing the RDM for many different subsystems \{\( A \)\}, all satisfying \( 1 << n_A << N \), and then using these RDMs to study the behaviour of the Binder cumulant as a function of temperature for all of these different subsystem sizes, we can diagnose the existence of such an Ising transition by demonstrating the existence of a crossing point at some non-zero \( T_c \).

Furthermore, if we wish to extract quantitative information about the critical behaviour of this transition, we could, for example, extend this procedure to the magnetic susceptibility, which, for a finite system of size \( n_A \), reaches a maximum at a pseudo-critical point, \( T_c (n_A) \). Combining this fact with our RDM procedure to extract \( T_c (n_A) \) for many different subsystem sizes, and then using the scaling relation [27]

\[
T_c^{-1} (n_A) = T_c^{-1} (\infty) - a n_A^{-1/\nu}, \tag{9}
\]


where $a$ is some constant and $T_c^{-1}(\infty)$ is the (inverse) critical temperature in the thermodynamic limit, it becomes possible to extract the critical exponent $\nu$ describing the divergence of the spin-spin correlation length. Since this analysis was performed using RDMs that were extracted from one individual energy eigenstate, this critical exponent must have been encoded in this state. A similar analysis could be performed for any other critical exponent of interest.

We mention here two important subtleties of this procedure, and argue why they should not substantially alter any of the conclusions reached above. First, there is some subtlety that is associated with the proper definition of $\hat{H}_A$, in particular, how the matter of boundary terms between the subsystem and its complement should be addressed. Here, when we must make such a distinction, we will adopt the simple (yet possibly less appropriate, see [24]) convention that $\hat{H}_A$ consists of all terms in the original Hamiltonian $\hat{H}$ with support on subsystem $A$, and disregard any terms which involve operators with support on the complementary region, or the boundary between the two. While the precise definition of $\hat{H}_A$ will have consequences for the satisfaction of equation 11 in a finite system, the distinction is expected to become irrelevant in the thermodynamic limit. Furthermore, if our interest is in merely extracting information about the critical point, our only concern is that the $\hat{H}_A$ we recover possesses a finite-temperature phase transition which is in the same universality class as the original Hamiltonian, which is a much weaker requirement.

Second, we emphasize that in our finite-size scaling analysis, all observable quantities, as a function of temperature, should be analytic. One may object to the procedure described above, in that we are taking a thermal density matrix which may correspond to a temperature on one side of the critical point of our model, and using it to extrapolate the behaviour of the subsystem to temperatures which are on the other side of the critical point. However, since there is no actual phase transition in a strictly finite system, there is no concern that we are attempting to extrapolate an observable quantity across a singularity.

III. NUMERICAL INVESTIGATION

Our theoretical argument outlined above rests on the assumption that the strong form of ETH will be satisfied in quantum systems with a finite-temperature phase transition, and that it is indeed possible to use one energy eigenstate of such a system to extrapolate observable quantities for a subsystem across a wide range of temperatures. We now provide numerical evidence in support of this claim. Our model Hamiltonian will be the transverse-field Ising chain

$$\hat{H} = -\sum_{i\neq j} J_{ij} \hat{\sigma}^z_i \hat{\sigma}^z_j - g \sum_i \hat{\sigma}^x_i,$$  \hspace{1cm} (10)

where $\hat{\sigma}^x_i$, $\hat{\sigma}^y_i$, and $\hat{\sigma}^z_i$ are the standard Pauli matrices on site $i$ of a one-dimensional lattice. The Ising interaction $J_{ij}$ is chosen to obey a power-law decay,

$$J_{ij} = \frac{J}{|i-j|^p}. \hspace{1cm} (11)$$

We set $J = 1$, which fixes the energy scale, and corresponds to a ferromagnetic Ising coupling. For the transverse term, we choose $g = 1.5$. Our boundary conditions are chosen to be open, so we do not make use of translation symmetry in diagonalizing the Hamiltonian. We do, however, make explicit use of spatial parity symmetry and Ising symmetry. In our work, we choose $N = 23$, as this is the largest system size for which we are able to find a significant number of exact energy eigenstates. We note that an individual energy eigenstate of the 23-site system lives within a single sector of the Ising and spatial parity symmetries, the RDMs which we will extract from these eigenstates live on the full Hilbert space of the subsystem they describe. It is a straightforward exercise to verify that such an RDM will obey the same symmetries as the subsystem Hamiltonian, so long as the original state it is extracted from is an eigenstate of the corresponding symmetries of the 23-site Hamiltonian.

Previous work [26] has studied the compatibility between spontaneous symmetry breaking and ETH in this model, for the case that $p = 1.5$, in which there is a second-order phase transition at finite temperature. Here we shall study this case, as well as the case $p = 3.0$, for which there is no finite-temperature phase transition. Both models possess an energy which scales extensively with system size, and thus a well-defined thermodynamic limit [29]. For the small system sizes we are able to study numerically, we find that ETH is best satisfied in the Ising chain, as opposed to the model defined on a square lattice, hence the reason for our particular choice of geometry; see [26] for details. We will not be interested in any quantum phase transitions which may occur at zero temperature as a result of adjusting any parameters in the Hamiltonian.

Figures 1 and 2 show the result of using this procedure to extrapolate the Binder cumulant as a function of temperature, for the $p = 1.5$ and $p = 3.0$ models, respectively. We perform this procedure for various different subsystem sizes, always with the RDM extracted from the center of the full system, and always from the same energy eigenstate. We also display a comparison against the results obtained from using the exact subsystem Hamiltonian to compute the thermal density matrix of the subsystem directly. While the results of this procedure vary slightly from state to state (see supplementary material), we find that most states produce qualitatively similar results, and so we choose to focus here on the 3,956th excited state of the even Ising, even parity symmetry sector for the $p = 1.5$ model, and the 3,986th excited state of the even Ising, even parity symmetry sector for the $p = 3.0$ model.

In order to aid in the visual comparison of these re-
results, we have rescaled the predictions from the RDM method by the temperature $T_\psi$ of these eigenstates, so that they appear on the same horizontal scale as the predictions of the exact Hamiltonian; however, we again emphasize that the knowledge of this $T_\psi$ is not necessary for the hypothetical extraction procedure we have outlined in the previous section. For the small system sizes considered here, we find that $T_\psi$ depends slightly on the choice of subsystem. The details of the numerical determination of this temperature can be found in the supplementary material.

We note that in both models, given an eigenstate with $T_\psi > 0$, all of the extrapolated curves approach their correct $T = 0$ values (close to 2/3 for the $p = 1.5$ model, and significantly less than 2/3 for the $p = 3.0$ model). In the case of the $p = 1.5$ model, there is a crossing at some intermediate temperature, indicating the presence of a phase transition, while no such crossing exists for the $p = 3.0$ model. In both cases, the scaling of the Binder cumulant with system size is correct. At sufficiently high temperature, this corresponds to a decreasing Binder cumulant with increasing system size for both models, while at low temperature, this scaling behaviour is reversed below the crossing point for the $p = 1.5$ model only. While the quantitative agreement here is not perfect (for example, the precise location of the crossing point for the $p = 1.5$ model is not correct), the qualitative agreement is still impressive, given our somewhat simple definition of the subsystem Hamiltonian which neglects the subtle issue of boundary terms, as well as the extremely small system sizes we have been restricted to, due to computational limitations.

We do not attempt to perform an actual finite-size scaling analysis of the critical exponents here, as we are limited to system sizes small enough that such a scaling analysis would not yield useful results. However, our numerics still provide strong qualitative evidence that such a procedure, given the eigenstate of a sufficiently large system, should be feasible, so long as the success of the extrapolation procedure we have seen here continues to improve with larger system sizes.

**IV. CONCLUDING REMARKS**

We have provided a theoretical argument in support of the claim that individual energy eigenstates of a non-integrable Hamiltonian should encode information about whether that Hamiltonian possesses a finite-temperature phase transition, as well as quantitative information about the critical behaviour of this transition. We have also provided numerical evidence in support of this claim,
though we have stopped short of actually extracting any quantitative information about such a transition, due to computational limitations. However, under the assumption that the extrapolation procedure we have outlined works for larger system sizes, the existence of such a procedure suggests that individual energy eigenstates, even at energy densities away from the critical point, should contain information about the finite-temperature phase transition of the Hamiltonian they originate from.

While this result strikes the authors as being primarily of interest for questions regarding the foundational principles of quantum statistical mechanics, we note one hypothetical scenario in which it could be of practical use. We imagine a Hamiltonian which is believed to satisfy ETH, and also possesses a sign problem, so that it is difficult to study in a traditional quantum Monte Carlo approach. If, for some reason, there existed a special ansatz that allowed for one to find some small fraction of the spectrum (perhaps, for example, the ground state and first excited state), in such a way that RDMs could be extracted and manipulated in a computationally tractable fashion, then our approach outlined here could be useful. This could have applications, for example, in the study of high-temperature superconductivity. However, at present, the authors do not possess any knowledge of such a hypothetical Hamiltonian or corresponding ansatz.

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