Universal Aspects of Eigenstate Thermalization

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Eigenstate Thermalization

\[ \langle E_\alpha | O | E_\beta \rangle = O(E) \delta_{\alpha \beta} + e^{-S(E)/2} f_0(E, \omega) R_{\alpha \beta} \]

\[ E = \frac{E_\alpha + E_\beta}{2} \quad \omega = E_\alpha - E_\beta \]

\[ O(E) = \text{microcanonical expectation value of } O, \]
\[ f_0(E, \omega) \text{ smooth function,} \]
\[ R \text{ random complex variable with zero mean and unit variance.} \]

Questions

• Which operators satisfy ETH? (e.g. projection operator onto an eigenstate doesn’t).

• How much information about a Hamiltonian is encoded in a single eigenstate?

• How large a subsystem of a closed system acts as a good bath?
Consider a finite subsystem \( A \) of an infinite system.

\[
\langle \psi | O | \psi \rangle = \frac{\text{tr}(O e^{-\beta H})}{\text{tr}(e^{-\beta H})}
\]

If above equation holds for all operators \( O \) with support only in region \( A \), then

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

where

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

“thermal reduced density matrix”
\[
\rho_A(\lvert \psi \rangle_\beta) \equiv \rho_{A,\text{th}}(\beta)
\]

Conceptually, two different thermodynamic limits:

1. \(V \to \infty\), with \(V_A\) held fixed.

2. \(V \to \infty, V_A \to \infty\) while the ratio \(V_A/V\) held fixed.
\[
\rho_A(|\psi\rangle_\beta) \overset{?}{=} \rho_{A,\text{th}}(\beta)
\]

Let's test this conjecture for 1D non-integrable spin Hamiltonians.

\[
H = \sum_i \left( -\sigma_i^z \sigma_{i+1}^z + h_x \sigma_i^x + h_z \sigma_i^z \right)
\]

\[h_x, h_z \approx 1\]

Also (see paper):

\[
H = - \sum_i \left[ (J_1 S_i^+ S_{i+1}^- + J_2 S_i^+ S_{i+2}^-) + \text{h.c.} \right] + \sum_i \left( V_1 S_i^z S_{i+1}^z + V_2 S_i^z S_{i+2}^z \right)
\]

TG, Garrison arXiv:1503.00729
Direct Comparison of Spectra

The figure shows the energy density for each eigenstate of an entanglement Hamiltonian for a subsystem size $L=21$, $L_A = 4$. The energy density is plotted against the eigenvalue index. The energy density of the state $|\psi\rangle_\beta \equiv e$ is also shown. The labels on the graph correspond to different energy calculations:

- $\frac{-1}{L_A \beta} \log [\rho_A, \text{th}(\beta)]$
- $\frac{1}{L_A} [H_A + c_A]$
- $\frac{-1}{L_A \beta} \log [\rho_A (|\psi\rangle_\beta)]$
- $\frac{1}{L_A} [\langle u_i | H_A | u_i \rangle + c_A]$

The graph demonstrates the comparison of spectra derived from different canonical counterparts corresponding to Eqns. 2a, 2b, the latter version being susceptible to boundary errors, which nevertheless are expected to vanish as $L_A$ increases. The condition (18) does not come into play while calculating the ground state energy density corresponding to temperature $T=\frac{1}{\beta}$.
Figure 8: Overlap between the Schmidt eigenvectors $\langle \varphi_i | u_j \rangle$ and the eigenvectors $| \varphi_i \rangle$ of the canonical density matrix, for an $L = 2$ system with $L_A = 0$, and subsystem sizes $L_A = 2, 3, 4, 5$. In each case, the eigenvectors are ordered from most significant (largest eigenvalue) to least significant (smallest eigenvalue).

Surprisingly, even though the entanglement spectrum does not match the actual spectrum beyond the energy density $E^\star$, the expectation values $\langle H_A | u_i \rangle | u_i \rangle / L_A$ 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. II C 2, the only way $\langle H_A | u_i \rangle | u_i \rangle$ can exceed the total energy $E$ is, if the $E$ boundary term, $E$ boundary $\sum_j r_j j_0 \langle \varphi_i | v_j | H_A | u_j \rangle$, 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. II C 2, Schmidt eigenvalues deviate from their ETH predicted value beyond $E^\star$ (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 $\| \rho_A - \rho_{\text{th}} \|$ between the reduced and canonical density matrices at various system sizes. The trace norm distance, defined as

$$ \| \rho_A - \rho_{\text{th}} \|_1 \leq \sqrt{\text{Tr} \left( (\rho_A - \rho_{\text{th}})^2 \right) } \leq \sqrt{\text{Tr} (\rho_A^2) \text{Tr} (\rho_{\text{th}}^2) }$$

places an upper bound on the probability difference that could result from any quantum measurement on the two density matrices. As such, it provides a 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.
Consequence #1: 

Thermodynamics using a single eigenstate.

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

would imply that Renyi entropies encode free energy at various temperatures.

\[ S_n(\ket{\psi}_\beta) = \frac{n}{n-1} V_A \beta (f(n\beta) - f(\beta)) \]

(holds only to leading order due to conical singularity)
Free energy density from a single eigenstate
Consequence #2:

Expectation value of observables at all temperatures using a single eigenstate.

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

+ corrections of order \(e^{-x/\xi_T}, e^{-y/\xi_T}\)
What about the limit $L_A \to \infty$, $L \to \infty$ such that $L_A/L$ is held a non-zero constant?
For random pure states, Renyi entanglement entropy density equals infinite temperature Renyi entropy density as long as $V_{A}/V < 1/2$. 

Lubkin 1978; Lloyd, Pagels 1988; Page 1993
For random pure states, Renyi entanglement entropy density equals thermal Renyi entropy density as long as $V_A/V < 1/2$.

Does the above plot holds true for finite energy density eigenstates of an ergodic system?
Scaling of Entanglement Entropy at fixed $L_A/L$

Entanglement entropy seemingly equals thermal entropy even at fixed $L_A < L/2$ at non-infinite temperatures as well.

Analytical evidence of conjecture from recent work on large central charge CFTs (Hartman et al (2014), Kaplan et al (2014)).
Scaling of Renyi Entropy at fixed $L_A/L$

Doesn’t seem to work as well as the von Neumann entropy!
Berry’s Conjecture for Hard-Sphere Gas

\[ \psi_\alpha(X) = N_\alpha \int d^{3N}P \, A_\alpha(P) \, \delta(P^2 - 2mU_\alpha) \, \exp(iP \cdot X/\hbar) \]

\[ A_\alpha(P) \] Gaussian random variable

\[ \langle A_\alpha(P) A_\beta(P') \rangle_{EE} = \delta_{\alpha\beta} \delta^{3N}(P + P')/\delta(P^2 - P'^2) \]

What’s the nature of reduced density matrix and quantum entanglement and for this system?

Berry 1977, See also Srednicki 1994
Perturbative Many-body Berry’s Conjecture

Consider an integrable system perturbed by an infinitesimal integrability-breaking term

$$H = H_0 + \epsilon H_1$$

e.g.,

$$H = \sum_{i=1}^{L} -Z_i Z_{i+1} - h_z Z_i + \epsilon X_i$$

$$\lim_{\epsilon \to 0} \lim_{L \to \infty} \langle \psi_m \rangle = \sum_{E_\alpha \in [E_m - \frac{1}{2} \Delta, E_m + \frac{1}{2} \Delta]} C_\alpha |s_\alpha \rangle$$

$$P(\{C_\alpha\}) \sim \delta(1 - \sum_\alpha |C_\alpha|^2)$$

Motivation: Deutsch 1991

TG, Lu arXiv:1503.00729
### Renyi Entropies assuming this conjecture:

\begin{align*}
S_2 &= - \log \text{Tr} \rho_A^2 = - \log \left[ \frac{\sum E_A e^{2S_A^M(E_A)+S_A^M(E-E_A)} + e^{S_A^M(E_A)+2S_A^M(E-E_A)}}{\sum E_A e^{S_A^M(E_A)+S_A^M(E-E_A)}} \right]^2 \\
S_3^A &= - \frac{1}{2} \log \left[ \frac{\sum E_A e^{S_A^M(E_A)+3S_A^M(E-E_A)} + 3e^{2S_A^M(E_A)+2S_A^M(E-E_A)} + e^{S_A^M(E_A)+2S_A^M(E-E_A)} + e^{3S_A^M(E_A)+S_A^M(E-E_A)}}{\sum E_A e^{S_A^M(E_A)+S_A^M(E-E_A)}} \right]^3 \\
S_n^A &= \frac{1}{1-n} \log \left[ \frac{\sum E_A e^{S_A^M(E_A)+nS_A^M(E-E_A)}}{\sum E_A e^{S_A^M(E_A)+S_A^M(E-E_A)}} \right]^n
\end{align*}

at the leading order as \( V \to \infty, V_A \to \infty \) while \( V_A/V \) is fixed.
**Saddle point approximation for Renyi Entropies in the thermodynamic limit**

\[
S_n^A = \frac{V}{1-n} \left[ f s(\epsilon_A) + n(1-f)s\left(\frac{\epsilon - \epsilon_A f}{1-f}\right) - ns(\epsilon) \right]
\]

where \(\epsilon_A\) satisfies

\[
\frac{\partial s}{\partial \epsilon} \Bigg|_{\epsilon_A} = n \frac{\partial s}{\partial \epsilon} \Bigg|_{\frac{\epsilon - \epsilon_A f}{1-f}}
\]

\(V = \text{total volume}, f = V_A/V, s = \text{thermal entropy density}, \epsilon = \text{energy density of the eigenstate} \)

**Only when** \(n = 1\) (von Neumann entropy), \(\epsilon_A = \epsilon\), and \(S^A/V_A\) is independent of \(f = V_A/V\) (⇒ no curvature i.e. Page curve)

(first noticed in a particle number conserving model at infinite temperature in TG, Garrison arXiv:1503.00729)
Example: $H_0$ with Gaussian density of states.

$$S_n = V f \left[ \log(2) - \frac{n}{2[1+(n-1)f]} \beta^2 \right]$$

Convex for $n > 1$,

Concave for $n < 1$.

$(f = V_A/V)$

No Page Curve for $S_n$, $n \neq 1$

Disagrees with “Canonical Thermal Pure Quantum State” calculation (Fujita et al 2017) which claims $S_n$ matches with thermal Renyi entropy (= finite temperature Page Curve).
Demonstration

\[ H = \sum_{i=1}^{L} Z_i + \epsilon \times \text{Random Matrix} \]
Non-perturbative Generalization

\[ H |\psi\rangle = E |\psi\rangle \]

\[ H = H_A + H_A^\perp + H_A^{\perp\perp} \]

\[ |\psi\rangle = \sum_{i,j} C_{ij} |E_i^A, E_j^{\perp}\rangle \]

“Ergodic Bipartition” Conjecture:

\[ P(\{ C_{ij} \}) \propto \delta(1 - \sum_{ij} |C_{ij}|^2) \prod_{i,j} \delta(E_i^A + E_j^{\perp} - E) \]

cf. Deutsch 2009: perturbative argument for von Neumann entropy wavefunction for

\[ H = H_A + H_A^\perp + \epsilon H_A^{\perp\perp} \]
Consequences

Reduced Density Matrix

$$\rho_A = \frac{1}{N} \sum_{\alpha} |s_{\alpha}\rangle \langle s_{\alpha}| e^{SM_{\bar{A}}(E-E_{\alpha})}$$

Renyi Entropies

Exactly same functional form as in the perturbative Berry’s conjecture:

\[ S_2 = - \log \text{Tr} \rho_A^2 = - \log \left[ \frac{\sum_{E_A} e^{2S_A^M(E_A)+S_A^M(E-E_A)} + e^{S_A^M(E_A)+2S_A^M(E-E_A)}}{\left( \sum_{E_A} e^{S_A^M(E_A)+S_A^M(E-E_A)} \right)^2} \right] \]

At leading order: \[ S_A^n = \frac{1}{1 - n} \log \left[ \frac{\sum_{E_A} e^{S_A^M(E_A)+nS_A^M(E-E_A)}}{\left( \sum_{E_A} e^{S_A^M(E_A)+S_A^M(E-E_A)} \right)^n} \right] \]

Once again, only \( S_1 \) (von Neumann entropy) follows Page Curve. For all other \( S_n \), curvature is non-zero in \( V \to \infty \) limit.
\[ H = \sum_i \left( -\sigma_i^z \sigma_{i+1}^z + h_x \sigma_i^x + h_z \sigma_i^z \right) \quad \text{with} \quad h_x, h_z \approx 1 \]
Finite Size Scaling and Comparison with Thermal Renyi
Finite Size Scaling and Comparison with Thermal Renyi

1. Von Neumann and Renyi entropy
   - By definition, the thermal entropy reaches a maximum at infinite temperature. Together with Eq. 35, this implies that when ETH holds, eigenstates at the infinite temperature point for a model with no conservation law (left panel, given by Eq. 30 at infinite temperature) are expected to form an inverted triangle shape, similar to the behavior of a random pure state. The entropy deviation at infinite temperature point is given by Eq. 30, with constants 21 and 27.

2. Figure 3 shows the scaling of von Neumann entropy $(\mathcal{A} S)$ with subsystem size $V_L$ and $V_A$. When the subsystem is taken to be a $V_A \times V_A$ triangle shape, similar to the behavior of a random pure state in the thermodynamic limit, the function $a(f \text{ vs } \log V_A)$ is expected to form an inverted triangle shape.

3. The grey vertical lines in Fig. 5 denote the entropy deviation at the infinite temperature point for a model with no conservation law (left panel, given by Eq. 30). Notice that the Renyi entropies at infinite temperature satisfy

$$S_k = \frac{1}{k} \log \text{Tr} \rho_k$$

for constant ratio $k \in (1, \infty)$.

4. The error bars represent one standard deviation away from the mean. Even when resolution limits the range of $(\mathcal{A} S_k)$, for $k = 1/2$ and $k = 1$, the error bars are very small, indicating high accuracy when comparing to the thermal distribution.

5. This implies that when ETH holds, eigenstates at the infinite temperature point for a model with no conservation law (left panel, given by Eq. 30) are expected to form an inverted triangle shape, similar to the behavior of a random pure state in the thermodynamic limit.

6. As seen in the limit $k \rightarrow 0$, the Renyi entropy deviation for eigenstates at the infinite temperature point for a model with no conservation law (left panel, given by Eq. 30) is finite, we calculate $(\mathcal{A} S_k)$ for $k = 1/2$ and $k = 1$.

7. This implies that when ETH holds, eigenstates at the infinite temperature point for a model with no conservation law (left panel, given by Eq. 30) are expected to form an inverted triangle shape, similar to the behavior of a random pure state in the thermodynamic limit.
Summary

• For many-body ergodic systems, a single eigenstate sufficient to extract Hamiltonian properties at arbitrary temperatures.

• As $V \rightarrow \infty$, with $V_A$ held fixed, reduced density matrix for region A is fully thermal.

• Many-body Berry conjecture/ergodic bipartition explains several intriguing features of entanglement scaling. Numerical evidence seems good. Specifically:

  1. von Neumann entropy density for an eigenstates equals thermal entropy density as long as $V_A < V/2$ ("finite T Page Curve"). One doesn’t need $V_A << V$.

  2. Renyi entropies follow a universal formula that depends only on the density of states, and unlike von Neumann entropy, have curvature as a function of $V_A/V$ as $V \rightarrow \infty$. 