Thermalization in Closed Quantum Systems

CQuIC Summer Course on Quantum Chaos

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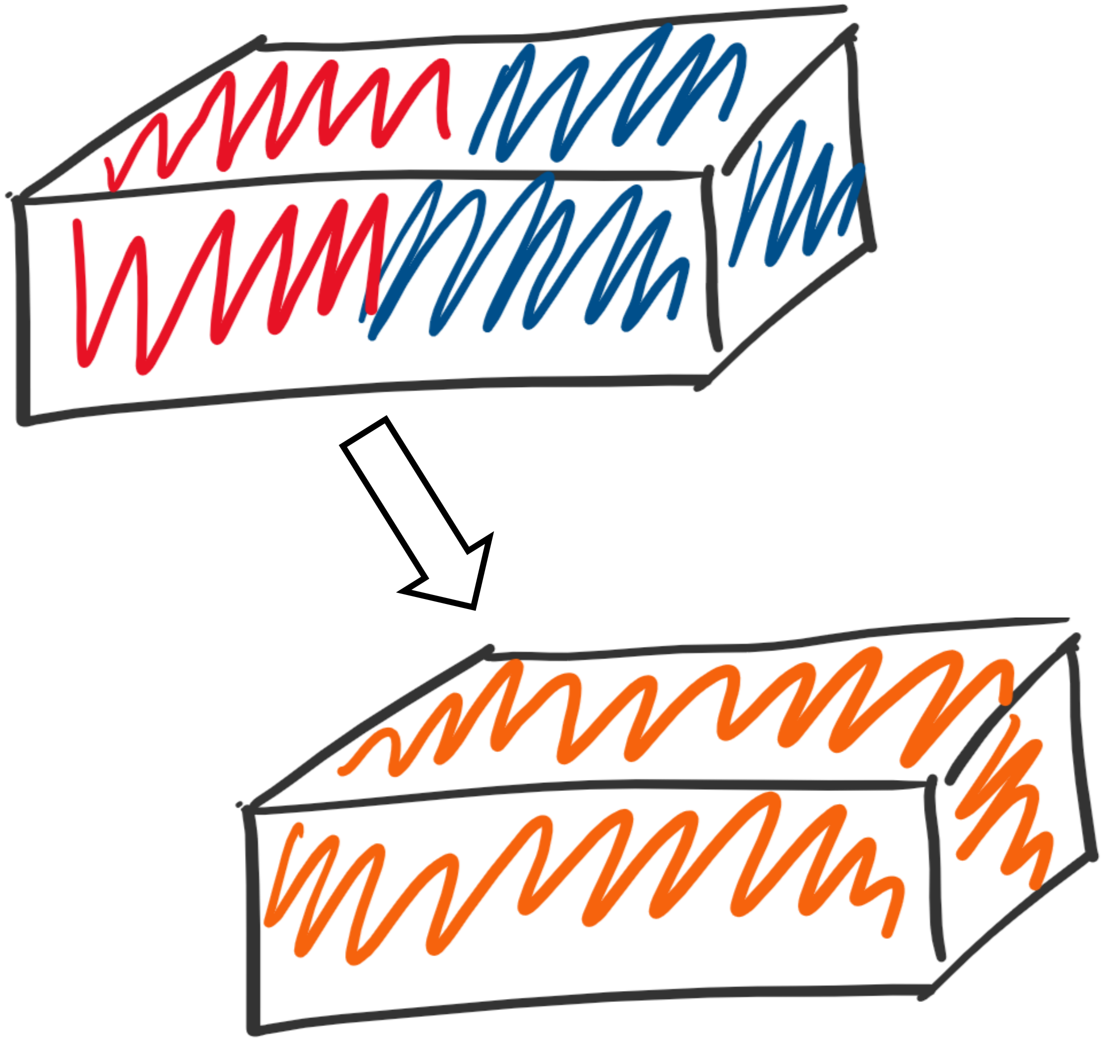
Outline

- Equilibration and Thermalization (Overview)
- Classical Thermalization Review
- Issues with Quantum Thermalization
- A Random Matrix Theory Approach
- Eigenstate Thermalization Hypothesis (ETH)
- ETH and Quantum Information

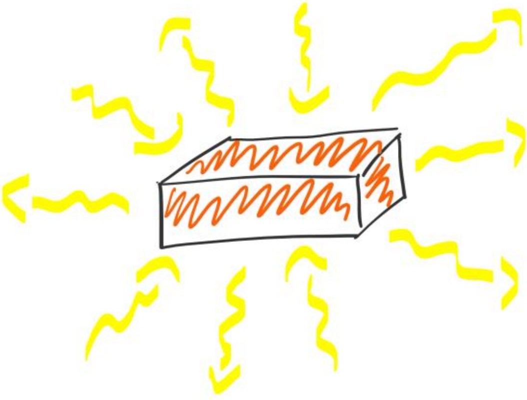
What is Thermalization?

- Equilibration
  - Approaching a state and remaining near that state for most time
- Thermalization
  - Equilibrium state only depends on certain macroscopic quantities, and given by relevant ensemble



Types of Thermalization

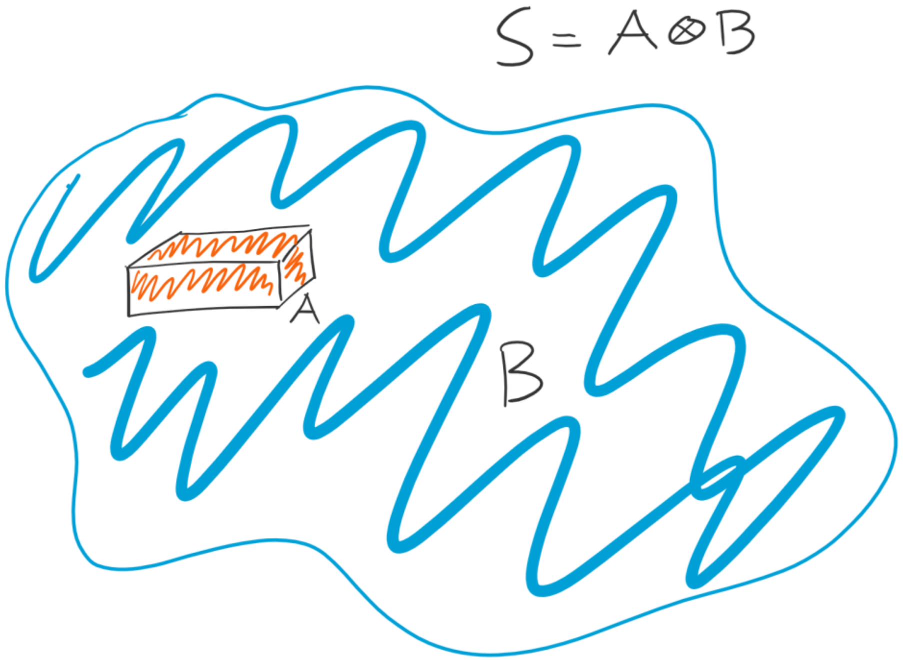
Open System



Canonical Ensemble

$$\mathrm{Tr}\frac{e^{-\beta H}\hat{O}}{Z}$$

Subsystem



Closed System

Microcanonical Ensemble

$$P(A) \propto \Omega(A)$$

Observable vs Subsystem Thermalization

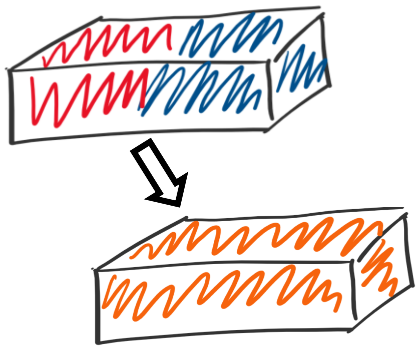
$$
\begin{tikzcd}[column sep=small]
 & O(\mathbf{q}(t), \mathbf{p}(t)) \\
O(t) \arrow[ur] \arrow[dr] & \\
 & \langle \psi(t) | \hat{O} | \psi(t) \rangle
\end{tikzcd}
$$

- Generally considering sets of observables

$$\hat{\rho}_S(t) = \mathrm{Tr}_{S^c} \left(e^{-iHt} |\psi\rangle\langle\psi| e^{iHt} \right)$$

- This can be viewed as a special case of the above

Equilibration on Average



$$O(t) \to O_{\mathrm{eq}}$$

- Observable approaches an equilibrium value

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T (O(t) - O_{\mathrm{eq}})^2 dt \approx 0$$

- Observable stays close to equilibrium value

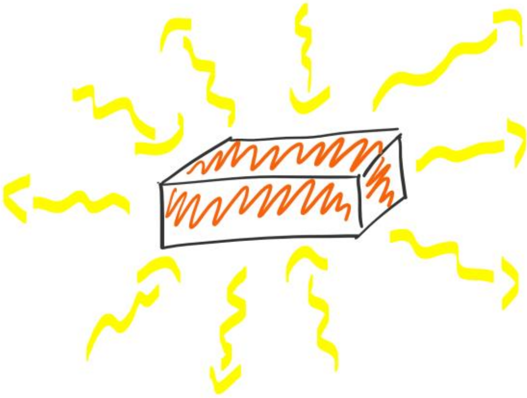
$$O_{\mathrm{eq}} \approx \lim_{T\to\infty} \frac{1}{T}\int_0^T O(t) dt$$

- Equilibrium value well-approximated by long-time average

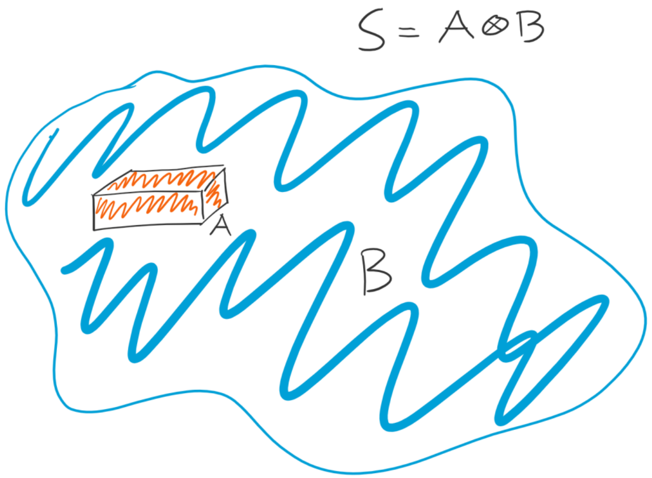
Analogous expressions hold for subsystem equilibration

Thermalization and Information

- Thermalization necessarily implies a loss of information
- Where did it go?



Lost to Environment



Inaccessible to local observables

Inaccessible to macroscopic observables

Classical Thermalization

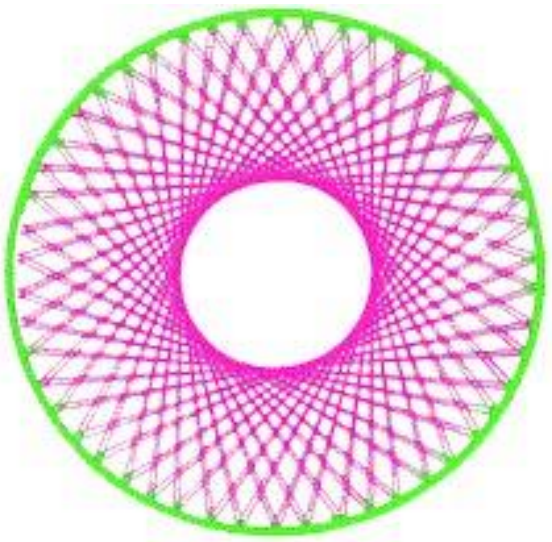
$$H(\mathbf{p},\mathbf{q}) \qquad \mathbf{z} = (\mathbf{q},\mathbf{p})$$

$$H(\mathbf{p}(t),\mathbf{q}(t)) = H(\mathbf{p}(0),\mathbf{q}(0)) = E$$

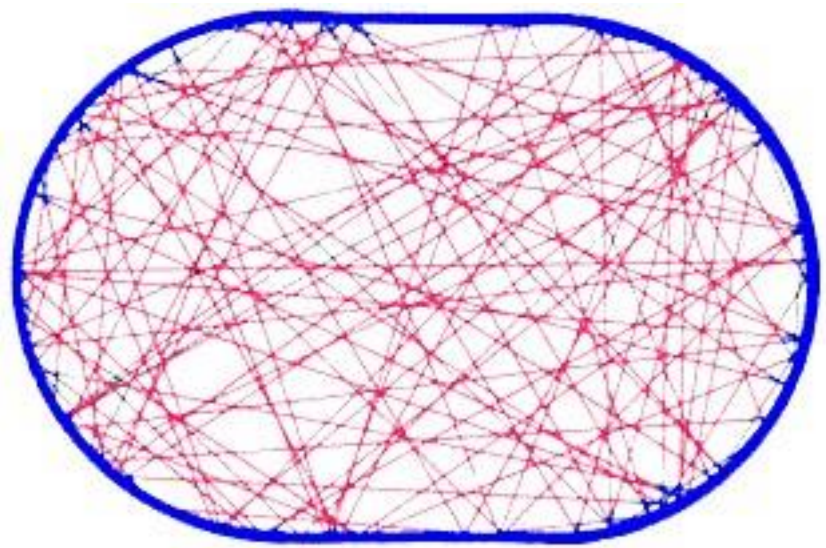
Equations of Motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

Integrable



Chaotic



Classical Thermalization

Chaos $\longrightarrow$ Mixing $\longrightarrow$ $\boxed{\text{Ergodicity}}$

Ergodicity
"Time average = Phase space average"
Orbits fill the entire energy shell uniformly

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T O(t)dt = \frac{\int_{S_E} O(z)dz}{\int_{S_E} dz}$$

$$\boxed{\frac{\int_{S_E} O(z)dz}{\int_{S_E} dz} \equiv \langle O\rangle_{\mathrm{micro}}}$$

Classical Thermalization (Closed System)

Consider a macroscopic observable O

$\Omega(A)$: Number or measure of microstates corresponding to observable value *A*

$$O_{\mathrm{eq}} = \lim_{T\to\infty} \frac{1}{T} \int_0^T O(t)dt = \frac{\int_{S_E} O(z)dz}{\int_{S_E} dz} \approx \operatorname*{argmax}_A \Omega(A)$$

Information about initial conditions cannot be resolved by macroscopic observable

Classical Thermalization (Subsystem)

Assume: S is in microcanonical ensemble at energy E and A,B can exchange energy

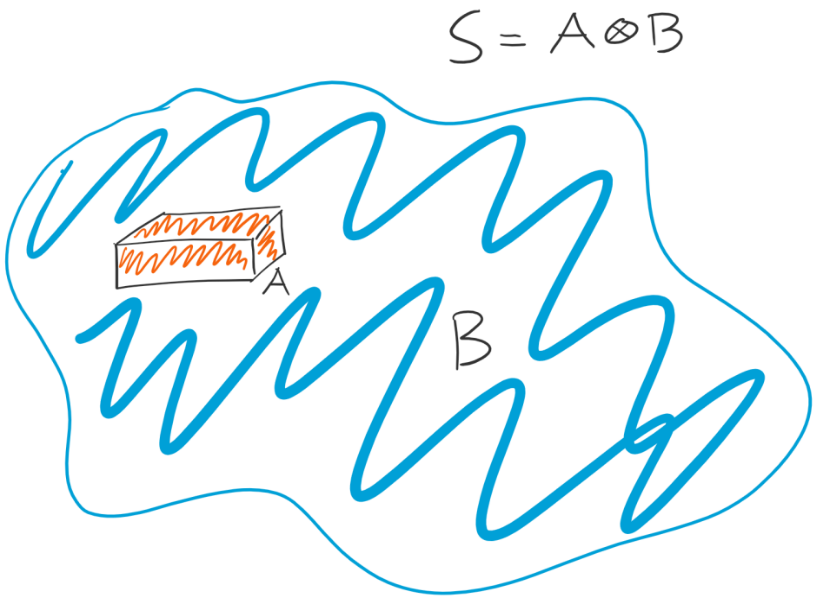
$$S(E) = k\log(\Omega(E))$$
$$\frac{1}{T} = \frac{\partial S}{\partial E}$$

$$\Omega_{AB}(E) = \Omega_B(E - E_A)\Omega_A(E_A)$$

$$\frac{\Pr(E_A)}{\Pr(E'_A)} = \frac{\Omega_A(E_A)}{\Omega_A(E'_A)} = \frac{\Omega_B(E - E'_A)}{\Omega_B(E - E_A)}$$

$$= e^{\frac{1}{k}(S(E-E_A)-S(E-E'_A))} \approx e^{-\frac{1}{kT}(E_A-E'_A)}$$

$$\implies \Pr(E_A) = \frac{e^{-\frac{E_A}{kT}}}{Z}$$ (Canonical Ensemble)



The initial information contained in A is spread throughout the whole system and becomes inaccessible to local observables.

Summary

Chaos → Ergodicity → Microcanonical Ensemble

Microcanonical Ensemble → Closed System Thermalization w.r.t Macroscopic Observable

Microcanonical Ensemble → Subsystem Thermalization to Canonical Ensemble

Transition to Quantum Thermalization

Immediate Issues

- No phase space (position and momentum don't commute)
- No well-defined trajectories, initial wave packets will spread
- No clear integrable vs nonintegrable definition
- Difficult to define chaos $\langle\psi(t)|\phi(t)\rangle = \langle\psi(0)|\phi(0)\rangle$

Transition to Quantum Thermalization

$$|\psi(t)\rangle = \sum_i c_i e^{-iE_i t}|E_i\rangle$$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\langle\psi(t)|\hat{O}|\psi(t)\rangle = \sum_i |c_i|^2\langle E_i|\hat{O}|E_i\rangle$$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt|\psi(t)\rangle\langle\psi(t)| = \sum_i |c_i|^2|E_i\rangle\langle E_i| \neq$$ Microcanonical ensemble

In general, long-time averages are sensitive to the initial conditions $c_i = \langle E_i|\psi(0)\rangle$

Equilibration Turns Out to be Quite General

$N(\epsilon)$: The maximal number of approximately degenerate energy gaps in an energy interval of width ϵ

$$\langle \hat{O}(t) \rangle = \langle \psi(t) | \hat{O} | \psi(t) \rangle$$

$$O_{\text{eq}} = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \langle \hat{O}(t) \rangle$$

$$\frac{1}{T} \int_0^T dt \left(\langle \hat{O}(t) \rangle - O_{\text{eq}} \right)^2 \leq C(|\psi(0)\rangle) \|\hat{O}\|^2 N(\epsilon) \left(1 + \frac{8 \log(\dim(H))}{\epsilon T} \right)$$

$$C(|\psi(0)\rangle) \sim \frac{1}{\dim(H)}$$

For states that populate a significant number of energy eigenstates

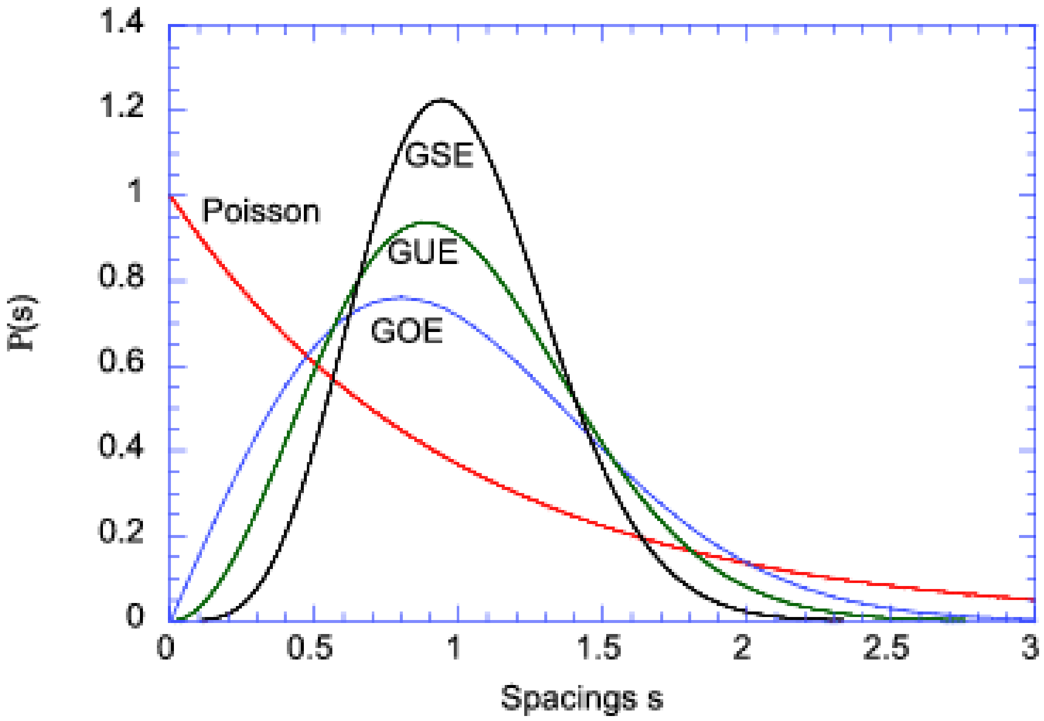
$$\langle \psi(t) | \hat{O} | \psi(t) \rangle = \sum_i |c_i|^2 \langle E_i | \hat{O} | E_i \rangle + \sum_{i \neq j} c_i c_j^* e^{-it(E_i - E_j)} \langle E_j | \hat{O} | E_i \rangle$$

While this addresses how quantum systems equilibrate, we still must show that they thermalize

[Gogolin and Eisert, 2016]

Random Matrix Theory

- Recall, The BGS conjecture states that quantum systems with chaotic classical counterparts have spectra with the same statistics as random matrices
- Since classical chaotic systems thermalize, consider an RMT approach to quantum thermalization
- The eigenvectors of a random matrix are essentially random unit vectors which are mutually orthogonal



Random Matrix Theory

$$\hat{O} = \sum_i O_i |O_i\rangle\langle O_i|$$

We can calculate the average matrix elements of observables in the random energy eigenbasis

$$O_{mn} = \langle E_m|\hat{O}|E_n\rangle = \sum_i O_i \langle E_m|O_i\rangle\langle O_i|E_n\rangle$$

$$\overline{\langle E_m|O_i\rangle\langle O_j|E_n\rangle} = \frac{1}{\mathcal{D}}\delta_{mn}\delta_{ij}$$

(Averaging $|E_m\rangle$ and $|E_n\rangle$ over the Haar measure)

$$\boxed{\overline{O_{mm}} = \frac{1}{\mathcal{D}}\sum_i O_i}$$

$$\boxed{\overline{O_{mn}} = 0} \qquad m \neq n$$

Random Matrix Theory

$$O_{mn} = \langle E_m|\hat{O}|E_n\rangle = \sum_i O_i \langle E_m|O_i\rangle\langle O_i|E_n\rangle$$

The fluctuations about the average of observables in the random energy eigenbasis can also be calculated

$$\boxed{\overline{O_{mm}^2} - \overline{O_{mm}}^2 = \overline{|O_{mn}|^2} - \overline{|O_{mn}|}^2 = \frac{1}{\mathcal{D}^2}\sum_i O_i^2}$$

(For GUE)

For the detailed derivation, see [D'Alessio et al., 2016]

RMT Observable Ansatz

Define: $\overline{O} \equiv \frac{1}{\mathcal{D}} \sum_i O_i$ $\qquad \overline{O^2} \equiv \frac{1}{\mathcal{D}} \sum_i O_i^2$

Ansatz: $O_{mn} \approx \overline{O}\delta_{mn} + \sqrt{\frac{\overline{O^2}}{\mathcal{D}}} R_{mn}$ $\qquad R_{mn}$ is a zero mean, unit variance random variable

Thermalizes*

$$O_{\mathrm{eq}} = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\langle O(t)\rangle = \sum_m |c_m|^2 O_{mm} \approx \overline{O}\sum_m |c_m|^2 = \overline{O}$$

No dependence on initial conditions!

RMT is Insufficient

$$O_{\rm eq} = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt \langle O(t)\rangle = \sum_m |c_m|^2 O_{mm} \approx \overline{O}\sum_m |c_m|^2 = \overline{O}$$

1. The equilibrium values in the RMT ansatz are independent of the system energy density

2. Relaxation times are observable dependent, and this information should be contained in off-diagonal matrix elements

Eigenstate Thermalization Hypothesis

Define: $\overline{E} \equiv \frac{1}{2}(E_m + E_n) \qquad \omega \equiv E_n - E_m$

Ansatz

$$O_{mn} = \mathcal{O}(\overline{E})\delta_{mn} + e^{-S(\overline{E})/2} f(\overline{E}, \omega) R_{mn}$$

$\mathcal{O}(\overline{E}), f(\overline{E}, \omega)$ are smooth functions of their arguments

R_{mn} is a zero mean, unit variance random variable

$e^{S(E)} = E \sum_{\alpha} \delta_{\epsilon}(E - E_{\alpha})$ is the thermodynamic entropy

Comparing ETH to RMT

RMT	ETH
$O_{mn} \approx \overline{O}\delta_{mn} + \sqrt{\frac{\overline{O^2}}{\mathcal{D}}} R_{mn}$	$O_{mn} = \mathcal{O}(\overline{E})\delta_{mn} + e^{-S(\overline{E})/2} f(\overline{E},\omega) R_{mn}$

1. The diagonal elements in ETH are not the same for all eigenstates, and more importantly, energy dependent

2. The off-diagonal elements in ETH depend on the envelope function $f(\overline{E},\omega)$ characterizing the relaxation time

The results of the ETH ansatz agree with the semi-classical predictions of the BGS conjecture [D'Alessio et al., 2016]

ETH Thermalizes

$$O_{mn} = \mathcal{O}(\overline{E})\delta_{mn} + e^{-S(\overline{E})/2} f(\overline{E}, \omega) R_{mn}$$

$$\boxed{e^{S(E)} = E \sum_{\alpha} \delta_{\epsilon}(E - E_{\alpha})}$$

$$\langle O \rangle_{\beta} \equiv \frac{\mathrm{Tr} e^{-\beta H} O}{\mathrm{Tr} e^{-\beta H}} = \frac{\int_0^{\infty} \frac{dE}{E} e^{S(E) - \beta E} \mathcal{O}(E)}{\int_0^{\infty} \frac{dE}{E} e^{S(E) - \beta E}} + O(e^{-S/2})$$

Solving this for $\mathcal{O}(E)$ (see [Srednicki, 1998] for proof)

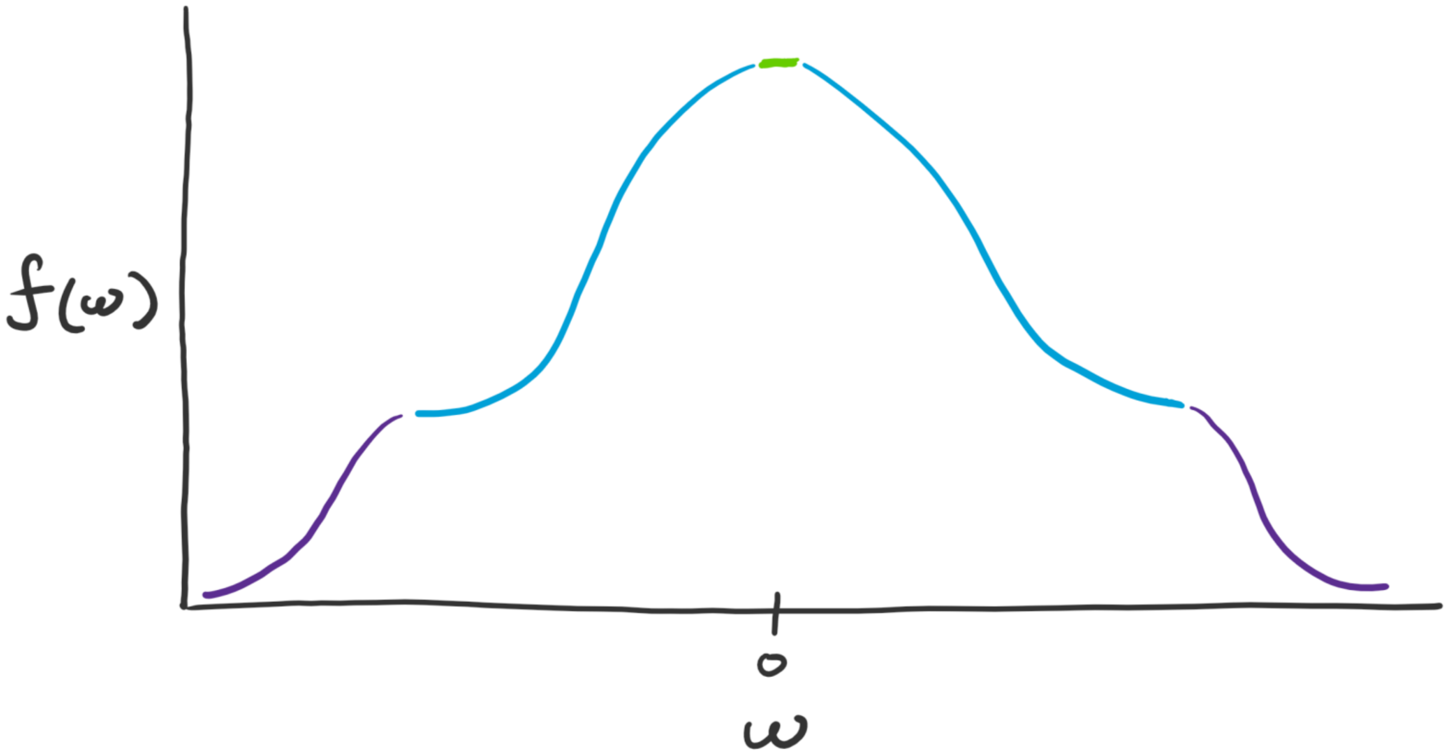
$$\boxed{\mathcal{O}(E) = \langle O \rangle_{\beta} + O(N^{-1}) + O(e^{-S/2})}$$

The Envelope Function $f(\overline{E},\omega)$

Ansatz: $O_{mn} = \mathcal{O}(\overline{E})\delta_{mn} + e^{-S(\overline{E})/2} f(\overline{E},\omega) R_{mn}$

- $f(\omega)$ is approximately constant
- $f(\omega) \propto \dfrac{\Gamma}{\omega^2 + \Gamma^2}$

  Markovian decay back to equilibrium from small fluctuations [Srednicki, 1998]
- $f(\omega)$ decays exponentially

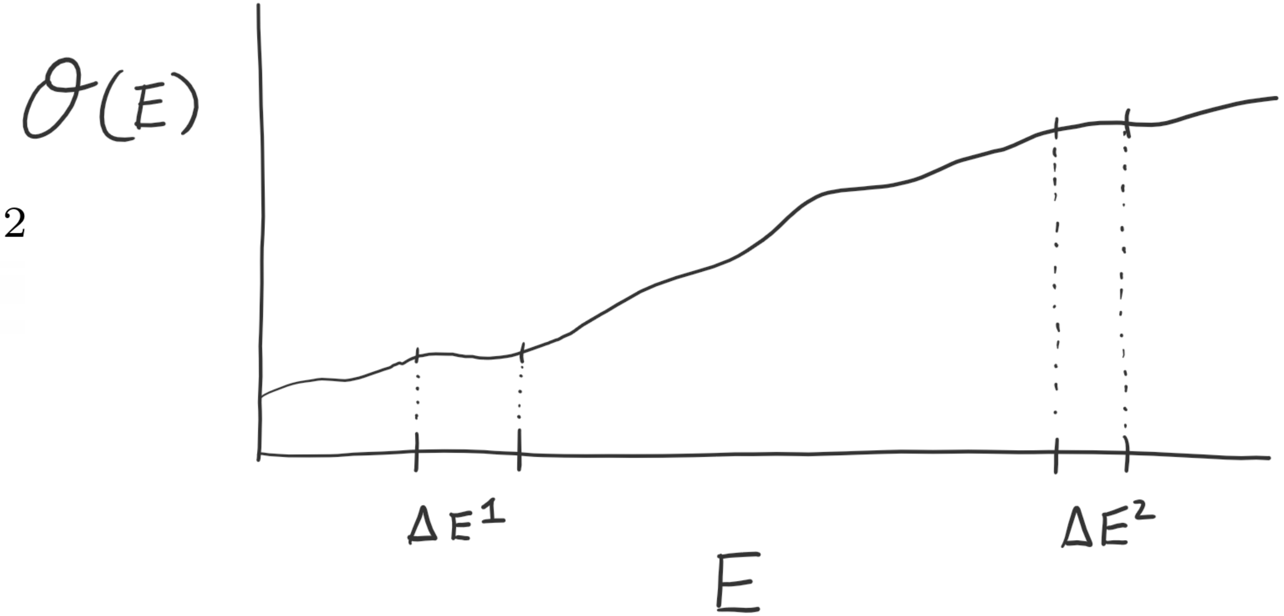


When Will Systems Thermalize?

- In order for a system to thermalize in ETH, the energy variance of the initial state should be small
- The energy eigenstates with appreciable populations should be contained in a region where $\mathcal{O}(E)$ does not vary significantly

$$|\psi(0)\rangle = \sum_{m:E_m\in\Delta E^1} c_m|E_m\rangle + \sum_{n:E_n\in\Delta E^2} c_n|E_n\rangle$$

$$O_{\mathrm{eq}}^{(\psi_0)} \approx \mathcal{O}(E^1)\sum_m |c_m|^2 + \mathcal{O}(E^2)\sum_n |c_n|^2$$



Depends on initial conditions, does not thermalize!

Validity of ETH

- For which observables?
  - ETH is expected to hold for all few-body observables
  - In [Garrison and Grover, 2015], it is conjectured ETH holds for observables with support on up to half of the system size
- For which parts of the spectrum?
  - ETH is expected to be valid for the bulk of the spectrum, not near the edges
  - Strong ETH: Holds everywhere in the bulk
  - Weak ETH: Holds for most eigenstates in the bulk

ETH Subsystem Formulation

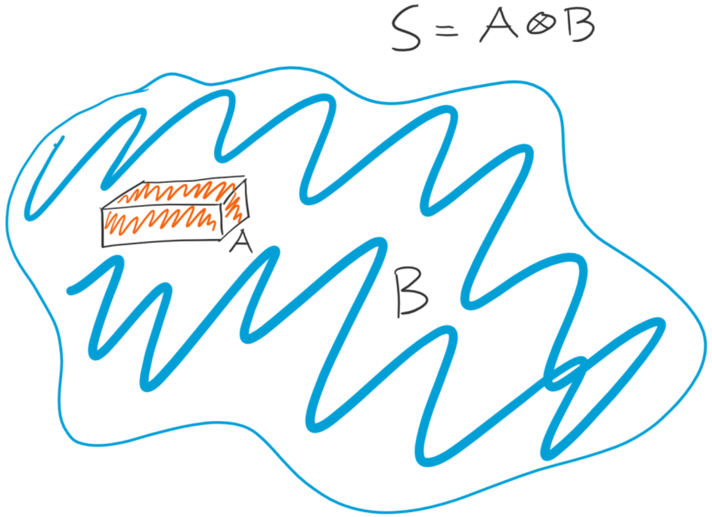
- Consider the set of all local observable on a subsystem *A* and assume ETH holds for each of them

$$\langle E_i|O|E_i\rangle = \langle E_j|O|E_j\rangle + O(e^{-S/2}) \qquad E_i, E_j \in \Delta E$$

$$\implies \mathrm{Tr}_B(|E_i\rangle\langle E_i|) = \mathrm{Tr}_B(|E_j\rangle\langle E_j|) + O(e^{-S/2})$$

$$\langle E_i|O|E_i\rangle = \langle O\rangle_\beta + O(N^{-1}) + O(e^{-S/2})$$

$$\implies \boxed{\mathrm{Tr}_B(|E_i\rangle\langle E_i|) \approx \mathrm{Tr}_B\left(\frac{e^{-\beta H}}{Z}\right) + O(N^{-1}) + O(e^{-S/2})}$$



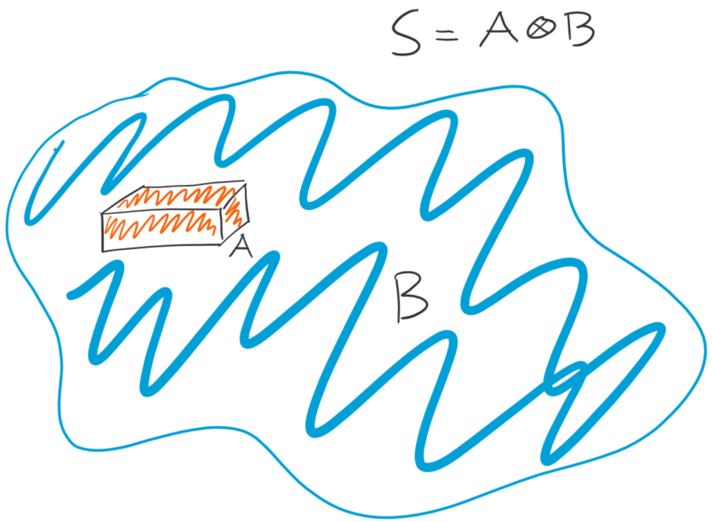
ETH Subsystem Formulation

- "Excited eigenstates are thermal"

$$\boxed{\mathrm{Tr}_B(|E_i\rangle\langle E_i|) \approx \mathrm{Tr}_B\left(\frac{e^{-\beta H}}{Z}\right)}$$

$$\overline{\rho}_T \equiv \lim_{T\to\infty}\frac{1}{T}\int_0^T |\psi(t)\rangle\langle\psi(t)|dt = \sum_i |c_i|^2|E_i\rangle\langle E_i|$$

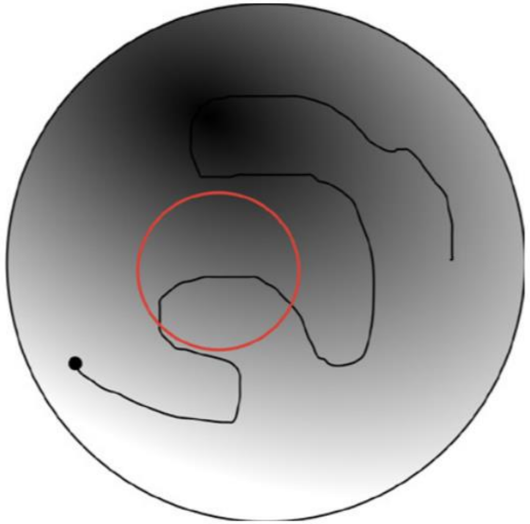
$$\mathrm{Tr}_B(\overline{\rho}_T) = \sum_i |c_i|^2\mathrm{Tr}_B(|E_i\rangle\langle E_i|) \approx \mathrm{Tr}_B\left(\frac{e^{-\beta H}}{Z}\right)$$



Classical vs Quantum Ergodicity

Classical ergodicity is a direct result of the dynamics of the system

Quantum ergodicity is not caused by the dynamics of the system, it is already present in the initial state



$$\langle\psi(t)|\hat{O}|\psi(t)\rangle = \sum_i |c_i|^2 \underset{\mathcal{O}(\overline{E})}{\underset{\approx}{\langle E_i|\hat{O}|E_i\rangle}} + \underbrace{\sum_{i\neq j} c_i c_j^* e^{-it(E_i-E_j)}\langle E_j|\hat{O}|E_i\rangle}_{\text{This will start to dephase and destructively interfere}}$$

ETH and Quantum Error Correction

- Recently, a connection between ETH, chaotic Hamiltonians, and quantum error correction was demonstrated in [Brandao, Crosson et al., 2018]
- If local errors are of the form of the ETH matrix ansatz, they satisfy the approximate Knill-Laflamme condtions where the codespace is the eigenstates contained in a small energy window

$$O_{mn} = \mathcal{O}(\overline{E})\delta_{mn} + e^{-S(\overline{E})/2} f(\overline{E},\omega) R_{mn}$$

$$\langle \psi_i | E | \psi_j \rangle = C_E \delta_{ij} + \epsilon_{ij}$$

ETH and Quantum Error Correction

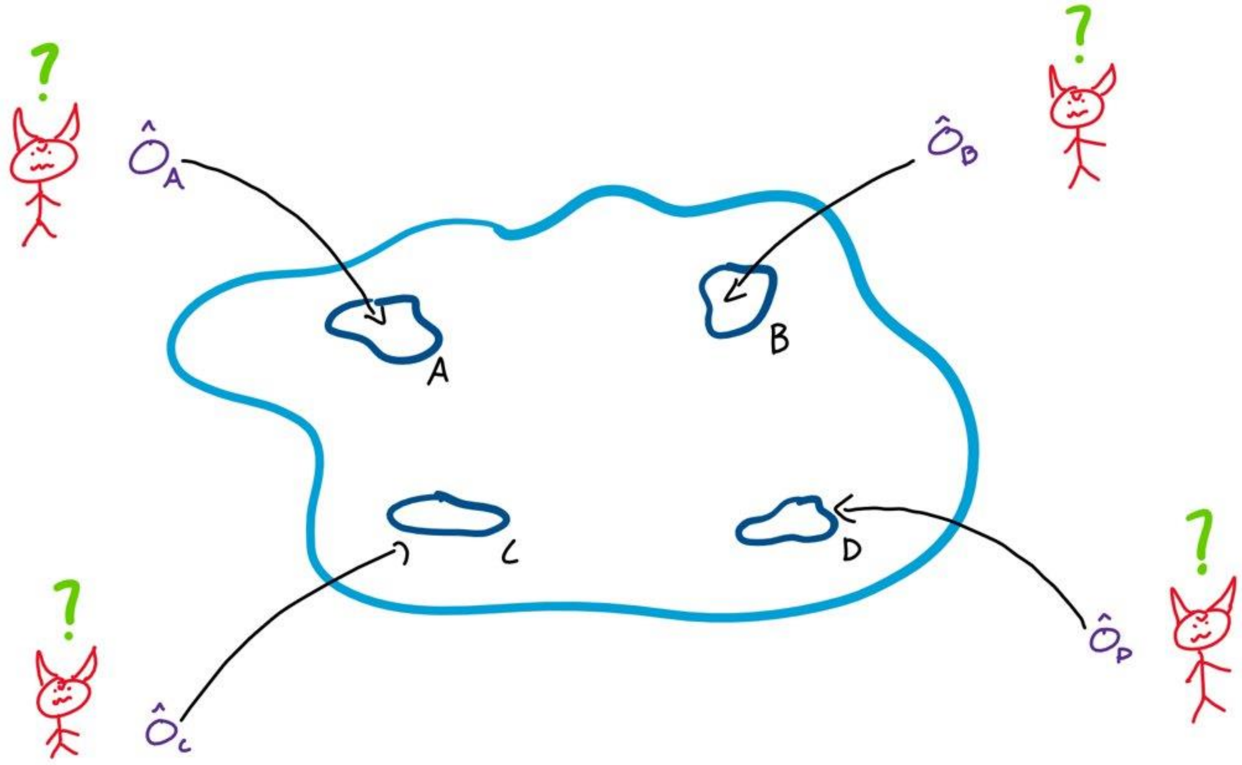
- A more physical formulation of this idea is introduced in [Bao and Cheng, 2019] which extends to a more general definition of chaotic Hamiltonians
- Recall that information about initial conditions in the subsystem picture must become distributed throughout the whole system and becomes inaccessible locally
- The method by which this is achieved via ETH and RMT is that nearby energy eigenstates are already locally indistinguishable

$$\mathrm{Tr}_B(|E_i\rangle\langle E_i|) \approx \mathrm{Tr}_B(|E_j\rangle\langle E_j|) \iff \langle E_i|O|E_i\rangle \approx \langle E_j|O|E_j\rangle$$

ETH and Quantum Error Correction

- If an adversarial environment cannot learn anything about the encoded information by local measurements, this implies an approximate quantum error correcting code [Beny and Oreshkov, 2010]

- Sets of nearby energy eigenstates in ETH form approximate quantum error correcting codes!



Further Topics

- Thermalization in integrable systems and the generalized Gibbs ensemble [D'Alessio et al., 2016, section 8] [Gogolin and Eisert, 2016, section 5.2]
- Other mechanisms of thermalization
    - Typicality [Gogolin and Eisert, 2016, section 6] [Deutsch, 2018]
    - Open System [Deutsch, 2018]
    - Maximum Entropy Principles [Gogolin and Eisert, 2016, section 5.1]
    - Quantum Ergodic Theorem [D'Alessio et al., 2016, section 4.1]

Summary

- In classical systems, there is a well-understood route to understanding thermalization through chaotic dynamics
- Notions of quantum chaos are quite different from classical chaos, requiring a different means of analyzing quantum thermalization
- Random matrix theory almost solves the thermalization problem, but does not contain any energy dependence or relaxation time information (non-physical)
- Modifying RMT yields the Eigenstate Thermalization Hypothesis, which characterizes thermalization for local observables

References

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