ETH
Eigenstate Thermalization Hypothesis

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Contents

What we will see:

1. review thermalization mechanism in classical systems
2. introduce eigenstate thermalization as a possible explanation for thermal behaviour in quantum systems
3. observe eigenstate thermalization in a particular class of systems

Main Results

More specifically:

1. Thermal behaviour in quantum systems *must* fundamentally differ from classical thermalization.
2. According to ETH, thermalization occurs at the level of individual eigenstates of a given Hamiltonian:

   Each eigenstate of the Hamiltonian implicitly contains a thermal state.

3. ETH correctly assesses thermal behaviour exhibited by low-density billiards in the semi-classical regime, provided Berry's conjecture (BC) holds:

$$\text{Berry's conjecture} \Longrightarrow \text{eigenstate thermalization}$$

1. CLASSICAL THERMALIZATION

Isolated Systems

Definition

An **isolated system** consists of N particles with total energy E confined within volume V. Its state is a point in phase space Γ:

$$(p, q) = (p_1, \dots, p_{3N}, q_1, \dots, q_{3N}) \in \Gamma.$$

Dynamics are specified by the Hamiltonian $\mathcal{H} = \mathcal{H}(p, q)$ via

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

Notes:

- any system will be assumed isolated, unless specified otherwise
- the system is part of a microcanonical ensemble, as suggested by the triple (N, V, E)

Fundamental postulate of stat. physics

Let all states satisfying the macroscopic boundary conditions be on the hypersurface $\Gamma_{N,V,E}$. In equilibrium all have an equal a-priori probability, i.e. they are uniformly distributed with a (stationary!) density:

$$\rho_{mc}(p,q) = \begin{cases} const. & \text{if } (p,q) \in \Gamma_{N,V,E} \\ 0 & \text{else} \end{cases}$$

ρ_{mc} is the density function of the microcanonical ensemble.

Definition

We denote by $\Gamma(E)$ the volume of phase space occupied by the microcanonical ensemble:

$$\Gamma(E) = \int_\Gamma d^{3N}p d^{3N}q \rho_{mc}(p,q)$$

Dynamical Chaos

- Classical systems are intrinsically deterministic.
- Nonetheless, they may exhibit (deterministic) chaos, i.e. dynamics highly sensitive to initial conditions
  - quantified: e.g. exponential growth of perturbations in the initial conditions with time (Lyapunov exponent)

For chaotic systems it is useful to:

1. address the issue of possible relaxation of certain measurable quantities to stationary values (thermalization)
2. attempt at a **statistical** description of a system in such thermal equilibrium

Ergodic Hypothesis (Boltzmann, 1871)

Definition

Let $A(p,q)$ be an integrable function, γ a trajectory on the hypersurface $\Gamma_{N,V,E}$, with parametrization $\gamma : \mathbb{R}_0^+ \to \Gamma_{N,V,E}, \quad t \mapsto (p(t), q(t))$. Let the (long-) time and microcanonical averages of A be defined as:

$$\bar{A} = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\ A(p(t), q(t)), \qquad \text{(time average)}$$

$$\langle A \rangle_{mc} = \frac{1}{\Gamma(E)} \int_\Gamma d^{3N}p d^{3N}q\ A(p,q)\ \rho_{mc}(p,q) \quad \text{(m.c. average)}$$

Then the system is ergodic iff

$$\bar{A} = \langle A \rangle_{mc} \tag{1}$$

Comments

- ergodicity justifies the use of the m.c. ensemble for calculating equilibrium values
- (1) is satisfied if the trajectory γ of the (individual) prepared system covers $\Gamma_{N,V,E}$, the constant energy manifold, homogenously
  - time evolution (dynamical chaos) **constructs** the thermal state
- more in the next talk

2. EIGENSTATE THERMALIZATION

The Problem

Task:
describe adequately thermal behaviour when exhibited by isolated quantum systems

$\longrightarrow$ ETH (eigenstate thermalization hypothesis)

- **assume** the system behaves thermally
- whether or not this assumption applies is a different problem (quantum chaos)
- idea: adapt and use ergodicity

Short Digression: Quantum Chaos

The problem: **When** does thermalization occur?

- search for property analogous to dynamical chaos in classical systems a quantum system must have in order to exhibit thermal behaviour
  - random matrix theory
  - e.g. for quantum billiards: validity of Berry's conjecture

A First Thought

Compared to its classical counterpart, any attempt at explaining the thermalization mechanism in quantum systems **must** be fundamentally different:

- time evolution in quantum systems is *linear* (time-dependent Schrödinger equation)

Furthermore:

$$\Delta x \Delta p \geq \hbar/2 \quad \Longrightarrow \quad \text{coarse graining, no phase space}$$

- no dynamical chaos in the classical sense

$\Longrightarrow$Time evolution cannot construct a thermal state.

The Setting

Quantum System

We shall consider isolated, bounded quantum systems with Hamiltonian $\hat{\mathcal{H}}$ and prepared in an initial state:

$$|\psi(t = 0)\rangle \equiv |\psi(0)\rangle.$$

- boundedness implies a discrete energy spectrum
- Let $\hat{\mathcal{H}}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$, where $\{|\psi_\alpha\rangle\}_\alpha$ is a complete orthonormal system. Then:

$$|\psi(0)\rangle = \sum_\alpha C_\alpha|\psi_\alpha\rangle, \quad C_\alpha = \langle\psi_\alpha|\psi(0)\rangle, \quad \sum_\alpha |C_\alpha|^2 = 1$$

Note: we call $|C_\alpha|^2$ the **eigenstate occupation numbers** (EON's).

Energy

Corollary

For the total energy of the system we obtain:

$$\langle E\rangle = \langle\psi(0)|\hat{\mathcal{H}}|\psi(0)\rangle = \sum_\alpha |C_\alpha|^2 E_\alpha$$

Generic Initial State

We will restrict our attention to initial states $|\psi(0)\rangle$ sufficiently narrow in energy, i.e. the distribution of the $|C_\alpha|^2$ is narrow. More precisely:

$$\Delta E = \left(\sum_\alpha |C_\alpha|^2 E_\alpha^2 - \langle E\rangle^2\right)^{1/2} = \left(\sum_\alpha |C_\alpha|^2 \Big(E_\alpha - \langle E\rangle\Big)^2\right)^{1/2} \ll \langle E\rangle$$

For our purposes such an initial state shall be called **generic**.

Time Evolution

1. The temporal evolution of the state vector is given by:

$$|\psi(t)\rangle = \sum_{\alpha} C_{\alpha} e^{-\frac{i}{\hbar} E_{\alpha} t} |\psi_{\alpha}\rangle$$

   - want to understand: how is thermal behaviour encoded in this equation

2. The time dependence of the expectation value of any obeservable A is given by:

$$\langle A(t)\rangle = \langle \psi(t)|A|\psi(t)\rangle = \sum_{\alpha,\beta} C_{\alpha}^{*} C_{\beta} e^{\frac{i}{\hbar}(E_{\alpha}-E_{\beta})t} A_{\alpha\beta} \qquad (2)$$

   where we define $\langle \psi_{\alpha}|A|\psi_{\beta}\rangle \equiv A_{\alpha\beta}$. Call $A_{\alpha\alpha}$ **eigenstate expectation value** (EEV).

Thermalization

To check whether a system is in thermal equilibrium, we must measure some observable(s) A belonging to the set $\mathcal{S}$ of *allowed* observables.

1. no general results for $\mathcal{S}$
2. concrete restrictions arise when one considers *specific classes* of systems (e.g. classically chaotic systems)

Definition

We say the quantum system exhibits thermal behaviour if for $A \in \mathcal{S}$, $\langle A(t) \rangle$ relaxes towards the thermal value prescribed by quantum statistical physics after some characteristic relaxation time.

Note: neglect fluctuations of A

Infinite-time average of an observable

The following average is mathematically tractable (use classical intuition):

Definition

The infinite-time average $\bar{A}$ is

$$\bar{A} \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \langle A(t) \rangle dt = \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha} \tag{3}$$

$\rightarrow$ Given A shows thermal behaviour, we assume the relaxation must be to this value.
(infinite time washes out nonthermal behaviour, contained within non-diagonal ($\alpha \neq \beta$) elements in the sum of eqn. (2))

"Quantum Ergodicity"

Let the system be truly isolated. The quantum statistical average is (microcanonical ensemble):

$$\langle A \rangle_{mc}(\langle E \rangle) = \frac{1}{N_{\langle E \rangle, \Delta E}} \sum_{\alpha : E_\alpha \in I} A_{\alpha\alpha}$$

where $I \equiv [\langle E \rangle - \Delta E, \langle E \rangle + \Delta E]$ is an energy window and $N_{\langle E \rangle, \Delta E}$ is the number of eigenstates contributing to the microcanonical average.
If A behaves thermally, it should also settle to the prediction of the microcanonical ensemble:

$$\bar{A} = \langle A \rangle_{mc}(E) \quad \Longleftrightarrow \quad \sum_{\alpha} |C_\alpha|^2 A_{\alpha\alpha} = \frac{1}{N_{\langle E \rangle, \Delta E}} \sum_{\alpha : E_\alpha \in I} A_{\alpha\alpha}$$

Deutsch: "ergodic quantum system".
This equation is problematic.

Thermodynamical Universality

$$\sum_{\alpha} |C_\alpha|^2 A_{\alpha\alpha} = \frac{1}{N_{\langle E\rangle,\Delta E}} \sum_{\alpha: E_\alpha \in I} A_{\alpha\alpha} \tag{4}$$

Concern: explain thermodynamical universality in this equation:

- l.h.s. of (4) depends on the initial conditions via $C_\alpha = \langle \psi_\alpha | \psi(0) \rangle$
- r.h.s. of (4) depends only on $\langle E \rangle = \sum_\alpha |C_\alpha|^2 E_\alpha$, which is the same for many sets $\{C_\alpha\}_\alpha$

A possible explanation: ETH

- restriction on A necessary: take e.g. $A = \mathcal{P}_\beta = |\psi_\beta\rangle\langle\psi_\beta|$

Eigenstate Thermalization

1. intuition: $A_{\alpha\alpha} = \text{const.}\ \forall\alpha$
2. idea: EEV's $A_{\alpha\alpha}$ almost don't vary between eigenstates which are close in energy (within I, c.f. generic initial state)

ETH (Deutsch '91, Srednicki '94)

Thermalization in isolated, bounded quantum systems happens at the level of **individual eigenstates** of the Hamiltonian:

$$A_{\alpha\alpha} = \langle A \rangle_{mc}(E_\alpha) \quad \forall\alpha \tag{5}$$

In other words, each eigenstate of the Hamiltonian implicitly contains a thermal state.

The (auxiliary) role of time

- no time variable t in eqn. (5)
- Role of time evolution:
  - initial state = superposition of eigenstates with "carefully" chosen phases C_α
  - revelation of the thermal state due to the dephasing effect of Hamiltonian time evolution in eqn. (2)
  - coherence between $A_{\alpha\beta}$ destroyed, $\bar{A}$ reached
- time evolution doesn't construct the thermal state, it only reveals it. The thermal state exists at t=0, but the coherence hides it (picture).

Second Approach

Lemma

$\bar{A}$ will depend on $\langle E \rangle$ and not on the details of the C_α if $A_{\alpha\alpha}$ is a smooth function of E_α with negligible variation over I:

$$A_{\alpha\alpha} = \Phi(E_\alpha). \tag{6}$$

Proof

Taylor 1st order: $\bar{A} = \Phi(\langle E \rangle)[1 + O(\Delta E / \langle E \rangle)]$. Assume generic state.

□

Notes:

1. argument E_α discrete, but close (quasi-continuous) within I
2. Φ approximately constant over I (up to small error)
3. (6) $\rightsquigarrow$ restriction for the allowed observables

Canonical Thermal Average

- idea c.f. picture

The (canonical) thermal average $\langle A \rangle_T$ is:

$$\langle A \rangle_T = \frac{1}{Z(T)} \sum_\alpha e^{-E_\alpha / k_B T} A_{\alpha\alpha} = \frac{1}{Z(T)} \int_0^\infty dE \; n(E) e^{-E/k_B T} \Phi(E)$$

with:

- $Z(T) = \sum_\alpha e^{-E_\alpha / k_B T}$: partition function
- $n(E) = \sum_\alpha \delta(E - E_\alpha)$: density of states

Eigenstate Thermalization

1. Approximating $n(E)$, one can show:

$$\langle A \rangle_T = \Phi(U)[1 + O(N^{-1/2})] \tag{7}$$

with $U(T) = T^2 Z'(T)/Z(T)$ the internal energy.

2. Ergodicity is satisfied if:

$$\bar{A} = \langle A \rangle_T \quad \Longleftrightarrow \quad N \gg 1 \text{ and } U(T) = \langle E \rangle.$$

3. Eigenstate thermalization: we have $A_{\alpha\alpha} = \Phi(E_\alpha)$

$$(7) \quad \Longrightarrow \quad A_{\alpha\alpha} = \langle A \rangle_{T_\alpha}, \text{ where } U(T_\alpha) = E_\alpha.$$

Eigenstate Thermalization: Validity

Results for a few restricted *classes* of systems:

1. ETH holds for integrable $\hat{\mathcal{H}}$ with weak perturbation (random Gaussian matrix) $\rightsquigarrow$ quantum chaos
(J.M. Deutsch)
2. For quantum systems with chaotic classical counterparts, ETH is valid sometimes, in particular if Berry's conjecture holds
(M. Srednicki)

Consider now an example of 2.

3. ETH: A SPECIFIC EXAMPLE

The ∞-hard-sphere gas

- representative example of a system which exhibits chaos classically in all its available phase space at any energy E
  - ergodic, mixing (Sinai, 1963)

Definition

The system consists of N identical particles in a box L^3, with mass m and radius a each. The Hamiltonian is:

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V(|x_i - x_j|), \quad i,j = 1,\dots N$$

where x_i is the position of the i-th particle and the potential is given by:

$$V(r) = \begin{cases} \infty & \text{if } r < 2a \\ 0 & \text{else} \end{cases}$$

- all following results are formulated specifically for this system (in particular BC)

Notation

Any wavefuntion $\psi(\vec{X})$, $\vec{X} = (x_1, ..., x_N) \in \mathbb{R}^{3N}$:

1. is defined on the domain D in coordinate space, where:

$$D = \{x_1, ..., x_N | -\frac{1}{2}L \leq x_{i1,2,3} \leq \frac{1}{2}L \; ; \; |x_i - x_j| \geq 2a\}$$

2. satisfies $\psi = 0$ on ∂D (∞ - potential).

Energy eigenfunctions:

1. are denoted by $\psi_\alpha(\vec{X})$, where:

$$\hat{\mathcal{H}}\psi_\alpha(\vec{X}) = E_\alpha \psi_\alpha(\vec{X})$$

2. in momentum space (semi-classical model):

$$\tilde{\psi}_\alpha(\vec{P}) \equiv h^{-3N/2} \int_D d^{3N}X \; \psi_\alpha(\vec{X}) e^{\frac{i}{\hbar}\vec{P}\cdot\vec{X}}$$

What we will see:

The line of thought is the following:

1. Berry's conjecture (BC)
2. *Assume* as initial state an energy eigenstate which satisfies BC
3. show that under this assumption the thermal behaviour of a particular observable is correctly explained by the ETH

Or more concisely:

$$\text{BC} \Rightarrow \text{ET}$$

Interlude: Thought Experiment

In our case $A = \hat{p}_1$, the momentum of a selected particle.

Thought Experiment

1. Prepare the system in an initial state $|\psi_i\rangle$
2. After some time t, measure $\hat{p}_1$
3. Repeat (same $|\psi_i\rangle$, same t, same particle)

Because of the inherent uncertainties in QM, we can hope to obtain a distribution for $\hat{p}_1$.

Berry's Conjecture

Berry's conjecture (Berry, 1977)

Let $\psi_\alpha(\vec{X})$ be an energy eigenfunction of the system at sufficiently high energy. Then $\psi_\alpha(\vec{X})$ can be written as:

$$\psi_\alpha(\vec{X}) = \mathcal{N}_\alpha \int d^{3N}P \; A_\alpha(\vec{P})\delta(\vec{P}^2 - 2mE_\alpha)e^{\frac{i}{\hbar}\vec{P}\cdot\vec{X}} \tag{8}$$

i.e. ψ_α is a superposition of plane waves with fixed wavelength (energy).

The amplitudes $A_\alpha(\vec{P})$ behave like Gaussian random variables with a two-point correlation function given by

$$\langle\tilde{\psi}^*_\alpha(\vec{P})\tilde{\psi}_\beta(\vec{P'})\rangle_{EE} = \delta_{\alpha\beta}\mathcal{N}^2_\alpha\delta(\vec{P}^2 - 2mE_\alpha)\delta^{3N}(\vec{P} - \vec{P'}) \tag{9}$$

Berry's conjecture II

Notes:

- EE = Eigenstate Ensemble: fictitious ensemble which contains all functions that have the properties of a "typical" eigenfunction. Individual eigenfunctions behave as if they were selected at random from that ensemble.
- $\mathcal{N}_\alpha$ from $\int_D d^{3N}X \ \psi_\alpha^2(\vec{X}) = 1$

Validity of Berry's conjecture

- uncertain, believed to hold in semiclassical classically chaotic systems (in most of their phase space)
- for our system, condition of **sufficiently high energy**
- rough criterion (Donald, Kaufman 1988): "thermal wavelength of each particle smaller than relevant length feature"(which produces classical chaos):

$$\text{thermal wavelength: } \lambda_\alpha \equiv O(1)\frac{h}{\sqrt{2mk_B T_\alpha}}$$

In our case this criterion would be $\lambda_\alpha \leq a$. Indeed:

$$\lambda_\alpha \leq a \Longleftrightarrow E_\alpha = \frac{3}{2}Nk_B T_\alpha \geq \ldots$$

(high energy requirement)

ETH and the hard-sphere gas

Theorem

Let $|\psi_\alpha\rangle$ be an energy eigenstate of the system which satisfies BC. In the limit of low density $Na^3 \ll L^3$, $|\psi_\alpha\rangle$ "predicts" a thermal distribution

$$f_{MB}(\vec{p_1}, T_\alpha) \text{ , where } T_\alpha \equiv \frac{2E_\alpha}{3Nk_B}$$

for the momentum $\vec{p_1}$ of a single constituent particle in the limit $N \to \infty$.

- This is precisely the eigenstate thermalization scenario: every eigenstate implicitly contains a thermal state.

Proof - An Outline I

Work in momentum space: $\tilde{\psi}_\alpha(\vec{P})$: energy eigenfunctions (FT: $\tilde{ }$)

- initial state:

$$\tilde{\psi}(\vec{P}, t = 0) \equiv \sum_\alpha C_\alpha \tilde{\psi}_\alpha(\vec{P})$$

$$\Longrightarrow \tilde{\psi}(\vec{P}, t) = \sum_\alpha C_\alpha e^{-\frac{i}{\hbar} E_\alpha t} \tilde{\psi}_\alpha(\vec{P}) \tag{10}$$

- joint probability density of all N particles: $|\tilde{\psi}(\vec{P}, t)|^2$

Proof - An Outline II

The probability of finding atom 1 with momentum in range d^3p around $\vec{p}_1$ is (marginal density):

$$f(\vec{p}_1, t) = \int d^3p_2 \dots d^3p_N |\tilde{\psi}(\vec{P}, t)|^2$$

Now consider an energy eigenstate as initial state:
$\exists \alpha : C_\alpha = 1, C_\beta = 0 \forall \beta \neq \alpha$. Then:

$$f(\vec{p}_1, t) = \int d^3p_2 \dots d^3p_N |\tilde{\psi}_\alpha(\vec{P})|^2 \equiv \phi_{\alpha\alpha}(\vec{p}_1)$$

which does not depend on time.

Proof - An Outline III

The trick (to be justified) is to average this time independent density over our fictitious EE, thereby using BC:

$$\langle \phi_{\alpha\alpha}(\vec{p}_1) \rangle_{EE} = \underbrace{\cdots\cdots}_{\text{BC, low density}} = \mathcal{N}_\alpha^2 L^{3N} \int d^3p_2 \ldots d^3p_N \; \delta(\vec{P}^2 - 2mE_\alpha)$$

At last:

$$\lim_{N\to\infty} \langle \phi_{\alpha\alpha}(\vec{p}_1) \rangle_{EE} = f_{MB}(\vec{p}_1, T_\alpha)$$

thereby defining T_α via:

$$E_\alpha = \frac{3}{2} N k_B T_\alpha$$

□

Comments

Note that:

1. n.t.s. small fluctuations (use *Gaussian* property):

$$\langle|\phi_{\alpha\alpha}(\vec{p}_1)|^2\rangle_{EE} - |\langle\phi_{\alpha\alpha}(\vec{p}_1)\rangle_{EE}|^2 \ll \langle\phi_{\alpha\alpha}(\vec{p}_1)\rangle_{EE}$$

   justify that EE is a good choice
2. Eqn. (6): $p_{1_{\alpha\alpha}} = \langle p_1\rangle_{MB}(E_\alpha)$ is a statement about the expectation value for the observable p_1
   - have shown corresponding densities are equal
3. symmetry assumptions for $\psi \rightsquigarrow$ FD-, BE- distributions