

Entanglement between system and environment III

Quantum mechanical evolution towards thermal equilibrium

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Outline

- Motivation
 - The Question
 - The Standpoint
 - One Step Further
- Setup
- Equilibration: 2 Theorems
- Initial State Independence: A Theorem
- Summary

The Question

Coffee and Beer cool down, or warm up and reach room temperature if you leave them alone for long enough time.

Thermalization as a fundamental fact of nature

How can one derive thermalization from basic dynamical laws ?

The Standpoint

Previous talks on *Entanglement between System and Environment*

Quantum mechanical treatment, density matrix formalism

Replacement of *equal a priori probability postulate* by a more *general canonical principle*

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Previous talks on *Entanglement between System and Environment*

Quantum mechanical treatment, density matrix formalism

Replacement of *equal a priori probability postulate* by a more *general canonical principle*

Almost all (pure) states of a large system are such that any small subsystem is in a canonical state.

At one **certain point in time**, kinematic result

One Step Further

This talk is about

Subsystems initially far from equilibrium

Time evolution, dynamical aspects

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 - The Model
 - Definitions
 - What do We Mean by *Thermalization* ?
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The Model

The system

Hilbertspace composed by a bath B and a subsystem S

$$H = H_B \otimes H_S$$

$$d_S, d_B < \infty$$

The Model

The Hamiltonian of the total system

$$H = \sum_k E_k |E_k\rangle\langle E_k|$$

only one assumption: **non-degenerate energy gaps**

extremely weak assumption

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Implications:

non-degenerate energy levels

Hamiltonian is fully interactive: $H \neq H_S + H_B$

Definitions

Pure state of the total system and its density matrix

$$|\Psi(t)\rangle \quad \rho = |\Psi(t)\rangle\langle\Psi(t)|$$

State of the bath B / subsystem S

$$\rho_B(t) = \text{Tr}_S \rho(t) \quad \rho_S(t) = \text{Tr}_B \rho(t)$$

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Time averaged state of the total system, B and S

$$\omega = \langle \rho(t) \rangle_t = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \rho(t) dt$$

note $\omega_{B,S} = \langle \rho_{B,S}(t) \rangle_t = \text{Tr}_{S,B} \omega$

Definitions II

Effective dimension of a (mixed) state ρ

tells us, how many pure states contribute to the mixture

$$d^{\text{eff}}(\rho) = \frac{1}{\text{Tr}(\rho^2)}$$

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Trace distance between two density matrices ρ_1 and ρ_2

characterizes their experimental distinguishability

$$D(\rho_1, \rho_2) = \frac{1}{2} \text{Tr} \sqrt{(\rho_1 - \rho_2)^2}$$

Thermalization ...

... is characterized by **four independent elements**

- Equilibration
- Bath state independence
- Subsystem state independence
- Boltzmann form of the equilibrium state

$$\rho_S = \frac{1}{Z} \exp\left(-\frac{H_S}{k_B T}\right)$$

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- **Equilibration: 2 Theorems**
 - Central Result in Words
 - Theorem 1
 - Theorem 2
 - Equilibration of Systems Far from Equilibrium
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Central Result in Words

Every pure state of a large quantum system that is composed of a large number of energy eigenstates and which evolves under an arbitrary Hamiltonian (with non-degenerate energy gaps) is such that every small subsystem will equilibrate.

Theorem 1

Consider any state $|\Psi(0)\rangle \in \mathcal{H}$ evolving under a Hamiltonian with non-degenerate energy gaps. Then the following inequalities hold:

$$\langle D(\rho_S(t), \omega_S) \rangle_t \leq \frac{1}{2} \sqrt{\frac{d_S}{d^{\text{eff}}(\omega_B)}} \leq \frac{1}{2} \sqrt{\frac{d_S^2}{d^{\text{eff}}(\omega)}}$$

This means: Whenever the state of the bath (total system) goes through many distinct states any small subsystem reaches equilibrium (since the mean fluctuation becomes very small)

Theorem 1

Q: In which cases (for which initial states $|\Psi(0)\rangle \in H$) does the total system go through many distinct states?

A: Almost all quantum states have this property.

From now on: restrict the initial state of the total system to a Hilbert subspace $H_R \subset H$ of dimension d_R .

$$|\Psi(0)\rangle \in H_R \subset H$$

Theorem 2

The average effective dimension $\langle d^{\text{eff}}(\omega) \rangle_{\Psi}$ where the average is computed over all uniformly random pure states $|\Psi(0)\rangle \in H_R \subset H$ is such that

$$\langle d^{\text{eff}}(\omega) \rangle_{\Psi} \geq \frac{d_R}{2}.$$

For a random state $|\Psi(0)\rangle \in H_R \subset H$, the probability that $d^{\text{eff}}(\omega)$ is smaller than $\frac{d_R}{4}$ is exponentially small, namely

$$\Pr_{\Psi} \left\{ d^{\text{eff}}(\omega) < \frac{d_R}{4} \right\} \leq 2 \exp(-c \sqrt{d_R}),$$

with $c \approx 10^{-4}$.

Equilibration of systems far from equilibrium

Q: Why can't we just plug in $H_R = H$ and $d_R = d$ in above formulas?

A: This does not cover initial **states far from equilibrium**, they are **not generic** states, they are quite rare.

Equilibration of systems far from equilibrium

Consider the following situation:

Bath with known macroscopic parameters (e.g. T)

Place a small subsystem into it, with arbitrary initial state

Initial state of the total system: $|\Psi(0)\rangle = |\phi(0)\rangle_B |\psi(0)\rangle_S$

Model macroscopic parameters: $|\phi(0)\rangle_B \in H_B^R \subset H_B$

Under the assumption $d_B^R \gg d_S^2$ we achieve:

For any initial state of the subsystem, and almost all initial states of the bath, the subsystem equilibrates.

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 - Subsystem State Dependence: Examples
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Theorem 3

Return to general model with $|\Psi(0)\rangle \in \mathbb{H}_R \subset \mathbb{H}_B \otimes \mathbb{H}_S$

ω_S depends on $|\Psi(0)\rangle$: ω_S^Ψ

The inequalities

$$\left\langle D(\omega_S^\Psi, \Omega_S) \right\rangle_\Psi \leq \sqrt{\frac{d_S \delta}{4 d_R}} \leq \sqrt{\frac{d_S}{4 d_R}}$$

hold true with $\Omega_S = \left\langle \omega_S^\Psi \right\rangle_\Psi$,

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hold true with $\Omega_S = \left\langle \omega_S^\Psi \right\rangle_\Psi$,

$$\delta = \sum_k \left\langle E_k \left| \frac{\Pi_R}{d_R} \right| E_k \right\rangle \text{Tr}_S \left(\text{Tr}_B (|E_k\rangle\langle E_k|) \right)^2 \leq 1,$$

where Π_R is the projector onto \mathbb{H}_R .

Bath State Independence

Consider once again subsystem and bath initially in the product state:

$$|\Psi(0)\rangle = |\phi(0)\rangle_B |\psi(0)\rangle_S \in \mathbb{H}_R = \mathbb{H}_R^B \otimes |\psi(0)\rangle$$

$$d_R = d_R^B$$

Given $d_B^R \gg d_S$,

almost all states of the bath lead to the same time averaged (equilibrium) state of the subsystem.

Subsystem State Independence

More complicated question, not yet completely solved

So far: all the used boundaries depended only on dimensions d , d_S , d_B , d_B^R .

Drastic counter-example: Atomic bomb

Equilibrium of subsystem may depend on its initial state.

Subsystem State Dependence

Examples:

- Conserved quantities on subsystem

$$H = \sum_{nm} E_{nm} |m\rangle\langle m|_B \otimes |n\rangle\langle n|_S$$

with observable $A = \sum_n a_n |n\rangle\langle n|_S$

Subsystem State Dependence

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- No conserved quantities on subsystem

Subsystem / bath consisting of 1 / many spins

$$H = E \sigma_S^z + H_{\text{int}} + H_B$$

$$E \gg 1, \quad -1 \leq H_{\text{int}}, H_B \leq 1$$

Subsystem State Independence

Provided, the energy eigenstates of the total system are far from product (from being product states of pure states of the subsystem and the bath), almost all initial states of the subsystem lead to the same time averaged state.

Proof: Apply Theorem 3 on the initial total state

$$|\Psi(0)\rangle = |\phi(0)\rangle_B |\psi(0)\rangle_S \in \mathbb{H}_R = |\phi(0)\rangle_B \otimes \mathbb{H}_S$$

Under the assumption on the form of $|E_k\rangle$, δ is small.

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