

Lecture 10 - Quantum quenches

(1)

Consider a closed quantum system with Hilbert space \mathcal{H} .

The system being closed means that it is completely isolated from its environment; there is no exchange of particles, energy or volume with the outside.

Is this ever a reasonable assumption? Aren't all systems somehow coupled to their environment?

Strictly speaking, yes — unless we take for \mathcal{H} the whole universe, which is not particularly interesting for our purposes. Interaction and coupling to the environment introduces a time scale τ_{env} , which is the time scale on which the interaction with the environment is relevant. Any experiment has associated with it a time scale τ_{exp} , which encompasses the time it takes to measure observables, as well as the time scales relevant for the phenomena being probed. For example, if we want to probe thermalization, we need $\tau_{\text{exp}} \gg \tau_{\text{th}}$ with τ_{th} the time scale over which thermalization takes place. So, the more exact question is: Can we construct experiments such that $\tau_{\text{exp}} \ll \tau_{\text{env}}$?

If yes, then for all practical purposes we can consider the experimental system a closed system.

Such closed quantum systems do actually exist and are under experimental control.

- Examples:
- ultracold atomic gases
 - trapped ions
 - nitrogen-vacancy centers in diamonds
 - ...

Non-equilibrium

A common protocol for studying non-equilibrium quantum dynamics in such system is a quantum quench. Quicky described, one prepares a system in an eigenstate of one Hamiltonian \hat{H}_0 ,

$$\hat{H}_0 |\psi_0\rangle = E_0 |\psi_0\rangle$$

often taken to be the ground state. One then abruptly changes the Hamiltonian to a different one \hat{H}_1 , and evolves the state with this Hamiltonian:

$$|\psi(t)\rangle = e^{-i\hat{H}_1 t} |\psi_0\rangle$$

Since \hat{H}_0 and \hat{H}_1 are different $|\psi_0\rangle$ is generally not an eigenstate of \hat{H}_1 , and the dynamics is therefore going to be non-trivial.

The switching between \hat{H}_0 and \hat{H}_1 can be done in different ways.

In a global quench, the parameters of the Hamiltonian are changed throughout all space, while in a local quench they are changed only locally, for a few degrees of freedom. One could for example imagine turning on some interaction \hat{V} as follows: define

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{V}$$

and take

$$\lambda(t) = \begin{cases} 0 & t < 0 \\ 1 & t \geq 0 \end{cases}$$

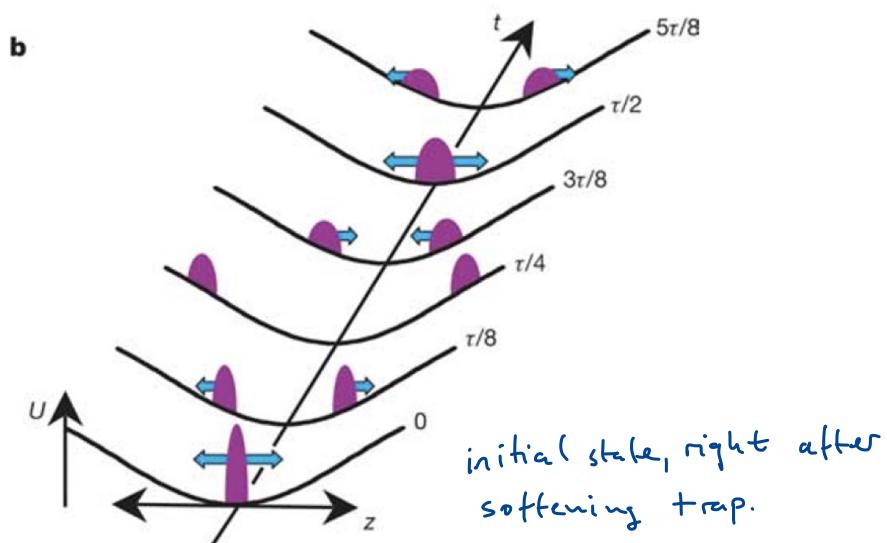
This is nice, but can it be done?

A quantum Newton's cradle

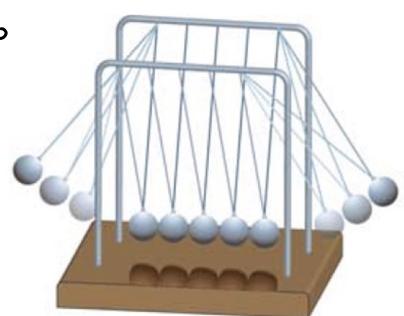
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Ref. Kinoshita, Wenger & Weiss, Nature 440, 900 (2016).

Here is an example of such experiment. This uses lasers to create a harmonic trap that can be loaded with a Bose gas of ^{87}Rb atoms. By some laser manipulations, an initial state consisting of two groups of atoms with opposite fixed velocity is created, both trapped at the bottom of the trap. This can be thought of as the eigenstate of \hat{H}_0 . The trap is then partially released and the two groups start moving. This is best explained by a cartoon:



The trap is such that the atoms are constrained to move only in one direction. This is therefore a 1D gas that is out of equilibrium. The two humps move up the remaining potential where they turn around, go through each other at the origin and up the hill again. And so on forever. This somehow reminded the authors/editors of Newton's cradle, only a quantum version, and they took the clever PR decision to call this



a quantum Newton's cradle.

OK, so far I only showed cartoons. The actual experimental data looks like this:

This is a pretty cool result, but is it what we expect? For a generic system, no! A generic system should thermalize and reach a steady state that has a thermal distribution of velocity for the atoms. This setup here is however not a generic system. Rather it is fine-tuned such that the Bose gas actually has no interactions. It is what we call integrable system, and that is the reason that it keeps bouncing back and forth, at least as long as the 1D gas can be kept isolated from the environment.

But, how can closed quantum systems thermalize? Remember that a density matrix obtained from a single wave function $|t\rangle$ is called pure.

A pure density matrix $\hat{\rho} = |t\rangle\langle t|$ satisfies

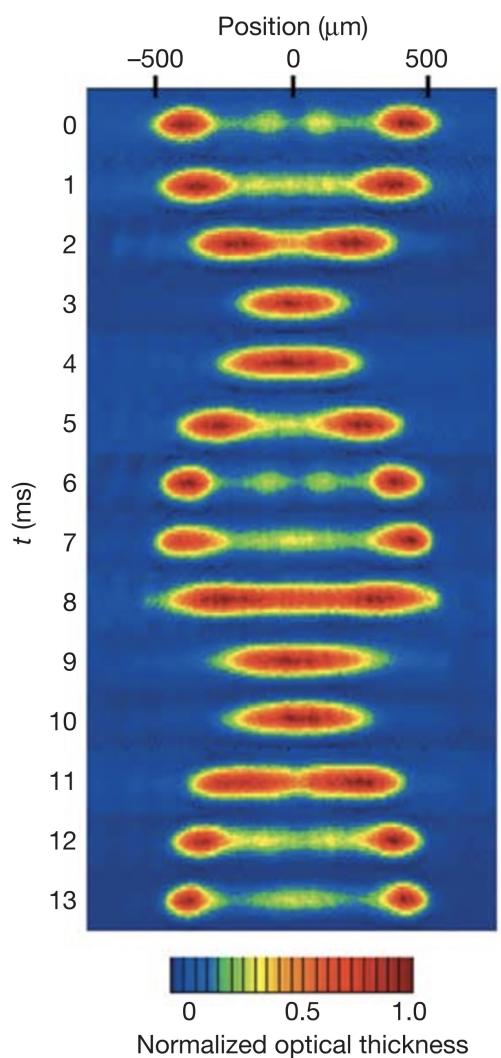
$$\hat{\rho}^2 = |t\rangle\langle t| |t\rangle\langle t| = |t\rangle\langle t| = \hat{\rho}$$

A mixed density matrix, such as $\hat{\rho} = \sum_i p_i |\varphi_i\rangle\langle\varphi_i|$ with $0 < p_i < 1$ satisfies

$$\hat{\rho}^2 = \sum_{ij} p_i p_j |\varphi_i\rangle\langle\varphi_i| \underbrace{|\varphi_j\rangle\langle\varphi_j|}_{\delta_{ij}} = \sum_i p_i^2 |\varphi_i\rangle\langle\varphi_i| \neq \hat{\rho}$$

unless $p_i = \begin{cases} 1 & \text{for } i = \bar{i} \\ 0 & \text{for all other } i \end{cases}$

in which case $\hat{\rho} = |\varphi_{\bar{i}}\rangle\langle\varphi_{\bar{i}}|$.



$$\text{A thermal density matrix } \rho_{\text{th}} = \frac{1}{Z} e^{-\beta H} \quad (5)$$

Take $\{|n\rangle\}$ the basis of eigenstates $H|n\rangle = E_n|n\rangle$. Then

$$\begin{aligned} \rho &= \sum_n \rho_{nn} |n\rangle \langle n| = \frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle \langle n| \\ &= \sum_n p_n |n\rangle \langle n| \end{aligned}$$

with $p_n = \frac{1}{Z} e^{-\beta E_n}$

Thermal density matrix always mixed (unless $\beta \rightarrow \infty$).

This leads us to the following puzzle:

Suppose we initialize our quantum system in the state $|\psi_I\rangle$. If the system is described by the Hamiltonian H , the state will time evolve according to the unitary time evolution operator $U = e^{iHt}$.

Initially $\rho(0) = |\psi_I\rangle \langle \psi_I|$ and $\rho^2(0) = \rho(0)$.

Under time evolution

$$\rho \rightarrow \rho(t) = |\psi(t)\rangle \langle \psi(t)| = U |\psi_I\rangle \langle \psi_I| U^\dagger$$

and

$$\rho^2(t) = U |\psi_I\rangle \underbrace{\langle \psi_I| U^\dagger}_{I \text{ since } U^\dagger U = I} U |\psi_I\rangle \langle \psi_I| U^\dagger$$

$$= U |\psi_I\rangle \langle \psi_I| U^\dagger = \rho(t)$$

$\Rightarrow \rho$ remains pure at all times!

→ Q: How can statistical mechanics emerge from quantum mechanics?

While this seems like a problem that can not be overcome, we have actually encountered a similar problem in the setting of classical mechanics.

(Compare $f(\bar{r}_1, \bar{p}_1; \dots; \bar{r}_N, \bar{p}_N)$ with $\frac{ds}{dt} = 0$ and $v(\bar{r}, \bar{p})$ with $\frac{ds}{dt} \geq 0$. In a sense, f knows everything about the system just as v does).

How do we solve this in quantum mechanics?

Von Neumann's insight

In a 1929 paper, quickly forgotten and only recently rediscovered, since some prominent physicist thought it was wrong, Von Neumann suggested that while states don't thermalize, (local) observables do!

That is, we should only expect something like:

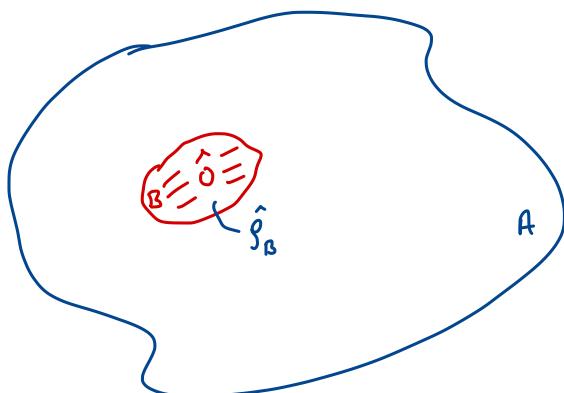
$$\lim_{t \rightarrow \infty} \langle \hat{O}(t) \rangle = \bar{O} = \text{Tr}(\hat{\rho}_{\text{th}} \cdot \hat{O})$$

With $\hat{\rho}_{\text{th}}$ the thermal density matrix.

What does this mean?

Since \hat{O} is local, we only need that the reduced density matrix that describes the space \hat{O} acts in becomes thermal, i.e., that

$$\hat{\rho}_B \sim \frac{1}{Z} e^{-\beta \hat{H}_B}$$



Somehow. Note that B here is a subsystem of the full Hilbert space, such that $H = H_A \otimes H_B$.

So this looks a bit like our open system setup. The main difference is that B is not special and is not separated from the rest. In fact, if we want the system to fully thermalize we should be able to pick any small subsystem, say \tilde{B} , and the $S_{\tilde{B}}$ should thermalize in the sense that $S_{\tilde{B}} \approx \frac{1}{2} e^{-\beta \hat{H}_{\tilde{B}}}$ with the same inverse temperature β . It is as if the rest of the system acts as an effective bath for any small subset of degrees of freedom.

Can we say something generic about states that thermalize in this sense, and what are the properties of Hamiltonians that lead to thermalizing dynamics?

First of, if we have $\hat{\rho}_B \sim \hat{\rho}_{th}$ then the entropy of $\hat{\rho}_{th}$ becomes the entanglement entropy of B with the rest of the system (up to a factor of k_B). Let's remind us a bit of entanglement entropies.

Entanglement entropy and reduced density matrices

Let's start with a system of two spins $H_A = H_B = \{| \uparrow \rangle, | \downarrow \rangle\}$

$$a) |\psi_F\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \equiv |\uparrow\uparrow\rangle$$

What is S_B ?

$$\rho = |\uparrow\uparrow\rangle \langle \uparrow\uparrow|$$

$$\begin{aligned} S_B &= \text{Tr}_A \rho = \langle \uparrow | \rho | \uparrow \rangle_A + \langle \downarrow | \rho | \downarrow \rangle_A \\ &= |\uparrow\rangle \langle \uparrow| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{aligned}$$

$|\psi_F\rangle = |\uparrow\uparrow\rangle$ is a product state.

$\rho_B^2 = \rho_B$ is a pure density matrix.

$$b) |\psi_s\rangle = \frac{1}{\sqrt{2}} (|1\uparrow 1\rangle - |1\downarrow 1\rangle)$$

$$\rho = \frac{1}{2} (|1\uparrow 1\rangle \langle 1\uparrow 1| + |1\downarrow 1\rangle \langle 1\downarrow 1| - |1\uparrow 1\rangle \langle 1\downarrow 1| - |1\downarrow 1\rangle \langle 1\uparrow 1|)$$

$$\Rightarrow \rho_B = \frac{1}{2} (|1\rangle \langle 1| + |1\rangle \langle 1|) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\rho_B^2 = \frac{1}{2} \rho_B \neq \rho_B$$

$|\psi_s\rangle$ not a product state. ρ_B is mixed.

c) What about $|\psi_0\rangle = \frac{1}{2}(|1\uparrow 1\rangle + |1\uparrow 1\rangle + |1\downarrow 1\rangle + |1\downarrow 1\rangle)$? Ex.

Note: Schmidt decomposition.

We can always write

$$|\psi\rangle = \sum_{\alpha} \lambda_{\alpha} |\alpha\rangle_A \otimes |\alpha\rangle_B \quad \text{with } \lambda_{\alpha} \geq 0$$

The states $\{|\alpha\rangle_A\}$ and $\{|\alpha\rangle_B\}$ are generally not a basis of \mathcal{H}_A and \mathcal{H}_B , but can be extended into a basis.

To see that this is true, one needs to do a singular value decomposition on Ψ_{n_A, n_B} thinking of it as a matrix. We will not go into details here but it's a fun exercise to look up what the singular value decomposition is and use it to demonstrate the Schmidt decomposition.

The state $|\Psi_F\rangle$ has no correlation between A and B.
The state is separable and A and B are not entangled.
In contrast, $|\Psi_S\rangle$ is maximally entangled. If I measure $|1\rangle$ in A I will measure $|1\rangle$ in B. $|0\rangle$ in A leads to $|1\rangle$ in B. The amount of entanglement between A and B can be obtained from the von Neumann entanglement entropy

$$S = -\text{Tr}_B S_B \log S_B = -\text{Tr}_A S_A \log S_A$$

Ex: In our example

$$|\Psi_F\rangle \rightarrow S_B = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad S = 0$$

$$|\Psi_S\rangle \rightarrow S_B = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad S = \log 2$$

OK, so what have we learned?

$$\text{If we want } \text{Tr}(S \hat{O}) = \text{Tr}_B(S_B \hat{O}_B) = \text{Tr}(S_{\text{th}} \hat{O}),$$

which is sometimes written as $S_B \sim S_{\text{th}}$ but should be understood as an equality between expectation values of local observables, then we need states with extensive entanglement. Roughly speaking,

$$S \rightarrow S_{\text{th}} \quad \text{which is extensive}$$

and therefore $S \sim L^d$ with d the spatial dimension of our system. Since L^d is the volume of the system, states with entropy that scales like that are said to have volume-law entanglement.

The reason for the name comes from the so-called area law of entanglement, which states that ground states of local gapped Hamiltonians follow an area law of entanglement:

$$S \sim L^{d-1}.$$

OK, so we need states with volume law entanglement. It turns out that for excited states, states with energy much higher than the ground state energy, this is generic. In fact, a randomly selected state in Hilbert space is almost guaranteed to have maximal entanglement. You will verify this in one of the problem sets.

But to know something more about the dynamics, we need to know something more about generic thermalizing Hamiltonians. In a quantum quench we start with $|\psi_0\rangle$ and then evolve with \hat{H} . Let's denote the eigenstates of \hat{H} with $|n\rangle$, i.e.,

$$\hat{H}|n\rangle = E_n|n\rangle$$

Since $\{|n\rangle\}$ is a basis we can expand the initial state in the eigenstates of \hat{H} , i.e.,

$$|\psi_0\rangle = \sum_n c_n |n\rangle \quad \text{with} \quad c_n = \langle n | \psi_0 \rangle.$$

The time evolved state then becomes

$$|\psi(t)\rangle = e^{-i\hat{H}t} |\psi_0\rangle = \sum_n c_n e^{-iE_n t} |n\rangle$$

We can now calculate the time evolution of an observable $\hat{\sigma}$

$$\langle \hat{\sigma}(t) \rangle = \langle \psi(t) | \hat{\sigma} | \psi(t) \rangle = \sum_{n,m} c_n^* c_m e^{-i(E_n - E_m)t} \delta_{mn}$$

with

$$O_{mn} = \langle m | \hat{O} | n \rangle.$$

So, we see that in order to understand the dynamics, we need to know two things:

- i) something about the spectrum of \hat{H} , in particular the distribution of level spacings $\Delta E_{ij} = E_i - E_j$
- ii) matrix elements of local observables in eigenstates of \hat{H} , namely O_{mn} .

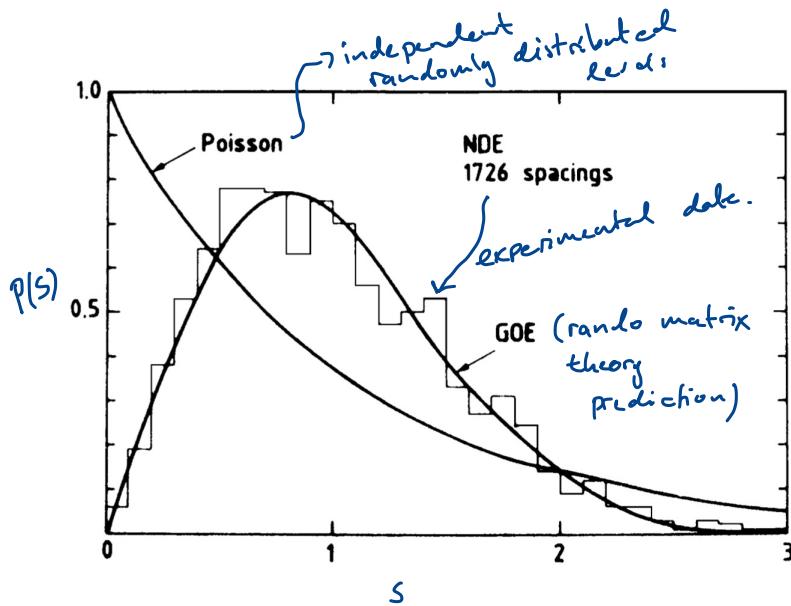
In a many-body Hamiltonian, whose dimension grows exponentially with system size, calculating these things exactly is an impossible task, except for special cases and/or small systems. How to make progress.

In the early days of quantum mechanics, Eugene Wigner was faced with a similar problem. He was trying to make sense of the spectra of large nuclei, i.e., he was trying to understand the spacings ΔE_{ij} , in particular the nearest level spacings $\Delta E_{i+1,i}$ (with E_i ordered such that $E_0 \leq E_1 \leq E_2 \leq \dots$). For low lying energies and small nuclei, one can use arguments similar to those used for atomic spectra (s,p,d,\dots , Hund's rule etc.), but quickly this becomes cumbersome and not very predictive. In either an act of desperation or a strike of brilliance (probably a bit of both), Wigner suggested that since the system was so complex, and the Hamiltonian equally so, the details were not so important, and maybe it was sufficient to replace \hat{H} with

a random matrix

$$\hat{H} \rightarrow \hat{H}_{\text{RMT}}$$

From the random matrix, Wigner could calculate the distribution of level spacing $P(s)$ with $s_i = \frac{E_{i+1} - E_i}{\Delta}$, where Δ is the mean level spacing. Here is what one gets, and comparison with experimental data



This was the birth of random matrix theory (RMT). It has been successfully applied to many aspects of both physics and math, and it is essential for our understanding of thermalization in quantum systems. We will discuss details in the next lecture.