LECTURE 17 DECEMBER

Quantum Many-Body Systems out of Equilibrium

So, today we'll start on a new topic ... { INTRODUCTORY SLIDE }

QUANTUM MATTER OUT OF EQUILIBRIUM. I'll begin discussing a particular problem, or better, "circle of problems", that has attracted enormous attention in the last 10-15 years: EQUILIBRATION OF ISOLATED QUANTUM MANY-BODY SYSTEMS

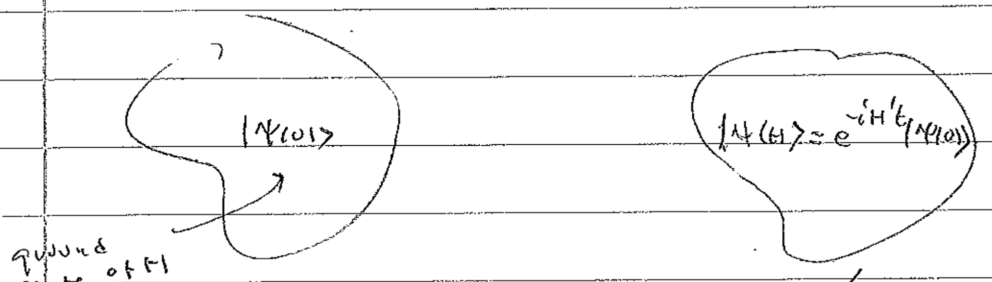
↳ time-evolution towards (time-independent observables)

This is a problem that goes back to the early days of Q.M., see links on the course home page:

I.1 Gogolin-Eisert review

4.1 d'Alessio review

What's the problem? Assume that we prepare a system in a pure state $|\Psi(0)\rangle$ that is not the ground state of the Hamiltonian which governs the dynamics. One simple and clear way of achieving this is via a QUANTUM QUENCH



$H = H(\alpha)$ $\xrightarrow{}$ $H' = H(\alpha' \neq \alpha) = H_{quench}$

↗ some parameter

"QUENCH": instantaneous change of $\alpha \to \alpha'$

This can easily be done experimentally in cold-atom systems (more about that later...)

(II.2

We can expand $|\Psi(t)\rangle$ in the eigenbasis of H' :

$$|\Psi(t)\rangle \overset{(\hbar=1)}{=} \sum_m C_m e^{-iE_m t} |m\rangle \qquad (\text{II}.1)$$

where $C_m = \langle m|\Psi(0)\rangle$, $H'|m\rangle = E_m|m\rangle$
$H' = H_{quench}$

The density matrix $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ will remain that of a pure state at all times, i.e. $\rho^2(t) = \rho(t)$.
It can never become a mixed density matrix !
No obvious equilibration towards a steady state long-time limit.

Let's look at the time evolution of an operator O :

$$O(t) \equiv \langle\Psi(t)|O|\Psi(t)\rangle = \sum_{m,n} C_m^* C_n e^{i(E_m - E_n)t} \underbrace{O_{mn}}_{\langle m|O|n\rangle}$$

$$= \sum_m |C_m|^2 O_{mm} + \sum_{m,n\neq m} C_m^* C_n e^{i(E_m - E_n)t} O_{mn} \qquad (\text{II}.2)$$

$$= \mathrm{Tr}(\rho(t) O)$$

$$= \sum_n \langle n|\Psi(t)\rangle\langle\Psi(t)|O|n\rangle = \sum_{n,m,m'} \langle n|e^{-iHt} C_m|m\rangle\langle e^{iHt} C_{m'}^* m'|O|n\rangle$$

$$= \sum_m |C_m|^2 O_{mm} + \sum_{m,n\neq m} C_m^* C_n e^{i(E_m - E_n)t} O_{mn}$$

Similarly $|C_m|^2 = \rho^{eq}_{mm} = \rho_{mm}(0) = \text{"}\rho_m\text{"}$

$$\rho(t) = \underbrace{\sum_m |C_m|^2 |m\rangle\langle m|}_{\rho_{eq}} + \underbrace{\sum_{m\neq m'} C_m C_{m'}^* e^{-i(E_m - E_{m'})t} |m\rangle\langle m'|}_{\text{vanishes by performing an infinite-time average}} \qquad (\text{II}.3)$$

"diagonal ensemble"

To have equilibration (in the strong sense):

$$\mathcal{O}(t) \xrightarrow{t \gg \tau_{rel}} \mathrm{Tr}(\rho_{eq}\,\mathcal{O}) \qquad (\mathrm{II}.4)$$

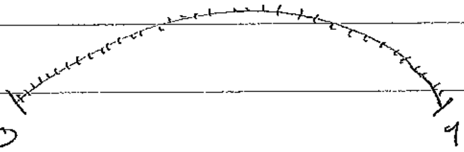
$= \mathrm{Tr}(\rho(t)\,\mathcal{O})$

* SEE NEXT PAGE (II.3 add)

One can prove a somewhat weaker result, equivalent to having (II.4) satisfied "for most of the time" in a sufficiently large time interval $[0, T]$.

$\underbrace{\text{sufficiently large time interval}}_{\text{what does it mean?}}$

Given an observable $\mathcal{O}$, with experimental resolution $\delta\mathcal{O}$ and range $\Delta\mathcal{O}$



"range-to resolution ratio"

$\Delta\mathcal{O}/\delta\mathcal{O}$ = # of possible measurement values $\sim 10^{20}$

Define

$$T_{\delta\mathcal{O}} \equiv \left\{ 0 < t < T : \left| \mathrm{Tr}(\rho(t)\,\mathcal{O}) - \mathrm{Tr}(\rho_{eq}\,\mathcal{O}) \right| \geq \delta\mathcal{O} \right\}$$

(large T)

THEOREM (Reimann, PRL 101, 190403 (2008))

$$* \quad \frac{T_{\delta\mathcal{O}}}{T} \lesssim \underbrace{\left(\frac{\Delta\mathcal{O}}{\delta\mathcal{O}}\right)^2}_{10^{40}\ !?!} \ \max_n \underbrace{\left\{ \rho_{nn}(0) \right\}}_{\text{VERY SMALL! BUT HOW SMALL? (NEXT PAGE!)}} \qquad (\mathrm{II}.5)$$

fraction of all times $t \in [0, T]$ for which there is an experimentally resolvable difference between the true expectation value $\mathrm{Tr}(\rho(t)\,\mathcal{O})$ and the time-independent equilibrium expectation value $\mathrm{Tr}(\rho_{eq}\,\mathcal{O})$.

[Note: $\rho_{nn}(0) = \rho^{eq}_{nn}$]

cf. (II.3)

* Intuitive guess:

$$\frac{T_{\delta\mathcal{O}}}{T} \sim \left(\frac{\Delta\mathcal{O}}{\delta\mathcal{O}}\right) \times \underbrace{\quad\cdots\quad}_{\text{function of } \rho_{eq}}$$

* One may try to prove a somewhat weaker result, asking about the long-time average of $O(t)$ ✡. Then, wouldn't the second time-dependent term vanish?
Yes, but maybe only on exponentially large time intervals, irrelevant for experiments (since the energy levels are so close, making $E_m - E_{m'}$ "exponentially small")
Somehow, to achieve that the second time-dependent term vanishes faster one needs "something more".
What is that? Answer: Dephasing of the initial state, making the relative phases random! This comes about from the generic incommensurability of the frequencies of the oscillating exponentials.

So, question is: Is the temporal dephasing sufficiently fast to produce "equilibration on average"?

Answer given in an influential paper by Peter Reimann, Phys. Rev. Lett. 101, 190403 (2008) with focus on what is experimentally relevant

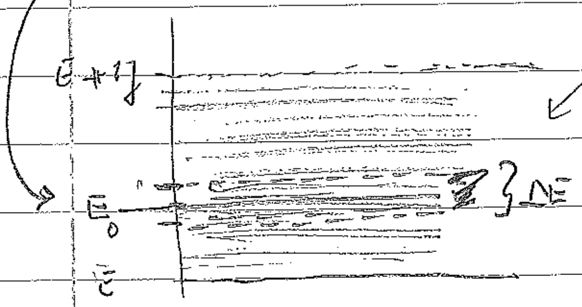
back to II.3

Let me sketch his argument...

✡ See discussion of long-time average in the introduction to d'Alessio et al.! Replace "long-time average" by "most likely behavior of $O(t)$ in a large time interval"? Maybe not necessary...?

Smallness of $\rho_{nn}(0)$

$E_0 = \langle \Psi_{init} | H_{quench} | \Psi_{init} \rangle$



How many levels M for N particles?

$M \sim 10^{O(N)} \sim 10^{10^{23}}$ macroscopically

Let δE be experimental resolution

Initialize the system with energy $\bar{E}$* with width $\Delta E \leq \delta E$. The energy window $[E_0 - \Delta E/2, E_0 + \Delta E/2]$ is macroscopically small (can't be resolved) but microscopically very large: $\Delta E \gg E_{n+1} - E_n$ (level spacing). # of energy levels in $[E_0 - \Delta E/2, E_0 + \Delta E/2] = D \gg 1$

* mean energy with subextensive fluctuations

ΔE signifies the interval where levels are significantly populated, given that the experimentally preset energy is $\approx E_0$. Population of levels outside of ΔE is negligible.

Assumption: None of the levels are macroscopically populated (hence we must exclude the groundstate from our consideration). This leads to the estimate that the largest population $\max \rho_{nn}(0)$ of a level is of the order

$$\max_n \rho_{nn}(0) \sim \frac{1}{\Delta E \cdot 10^{O(N)}} \qquad (\text{II}.6)$$

It follows from (II.5) and (II.6) that $\overline{\Gamma}_{\delta\rho}$ is vanishingly small.

Let's look at a simulation FIG 2 p 22 Gogolin-Eisert

DISCUSSION OF RECURRENCE: Gogolin thesis SLIDES

WHAT KIND OF EQUILIBRIUM STATE?

This proves EQUILIBRATION under weak conditions — "THERMALIZATION" ("GIBBS ENSEMBLE") "LOSS OF MEMORY"! / SOMETHING ELSE ? ?

(II.5

The next thing to inquire about: To what extent is the equilibrium expectation value $\mathrm{Tr}(\rho_{eq} O)$ in agreement with the corresponding microcanonical expectation value, as predicted by the text books. In other words, does the system thermalize ? Σ ▶

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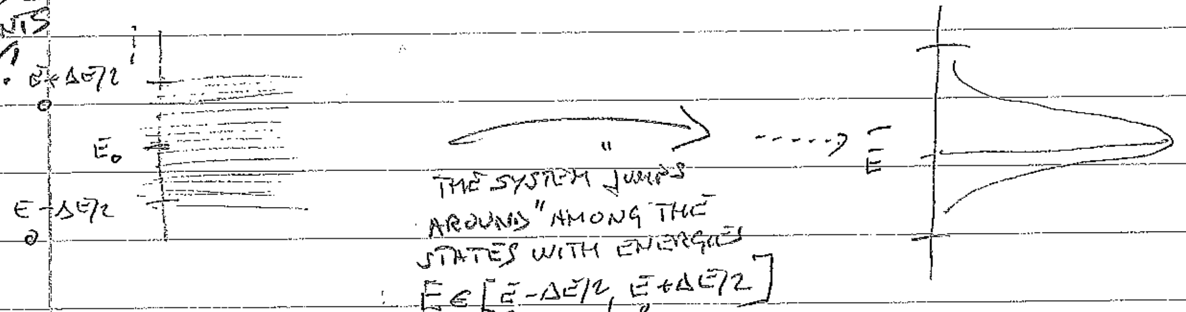
THIS DISCUSSION MORE RELEVANT FOR THERMALIZATION OF SUBSYSTEMS

REVIEW OF THERMALIZATION AND THE CANONICAL ENSEMBLE.

COMMENTS BELOW?



$t=0$ (NON-EQUILIBRIUM) $\qquad t>0 \qquad t\to\infty$

EXPECTATION VALUE OF E = TIME-AVERAGE OF E AT $t\to\infty$

$$\bar{E} = \frac{1}{Z}\sum_{n\in I} e^{-\beta E_n} E_n$$

summation $n\in I$ over accessible states

= "THERMAL EXPECTATION VALUE" WITH $\beta = 1/k_B T$ DETERMINED BY $\bar{E}$.

("EFFECTIVE" TEMPERATURE $1/k_B T_{eff}$ SINCE NO THERMAL RESERVOIR.

KEY POINT: OBSERVABLES ARE GIVEN BY

$$\langle O\rangle = \frac{1}{Z}\sum_n O_n e^{-\beta E_n}$$

FOR SUFFICIENTLY LARGE t.

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$$E = \langle \Psi_{init} | \hat{H}_{quench} | \Psi_{init} \rangle \qquad (\text{II}.6)$$

So again we prepare the system in a non-equilibrium state with energy E (w.r.t. the final ("quench") Hamiltonian $\hat{H}$) with width ΔE (cf. discussion on p. II.4)

"micro canonical window" $\rightarrow$ $$I_{mic} = [E_0 - \Delta E/2,\ E_0 + \Delta E/2] \qquad (\text{II}.7)$$

Corresponding microcanonical ensemble:

"THERMALIZATION OF ISOLATED SYSTEM GIVEN BY THE MICROCANONICAL ENSEMBLE."

CF. FUNDAMENTAL POSTULATE OF STATISTICAL MECHANICS

$$\rho_{mic} = \frac{1}{D} \sum_{mic} |n\rangle\langle n| , \qquad (\text{II}.8)$$

D = # of levels $\in I_{mic}$

implying that $\rho^{mic}_{nn} = \frac{1}{D}$ if $E_n \in I$, 0 otherwise.
We then have for an arbitrary observable $\mathcal{O}$:

$$\mathrm{Tr}(\rho_{mic}\,\mathcal{O}) = \sum_n \rho^{mic}_{nn}\,\mathcal{O}_{nn} = \frac{1}{D} \sum_{\substack{n \\ |E-E_n|<\Delta E}} \mathcal{O}_{nn} \qquad (\text{II}.9)$$

to be compared with our equilibration result from above

$$\mathrm{Tr}(\rho_{eq}\,\mathcal{O}) \approx \sum_{\substack{n \\ |E-E_n|<\Delta E}} \rho_{nn}(0)\,\mathcal{O}_{nn} \qquad (\text{II}.10)$$

$\leftarrow$ cf. Reimann's argument

The challenge is to explain how $\mathrm{Tr}(\rho_{mic}\mathcal{O}) \approx \mathrm{Tr}(\rho_{eq}\mathcal{O})$.
At first glance: "Implausible! $\mathrm{Tr}(\rho_{eq}\mathcal{O})$ retains knowledge about the initial state, $\mathrm{Tr}(\rho_{mic}\mathcal{O})$ doesn't!"

through dependence on ρ_{nn}!

Standard theory that resolves this apparent paradox:
Eigenstate thermalization hypothesis.

EIGENSTATE THERMALIZATION HYPOTHESIS

Deutsch, Phys. Rev A 43, 2046 (1991)

Srednicki, Phys. Rev E 50, 888 (1994); J. Phys. A 29, L75 (1996)

Looking at (II.9) and (II.10) we see that

$$\sum_{\substack{n \\ |E-E_n|<\Delta E}} |c_n|^2 O_{nn} \approx \frac{1}{D} \sum_{\substack{n \\ |E-E_n|<\Delta E}} O_{nn} \qquad \text{(II.11)}$$

if the two ensembles are to give the (approximately) same result. What mechanisms are possible?

1. For physically interesting initial conditions: Fluctuations in $|c_n|^2$ and O_{nn} are uncorrelated → a given initial state then performs an unbiased sampling of the distribution of A_{nn} resulting in (II.11)

ETH

2. $|c_n|^2$ practically do not fluctuate between eigenstates close in energy (= sufficient but not necessary condition for thermalization)

3. O_{nn} practically do not fluctuate between eigenstates that are close in energy

Let's look at results from numerics (exact diagonalization on a small system): FIG 1A, 1B (supporting that thermalization does happen; FIG 3C (supporting ETH and ruling out scenario 2)

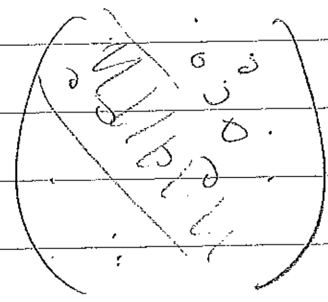
SLIDE

FIG 2 ← SHOWS THAT EACH EIGENSTATE WITH ENERGY VERY CLOSE TO E, BEHAVE AS A THERMAL STATE!

But how can an observable $\mathcal{O}$ "feel" whether two eigenstates $|m\rangle$ and $|n\rangle$ of the Hamiltonian H' belong to similar energies or not without any a priori knowledge about the Hamiltonian H' ?!

$$H = H_0 + V \qquad (\text{II}.12)$$

$H' = H(\alpha') = H_{quench}$; $H_0 = H(\alpha)$; V: perturbation (from $\alpha \to \alpha'$) assumed to be weak



$$\begin{cases} H|n\rangle = E_n |n\rangle , & E_{n+1} \geq E_n \\ H_0 |n\rangle_0 = E_n^0 |n\rangle_0 , & E_{n+1}^0 \geq E_n^0 \end{cases}$$

Frequently: ${}_0\langle m|V|n\rangle_0 \equiv V_{mn}^{(0)}$ = matrix elements of a banded, sparse matrix.

DISCUSS!

NOT AS WEIRD AS IT MAY FIRST APPEAR!

Sample this from an ensemble of RANDOM MATRICES which imitate the "true" perturbation V (band structure, sparsity, etc.)

The randomness of $V_{mn}^{(0)}$ implies a randomization of the eigenstates of H and hence of the basis transformation matrix $U_{mn} = {}_0\langle m|n\rangle$ ($|n\rangle = \sum_m |m\rangle_0 \, {}_0\langle m|n\rangle$). It follows that $\mathcal{O}_{mn} = \langle m|A|n\rangle$ will be elements of a random matrix

$\mathcal{O}$: observable

$A_{jk}^0 = {}_0\langle j|A|k\rangle_0$

$$\mathcal{O}_{mn} = \sum_{j,k} U_{mj} \, \mathcal{O}_{jk}^0 \, U_{nk}^* \qquad (\text{II}.13)$$

since $U^{-1} = U^+$

To prove ETH amounts to proving that

$$\mathcal{O}_{mm} - \mathcal{O}_{nn} \qquad (\text{II}.14)$$

is VERY! small for most V and sufficiently close m and n. This is done by exploiting the machinery of RANDOM MATRIX THEORY! Requires a formal/detailed analysis!

DISCUSS... ETH is still a hypothesis in the sense that the RANDOM MATRIX analysis must be supplemented with some (weak) assumptions. Strong support from numerics! (See the paper by Rigol et al. on the course home page.)

ADDED NOTE: Here we have discussed ETH/random matrix theory for the full isolated system. There is a variant of this approach, pioneered by von Neumann in 1929, where the focus is on a subsystem (coded by a REDUCED DENSITY MATRIX) with the rest of the isolated system acting as an environment. To make this approach consistent one applies ETH/random matrix theory pretty much in the same way as above but with the microcanonical ensemble replaced by an effective canonical ensemble with Boltzmann weights $e^{-E_n/k_B T_{eff}}$

Interesting connection to entanglement (with the environment) and the measurement problem!

see page II.5