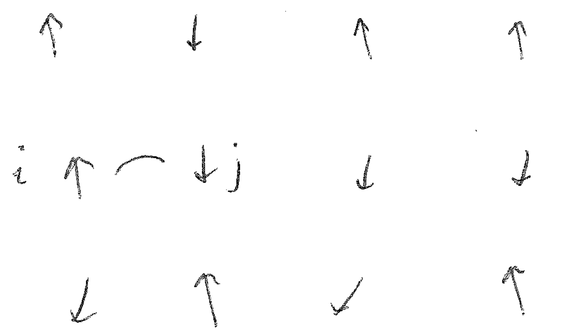
Ergodicity, entanglement, and Many-body localization

Lecture 1: Motivation, outline of the course. Eigenstate Thermalization Hypothesis.

Consider an isolated quantum many-body system
For example, a system of interacting spins-$\frac{1}{2}$



$$H = \sum_{\langle ij \rangle} h_{ij}$$ - Hamiltonian, $\langle ij \rangle$ - nearest neighbors [or more generally nearby spins]

Assume locality of interactions (physically reasonable, applies to most systems)

Thought experiment: ① Initialize the system in state $|\psi_0\rangle$ at time $t=0$.
② Let the system evolve according to unitary evolution by H:

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$$

Question: What happens during this evolution?
What are different "universality classes" of q-systems, from the point of view of dynamics?
Long-time steady state? Approaching the steady state?

Formally, understanding dynamics reduces to understanding spectrum and wave functions of (many-body) eigenstates: We denote eigenstates by $\{|\alpha\rangle\}, \alpha=1..D$ where D is the Hilbert space dimension, energies E_α:

$$H|\alpha\rangle = E_\alpha|\alpha\rangle$$

We can decompose any initial state $|\Psi_0\rangle$ via eigenstates:

$$|\Psi_0\rangle = \sum_\alpha C_\alpha |\alpha\rangle$$

$$|\Psi(t)\rangle = \sum_\alpha C_\alpha e^{-iE_\alpha t} |\alpha\rangle$$

The value of a physical observable described by operator $\hat{O}$:

$$O(t) = \langle\Psi(t)|\hat{O}|\Psi(t)\rangle = \sum_{\alpha,\beta} C_\alpha C_\beta^* e^{i(E_\beta - E_\alpha)t} O_{\alpha\beta} =$$

$$= \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} + \sum_{\alpha\neq\beta} C_\alpha C_\beta^* e^{i(E_\beta - E_\alpha)t} O_{\alpha\beta},$$

$O_{\alpha\beta} = \langle\beta|\hat{O}|\alpha\rangle$ - matrix element.

Thus, need to understand many-body, excited eigenstates & matrix elements.

<u>This is a conceptually new challenge</u>:

- In condensed matter, we often study ground states and low-energy excitations above them (Superconductivity, BEC, ..)
  * Here, need to understand highly excited states. This is a much harder problem (see below)
- In cond-mat, we usually work with thermal states. Assume that density matrix $\rho \propto e^{-\beta H}$, study linear response functions

* Here, we want to understand dynamics of <u>highly non-thermal</u> states

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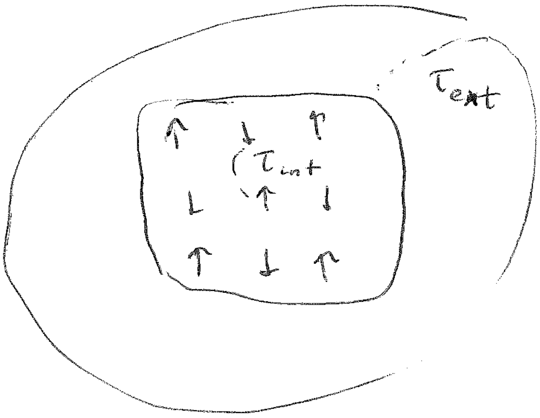
Does it make sense to study isolated systems? Why now? (its an old problem)



Environment

Recent experimental breakthroughs: There are "synthethic" quantum systems which are well (but not perfectly!) isolated from the external world.

Examples include: cold atoms, trapped ions, q-bits, ...

τ_{int} - "internal" time scale

τ_{ext} - external time scale, due to coupling to ext. world

We need observation time

$$\tau_{int} \lesssim t \lll \tau_{ext}.$$

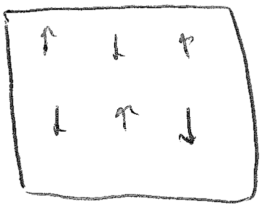
This indeed has been achieved in experiments

[Note that in solid state systems, often τ_{int} is very small, and $t \gg \tau_{int}$ - this makes it difficult to characterize dynamics in those systems]

"Synthethic" systems were initially developed to simulate solid-state systems (e.g. Hubbard model)

But they turn out to be ideal for probing non-equilibrium quantum states.

Currently we know two generic kinds of systems with very different dynamics



$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$$

Thermalization
$|\psi(t)\rangle$ has thermal physical observables
Natural possibility; stat. mechanics applies

Many-body localization
$|\psi(t)\rangle$ is highly non-thermal
Retain memory of $|\psi_0\rangle$
Stat mech does not apply

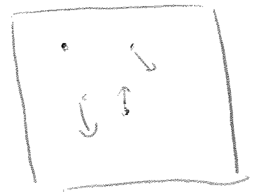
We will mostly focus on Thermalization & MBL.
Additionally, will consider "Floquet" systems in which Hamiltonian is varied periodically in time

$H(t+T)=H(t)$. For example, system interacts with external EM field.

Periodic driving: an Efficient tool of quantum control.

Reminder: Classical systems

[our discussion will be superficial, useful for analogues]



Classical system with N degrees of freedom is described by $2N$ variables: positions & momenta

$$(p_i, q_i), \quad i = 1 \ldots N$$

Usually, one considers an ensemble of systems. ~~Here~~ Then, it is assumed that microcanonical distribution applies:

$$\rho(\underbrace{p, q}_{N \text{ pairs}}) \propto \delta(E(p,q) - E)$$

Assuming that energy is the only integral of motion

We are interested in dynamics of a <u>single system</u>

Time-averaged distribution f-n is given by microcanonical distribution, if the system is <u>ergodic</u>

That is, under time evolution system explores all points in the phase space, given energy conservation

Often, term <u>ergodicity hypothesis</u> is used. Very difficult to prove even in special cases

A closely related (but not equivalent) is notion of <u>chaos</u>. Chaotic systems, effectively, "forget" their initial conditions. Slightly different initial conditions lead to diverging trajectories at later times

$x_0 = (p_0, q_0)$ - initial condition

$x_0 + \delta x_0 = (p_0 + \delta p_0,\ q_0 + \delta q_0)$ $\quad \delta x_0$ is small

In chaotic systems, $|\delta x(t)| \sim e^{\lambda_L t} |\delta x_0|$

λ_L - Lyapunov exponent

Most classical systems are chaotic, even for a few degrees of freedom.

But there is an important exception:

<u>Integrable systems</u>

$I = (I_1 \quad I_N)$ - integrals of motion:

$$\{I_1, H\} = 0 \quad , \quad \{I_i, I_j\} = 0$$

$\{f, g\}$ is the Poisson bracket

$$\{f, g\} = \sum_{i=1..N} \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial q_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}$$

$\exists$ a canonical transformation

$(p, q) \Rightarrow (I, \theta)$ action-angle variables

One can predict time evolution:

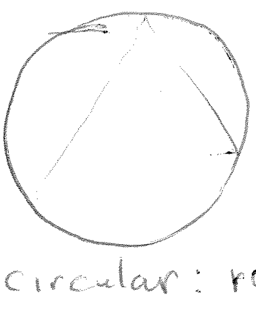
$$\left.\begin{aligned} I_j(t) &= I_j^0 = \text{const} \\ \theta_j(t) &= \Omega_j t + \theta_j(0) \end{aligned}\right\}$$

In this variables, trajectories are <u>tori</u> in the phase space

<u>Motion is periodic</u>

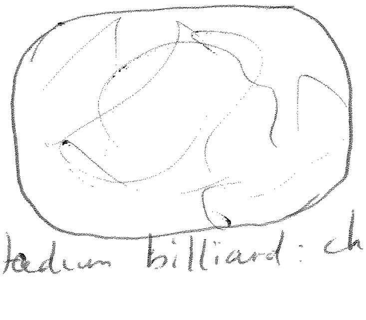
(assuming Θ is compact)

Simple example: billiards



IOM: angular momentum
energy

circular: regular motion

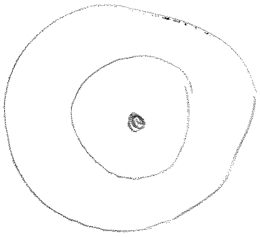


stadium billiard: chaotic

Integrability seems to be a fine-tuned property.

Yet, we know systems with (quasi) periodic motion.

Solar system!



Kolmogorov-Arnold-Moser theory (KAM)

If ~~into~~ integrable system is weakly perturbed, most invariant tori are deformed, ~~but~~ survive given that periods (of different IOMs) are sufficiently irrational.

This assumption is crucial to avoid resonances

Thus, KAM says that motion is quasiperiodic for a large set of initial conditions.

(Many-body localization has interesting analogy to KAM theory)

Quantum systems

Defining quantum chaos is challenging!

Indeed, naively, one could, say, consider $|\psi\rangle$ as analogue of (p,q). But since evo is unitary, difference in the initial condition stays constant

$$|\psi_0\rangle \qquad |\psi_0'\rangle \qquad \langle\psi_0|\psi_0'\rangle = 1-\varepsilon \ , \ \varepsilon \ll 1$$

$$\langle\psi'(t)|\psi(t)\rangle = \langle\psi_0'|e^{iHt}e^{-iHt}|\psi_0\rangle = 1-\varepsilon.$$

There is no notion of trajectory, which goes back to uncertainty principle.

Random matrix theory

One could try to take a classically chaotic system and quantize it.

(Quantizing classically integrable system is easy:

$$\oint p\, dq \simeq 2\pi \hbar n \quad \text{- Bohr-Sommerfeld})$$

However, Wigner realized that rather than focusing on individual energy / eigenfunctions (which is hopeless) one should focus on their statistical properties

Motivated by spectra of complex nuclei (many strongly interacting degrees of freedom)

Crucial step: study an ensemble of random matrices where different degrees of freedom interact.
(Natural for a system like a heavy nucleus)

Simplest ensemble: random Hermitian matrix

$$P(\hat{H}) \propto \exp\left[-\frac{\beta}{2a^2} \mathrm{Tr}\,(\hat{H})^2\right] = \exp\left[-\frac{\beta}{2a^2}\sum_{ij}|H_{ij}|^2\right]$$

$$H_{ij} = H_{ji}^*$$

Matrix elements are independent Gaussian variables of the same order.

Main idea: study statistics of energy levels (Wigner-Dyson)

Energy level repulsion.

See already in 2×2 example

$$H = \begin{bmatrix} \varepsilon_1 & \frac{V}{\sqrt{2}} \\ \frac{V^*}{\sqrt{2}} & \varepsilon_2 \end{bmatrix} \qquad \varepsilon_1, \varepsilon_2, V \text{ - random Gaussian variable}$$

$$E_{1,2} = \frac{\varepsilon_1+\varepsilon_2}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_1-\varepsilon_2)^2+2|V|^2}$$

Statistics of level separation:

$$P(E_1 - E_2 = \omega) = P(\omega)$$

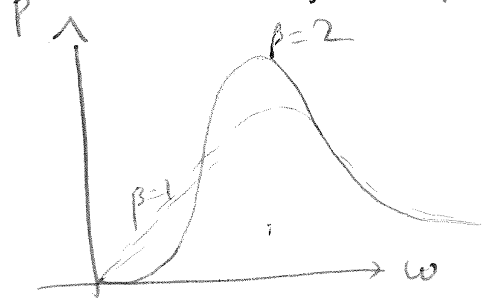
V - real (orthogonal ; TRS):

$$P(\omega) \propto \frac{\omega}{2\sigma^2}\, e^{-\omega^2/4\sigma^2}$$

V - complex (unitary, no TRS)

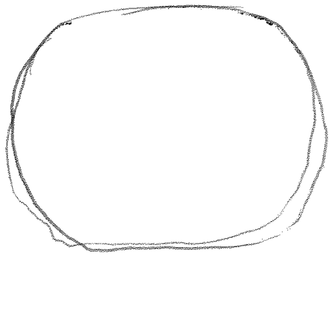
$$P(\omega) = \frac{\omega^2}{2\sqrt{\pi}\,(\sigma^2)^{3/2}} \cdot e^{-\omega^2/4\sigma^2}$$

$$P(\omega) = A_\beta \cdot \omega^\beta e^{-B_\beta \omega^2}$$ $\beta = 1(2)$ for ~~orthogonal~~ orthogonal (unitary)



For large matrices, energy level statistics is described by Wigner-Dyson distribution. which has similar structure at small separations.

WD statistics applies to many systems.



Stadium billiard
energy level repulsion

WD statistics often used as an indicator of quantum chaos (belief based on case studies, not a rigorous result)

What is important, Also holds in thermal many-body systems!

Eigenstates of RMT.

$(\psi_1 \ldots \psi_N)$ – components of wave functions in some basis

$$P_{GOE}(\psi_1 \ldots \psi_N) \propto \delta\left(\sum_j \psi_j^2 - 1\right), \quad P_{GUE} \propto \delta\left(\sum_j |\psi_j|^2 - 1\right)$$

This is because of the orth. (unitary) invariance of random matrix ensembles.

Essentially, eigenstates are random vectors (either real or complex)

[But: eigenstates are very sensitive to small changes of the Hamiltonian. $H_0 + V$ looks like a random matrix in the basis of eigenstates of H_0]

Matrix elements ("observables")

Observable O

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

For a given random Hamiltonian, eigenstates

$$H|m\rangle = E_m |m\rangle$$

$$O_{mn} = \langle m|\hat{O}|n\rangle = \sum_i O_i \langle m|i\rangle\langle i|n\rangle =$$

$$= \sum_i O_i (\psi_i^m)^* \psi_i^n, \quad \psi_i^m = \langle i|m\rangle$$

$$\overline{(\psi_i^m)^* \psi_j^n} = \frac{1}{D}\delta_{mn}\delta_{ij} \qquad D \text{ – Hilbert space dimension}$$

(since $|n\rangle, |m\rangle$ are random independent vectors)

Diagonal: $\overline{O_{mm}} = \frac{1}{D} \sum_i O_i \equiv \bar{O}$

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

$$\overline{O_{mm}^2} - \overline{O_{mm}}^2 = \frac{3-\beta}{D} \overline{O^2}$$ – fluctuation are <u>small</u>

$$\overline{|O_{mn}|^2} = \sum_i O_i^2 \overline{|\psi_i^m|^2 |\psi_i^n|^2} = \frac{1}{D} \overline{O^2}$$

$$O_{mn} \simeq \bar{O} \, \delta_{mn} + \sqrt{\frac{\overline{O^2}}{D}} \, R_{mn}$$ ← random number

In deriving this, we averaged over an ensemble of fictitious Hamiltonians. But since fluctuations are suppressed, one can use this ansatz for a given fixed Hamiltonian

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Remarkably, RMT (in some sense) applies to 'many-body systems with local interactions

The eigenstate thermalization hypothesis

Quantum many-body system $\uparrow \downarrow \uparrow \downarrow \uparrow$
with <u>local</u> interactions. (RMT - nonlocal!)
Locality is crucial.

ETH: an ansatz for matrix elements in the basis of eigenstates of H

$$\boxed{O_{mn} = O(\bar{E})\,\delta_{mn} + e^{-S(\bar{E})/2} \cdot f_O(\bar{E}, \omega)\, R_{mn}}$$

$\bar{E} = (E_m + E_n)/2$, $\omega = E_n - E_m$, $S(E)$ - thermodynamic entropy at energy E

$O(\bar{E})$ - smooth function, $O(\bar{E})$ is identical to the exp. value of the microcanonical ensemble

$$O(\bar{E}) = O(E)_{\text{microcan}}$$

single eigenstate)

$f_O(\bar{E}, \omega)$ - smooth function which characterizes response function of observable $\hat{O}$.

R_{mn} - random numbers, zero mean $\overline{R_{mn}} = 0$

$\overline{R_{mn}^2} = 1$ unit variance

This ansatz is similar to RMT, but $O(\bar{E})$, $f_O(\bar{E}, \omega)$ are new ingredients

ETH implies thermalization

$$|\psi_0\rangle = \sum C_m |m\rangle$$

$$\bar{O} = \lim_{t_0 \to \infty} \frac{1}{t_0} \int_0^{t_0} dt\, O(t) = \sum_m |C_m|^2 O_{mm}$$

As long as energy fluctuations are small (subextensive).

$$\delta E = \sqrt{\langle \psi_0 | \hat{H}^2 | \psi_0 \rangle - \langle \psi_0 | H | \psi_0 \rangle^2},$$

$\bar{O}$ will agree to leading order with microcanonical prediction

$$\bar{O} = O(\langle E \rangle) = O_{Microcan.}$$

Deviations:

$$O_{mm} \simeq O(\langle E \rangle) + (E_m - \langle E \rangle) \left.\frac{dO}{dE}\right|_{\langle E \rangle} + \frac{1}{2}(E_m - \langle E \rangle)^2 \left.\frac{d^2 O}{dE^2}\right|_{\langle E \rangle}$$

$$\bar{O} = O(\langle E \rangle) + \frac{1}{2}(\delta E)^2 \cdot O''(\langle E \rangle) \approx \cancel{O_{Microc} + \frac{1}{2}\left[(\delta E)^2 - (\delta E_{microcan})^2\right] \cdot O''(E)}$$

$$= O_{Microcan} + \frac{1}{2}\left[(\delta E)^2 - (\delta E_{Microcan})^2\right] O''(\langle E \rangle)$$

If (δE) is subextensive, then the second term is negligible

Strong thermalization: ~~The observable~~

Prepare system in a non stationary state with some mean energy and subextensive energy fluctuations. An observable thermalizes if during time evolution it relaxed to its microcanonical value & remains there at most later times

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Off-diagonal matrix elements determine relaxation (and other response functions)

For example, compute long-time average of temporal fluctuations:

$$\sigma_O^2 = \lim_{t_0 \to \infty} \int_0^{t_0} dt \cdot \left([O(t)]^2 - \bar{O}^2 \right) =$$

$$= \lim \int dt \cdot \sum_{mnpq} O_{mn} O_{pq} \cdot c_m^* c_n c_p^* c_q \cdot e^{i(E_m - E_n + E_p - E_q)t} -$$

$$- \bar{O}^2 = \sum_{m,\, n \neq m} |c_m|^2 |c_n|^2 \underline{\underline{|O_{mn}|^2}} \le \max |O_{mn}|^2 \sum_{m,n} |c_m|^2 |c_n|^2$$

$$= \max |O_{nm}|^2 \propto \exp[-S(\bar{E})]$$

Fluctuations exp. small in system size

At almost all time $O(t) = \bar{O}$.

f_O determines response f-ns

$$\langle n|\mathcal{O}(t)\,\mathcal{O}(0)|n\rangle = \sum \langle n|\mathcal{O}(t)|m\rangle\langle m|\mathcal{O}(0)|n\rangle =$$

$$= \sum e^{+i(E_n-E_m)t}|\mathcal{O}_{nm}|^2 = \sum_{n,m} e^{i\omega t}\,|f_O(\bar{E},\omega)|^2 e^{-S(E)} R^2_{nm}$$

R^2_{nm} averages to one

$$\propto \int e^{i\omega t}\,|f_O(\omega)|^2\,d\omega$$

Also spectral function (absorption rate, e.g. ~~if ext~~ perturb. $\lambda\hat{O}e^{i\omega t}$ is applied:

$$A(\omega) \propto |f_O(\omega)|^2$$

Thus, f_O determines time-dependent observables. Put in "by hand".

Consider one-dimensional system

$\mathcal{O}(t) = \hat{n}_1(t)$ - density on a site. Assume system is diffusive.

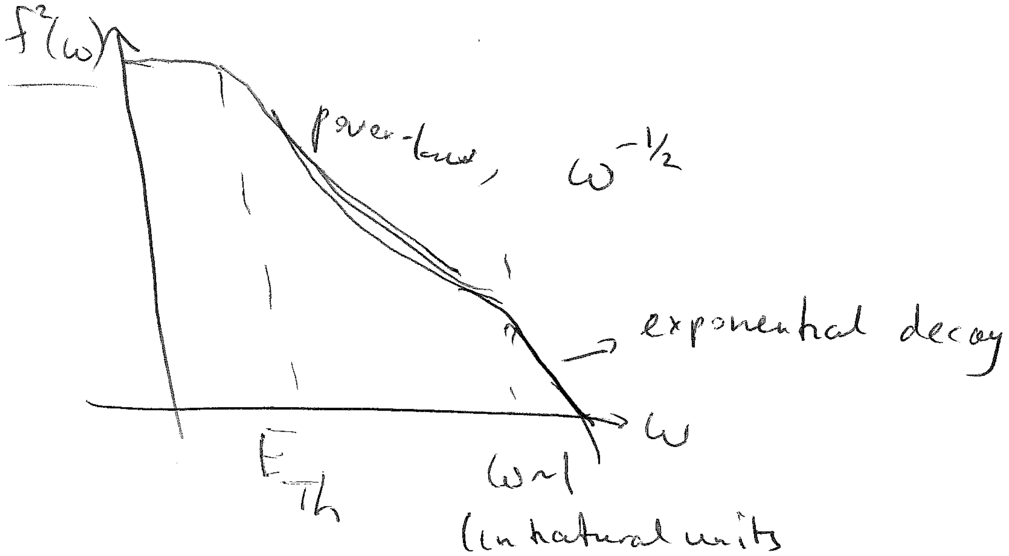
$$\langle n|\mathcal{O}(t)\,\mathcal{O}(0)|n\rangle \sim \frac{1}{t^{1/2}}$$

$$|f^2(\omega)| \sim \frac{1}{\omega^{1/2}}.$$

But: In a finite system, diffusion "saturates" after time

$$\tau_{Th} \approx \frac{L^2}{D} \quad \text{- Thouless time}$$

$$E_{Th} = \hbar D/L^2 \quad \text{- Thouless energy}$$


$f^2(\omega)$
power-law, $\omega^{-1/2}$
exponential decay
ω
E_{Th}
$\omega \sim 1$
(in natural units