Rough notes for Boulder School, July 2021

– D. Huse (use with care)

topics of these lectures:

- Many-body quantum dynamics
- Thermalization
- Many-body localization (MBL)

We will consider closed many-body systems.

No external environment

N degrees of freedom $N \gg 1$ spins, q-bits, sites of an optical lattice, ..., dynamics due to $H(t)$. (Hamiltonian) strongly-interacting, not low ~~temperature~~ entropy density (Can put some "environment" inside.)

Can be well-approximated in the lab these days.

→ May not use weak interaction or low temperature approximations.

One basic question: Does our system, under the dynamics due to $H(t)$, go to thermal equilibrium? Is it a "bath" for itself?

YES = thermalization

NO: one case is MBL: many-body localization.

Also:
How does the apparent irreversibility of thermalization emerge from the reversible unitary dynamics due to $H(t)$?

Cases: • Fully isolated, time-independent $H(t) = H$.
Has extensive conserved energy.

"Get" eigenstates and eigenenergies:

$$H|n\rangle = E_n|n\rangle$$ ← many-body eigenstate of H

Dynamics looks then "simple": (Schrödinger picture)

initial state

$$\rho(t) = \sum_{nm} \rho_{nm}(0)\,|n\rangle\, e^{i(E_m - E_n)t} \langle m| \qquad (\hbar = 1)$$

or for a pure state: $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$

initial state

$$|\psi(t)\rangle = \sum_n e^{-iE_nt}\,|n\rangle\langle n|\psi(0)\rangle$$

This apparent Simplicity is an illusion: $\{|n\rangle\}$ and $\{E_n\}$ contain (hide) all the complexity that is really there.

- Driven ~~b~~ut closed: $H(t)$ depends on t.

External drive producing time-dependence of $H(t)$ must be "classical", so system can not get entangled with it.

(coherent states can approximate this well)

Dynamics:

$$i\frac{d\rho(t)}{dt} = [H(t), \rho(t)]$$

- Special case of interest: Floquet system:

$H(t)$ is periodic: $H(t+T) = H(t)$

Can be viewed as discrete time (set period $T=1$)

$$\rho(t+1) = U\rho(t)U^{\dagger}$$

U is unitary operator that evolves forward in time by one period: $U = \hat{T}\, e^{-i\int_0^T dt\, H(t)}$

time ordering operator.

(there is also "micromotion" within one period.)

Floquet systems have eigenstates (of U), but no extensive conserved energy:

$$U|\alpha\rangle = e^{i\phi_\alpha}|\alpha\rangle$$

$$\rho(t=n) = \sum_{\alpha,\beta} \underbrace{\rho_{\alpha\beta}(0)}_{\text{initial state}} |\alpha\rangle e^{in(\phi_\alpha - \phi_\beta)} \langle\beta|$$

is the unitary dynamics of a Floquet system.

Closed system dynamics:

more symmetries $\longrightarrow$

Unitary
no symmetries $\longrightarrow$ Unitary with more symmetries

make $H(t)$ periodic

Floquet:
hase eigenstates $\longrightarrow$ Floquet with more symmetries

$H(t)=H$

Hamiltonian:
also has extensive conserved energy $\longrightarrow$ Hamiltonian with more symmetries

simplest place to study thermalization

MBL "needs" eigenstates, so this is the simplest place to study MBL

Additional symmetries could be particle number, magnetization, integrability, many others.

Limit $N \to \infty$ is conceptually useful.

Thermalization, Thermodynamics, phase transitions, etc. become sharply defined in this limit.

Laboratory systems can be large enough so this limit is a very useful reference point.

All observables are Hermitian operators.

But, in the $N \to \infty$ limit <u>almost all</u> Hermitian operators are <u>not</u> observable.

Observable: operator that is a product of a <u>finite</u> number of <u>local</u> operators. → (spins, raising & lowering operators at a site.)
sums of observable are observable, products of observable need not be observable.

Example N spin-$\frac{1}{2}$'s or qubits.

This system has 4^N linearly-independent operators.

Each spin has 4 Pauli operators: $1, X, Y, Z$

Any outer product of Pauli operators over all N spins is a many-body Hermitian operator.

Observables in limit $N \to \infty$ are identity on all but a finite number of the spins.

E.g., $X_{22} \otimes Z_{483} \otimes Y_{781} \otimes$ identity on all other spins.
3-spin operator ↗

Why give <u>local</u> operators a special status?

consider:

$$H = \sum_n |n\rangle E_n \langle n| \qquad \text{or} \quad U = \sum_n |n\rangle e^{i\phi_n} \langle n|$$

If we "allow" all Hermitian operators to be considered observable, then $|n\rangle\langle n|$ are all conserved operators. Under this (inappropriate) assumption, Any H (or U) is integrable and does not thermalize. (Lychkovskiy, 2013)

So to make a meaningful distinction between systems that are: chaotic or not / thermalize or not, we need to ~~privileged~~ restrict the set of observables to a ~~vanishing~~ special subset of all operators in the $N \to \infty$ limit.

What is thermal equilibrium of a closed system?

It is only sharply defined in the limit $N \to \infty$.

If we have conserved energy, or any other <u>extensive</u> conserved quantities, need to specify the <u>density</u> of each extensive conserved quantity (e.g. energy, particle number, magnetization, ...), or corresponding temperature, chemical potential, field, ... thermodynamic parameter.

At thermal equilibrium, the entropy is maximized, given the conserved densities. So average over all states with those densities ~~(to within subextensive precision)~~ (take constraint so → Dirac delta function of density in $N \to \infty$ limit). This constrained average over states gives probability distributions for all observables.

A thermal state is <u>any</u> state (mixed or pure) that has these same thermal equilibrium probability distributions for all observables.

You are familiar with microcanonical, canonical, $\rho = e^{-\beta H}/Z(\beta)$ grand canonical ensembles, $\rho = \dfrac{e^{-\beta(H-\mu N)}}{Z(\beta,\mu)}$ which are all thermal states. But these are only some examples and the set of all thermal states is <u>much</u> much larger than this.

Thermalization as a dynamical process:
(Is not proven for any physically realistic system. But appears to be true for many such systems.)

Start in an initial state that is out of ~~equil~~ thermal equilibrium. But has well-defined densities of all extensive conserved quantities in $N \to \infty$ limit.

This means there is a set of observables $\{A\}$ that have probability distributions different from thermal equilibrium (e.g., optical lattice sites with high or low occupation).

Under time evolution observable A becomes at later time: $A(t) = U^{\dagger}(t) A U(t)$
(Heisenberg picture)
and it is this "less-observable" operator that is now out of thermal equilibrium. In limit $t \to \infty$ $A(t)$ stops being observable, so can not be seen to be out of thermal equilibrium.

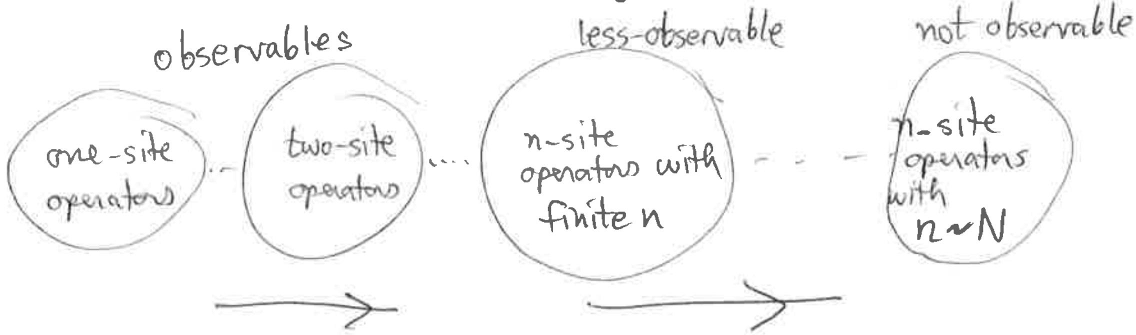
For systems that do thermalize, all non-conserved observables $A(t)$ "spread" over many local degrees of freedom, becoming first less-observable and finally non-observable, in the limit $t \to \infty$.

At late time t, observable $B(t)$ has the distributions that $B(0) = U(t) B(t) U^{\dagger}(t)$ had in the initial state. But this $B(0)$ (non-observable for $t \to \infty$) is a highly nonlocal complex operator that was not controlled or controllable in the initial state, so ~~ends~~ has the distribution that maximizes the entropy: the thermal equilibrium distribution.
(for systems that thermalize)

Thermalization: ~~Th~~ The initial state was ~~not~~ observably not in thermal equilibrium. But goes to thermal state for $t \to \infty$.

This "information" about non-eq initial state remains in the system at all times, but gets "hidden" in the probability distributions of nonobservable operators.

For $t \to \infty$ from almost all nonequilibrium initial states, the system $\to$ a thermal state.



Under dynamics of H or U of closed system, there is a flow in operator space that is almost purely from observable $\to$ nonobservable. This is the "cause" of the apparent irreversibility. And of 2nd law of thermodynamics.

There are special nonobservable operators that will evolve to become observable. But they, (being nonobservable) can not be controlled in the initial state preparation, so ~~one is~~ have random (thus thermal equilibrium) initial ~~state~~ distributions.

Eigenstate Thermalization Hypothesis (ETH).

Landau+Lifshitz, Jensen+Shankar 1985, Srednicki 1994, ...

If our system has H or U and ~~this~~ eigenstates of the dynamics, and it dynamically does thermalize from all initial states (that have given densities in $N \to \infty$ limit), then all eigenstates must be thermal states. (since eigenstate for $t \to \infty$ is same as for $t=0$)

This appears to be true for many (but not all) systems (under numerical tests).

If ETH is true, then the appropriate microcanonical "ensemble" is a single many-body eigenstate of the full system.

Dynamics of an observable A (now in Schrödinger picture): in terms of eigenstates of H:

$$\rho(t) = \sum_{nm} \rho_{nm}(0)\, |n\rangle\, e^{i(E_m - E_n)t} \langle m|$$

$$\langle A \rangle_t = \mathrm{Tr}\{A\rho(t)\} = \sum_n \langle n|A|n\rangle \rho_{nn}(0) + \sum_{n \neq m} \langle m|A|n\rangle \rho_{nm}(0) e^{i(E_m - E_n)t}$$

diagonal part of ETH: $\langle n|A|n\rangle$ is thermal equilibrium value of $\langle A\rangle_T$, so independent of $|n\rangle$ when all $|n\rangle$ are at same "temperature" (also any other thermodynamic parameters, like μ...)

$$\langle A \rangle_t = \langle A \rangle_T^{eq} + \underbrace{\sum_{n \neq m} \langle m|A|n\rangle \rho_{nm}(0) e^{i(E_m - E_n)t}}$$

off-diagonal part of ETH: (not fully formulated) What are the "statistical" properties of $\langle m|A|n\rangle$?

this must be nonzero in noneq'm initial state in $N \to \infty$ limit so $\langle m|A|n\rangle$ must be large enough to allow this

must go to zero for $t \to \infty$, $N \to \infty$ for all initial states, (due to pseudorandom phases) so $\langle m|A|n\rangle$ must be small enough for this to be true

Off-diagonal part of ETH:

Srednicki: $\langle n|A|m\rangle$ for a thermalizing system:
1994

$$\langle n|A|m\rangle \sim D^{-1/2} f_A(|E_n - E_m|)\, R_{nm}(A)$$

D = dimension of Hilbert space of states at that thermodynamic condition (follows from approxing states as random)

f_A: some ~~real~~ real nonnegative function (not universal) falls off with increasing energy diffn (but can be nonmonotonic)

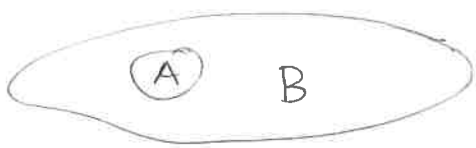
R_{nm}: pseudorandom numbers, variance 1. But really contains many correlations, since H contains few parameters, but there are D^2 (R_{nm}'s). e.g., Chan, De Luca, Chalker 2019 shows locality implies some strong correlations in R_{nm}'s

Exactly what correlations R_{nm} must have, and what correlations it must not have, is not yet fully known.

Entanglement (bipartite)

Put our full system in a pure state $\rho = |\psi\rangle\langle\psi|$.

Divide the degrees of freedom in to two parts A, B.



specifically, take limit $N \to \infty$ by $B \to \infty$, keeping A finite.

A need not be compact in real space.

Full Hilbert space $\mathcal{H}_{AB}$ is contained in outer product of ~~two~~ subsystems' Hilbert spaces:

$$\mathcal{H}_{AB} \in (\mathcal{H}_A \otimes \mathcal{H}_B)$$

usually $=$, but there might be some strict constraints making $\mathcal{H}_{AB}$ smaller.

If full system is in the pure state $|\psi\rangle_{AB}$ the state of subsystem A is

$$\rho_A = \operatorname{Trace}_B \{|\psi\rangle\langle\psi|\}$$

and is in general mixed, due to entanglement between A and B

~~partial~~ trace over all of B, not A

If $|\Psi\rangle$ is a thermal state, then ρ_A is the thermal equilibrium density matrix of subsystem A (A finite, $B \to \infty$).

Entropy density ~~of~~ of A is the thermal value. "volume-law"
entropy ~ volume of A.

If full system's state $|\Psi\rangle$ is pure, so has zero von Neumann entropy $S_{AB} = -\mathrm{Trace}\{\rho \ln \rho\} = 0$

Can say:
All of the entropy of A is then entanglement entropy, due to A being entangled with B. so generally ρ_A contains all the info about how A, B are entangled.

Classically, thermalization is weaker than quantum: since classical Newtonian system do not become entangled.

quantum pure state: $\rho = |\Psi\rangle\langle\Psi|$

classical pure state: a single classical configuration.

closed system under $\left\{\begin{matrix}\text{quantum} \\ \text{classical Newtonian}\end{matrix}\right\}$ dynamics initially pure
→ state remains pure at all times.

Quantum system that thermalizes becomes highly-entangled; this allows all subsystems to be in thermal equilibrium mixed states: System at fixed large time t in state $|\Psi(t)\rangle$ is thermal.

Classical system at fixed time t is in some specific "pure" classical configuration; each subsystem is also in a "pure" configuration (no entanglement). So state never becomes thermal in the same sense entangled quantum pure states do. ~~Them~~ Classical thermalization requires either a time-average, or a mixed initial state.

Not all systems thermalize:
exceptions:

- Quantum many-body "scars": Some of the eigenstates of the system's dynamics are non-thermal, most eigenstates are thermal.

  There are many such "fine-tuned" models. Probably these models are not robust to arbitrary small changes to H or U, and will be unstable to thermalization.
  Not part of these lectures

- Integrable systems: Number of conserved observables $\to \infty$ as $N \to \infty$.

  - "traditional" integrable systems (e.g. Bethe ansatz) conserved observables are delocalized: sums of observables ~~over~~ with "weight" spread ~~fairly~~ uniformly over all local degrees of freedom. ~~not concentrated on a f~~

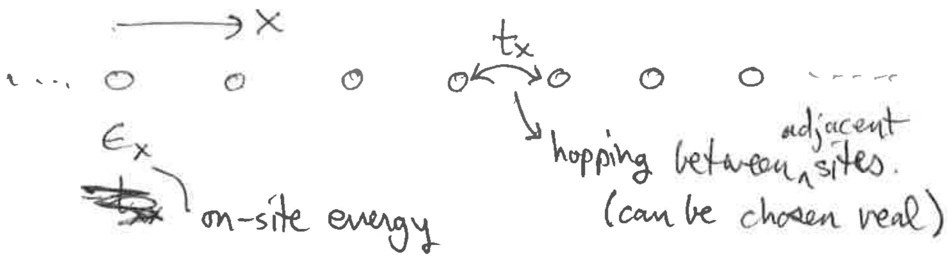
    These also ~~do not~~ appear to be unstable to thermalization under small generic changes to H or U. Not part of these lectures.

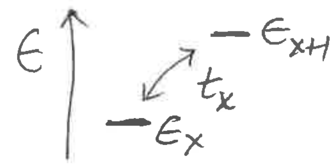
  - Many-body localized (MBL) systems.

    Conserved observables are <u>localized</u> operators, with their support concentrated on of order one local degrees of freedom (with "tails" that decay exponentially in space). MBL appears to be stable to small <u>local</u> changes in H or U. MBL is what we will now focus on.

Single-particle Anderson localization as MBL:

Consider noninteracting particles hopping along a 1D chain of sites:





$$H = \sum_x \left[\epsilon_x c_x^\dagger c_x + t_x (c_x^\dagger c_{x+1} + h.c.) \right]$$

We will work in the strong localization limit, where typically $t_x \ll |\epsilon_x - \epsilon_{x+1}|$ (so typically only weak "hybridization" of single-particle eigenstates) and treat t_x perturbatively in the "locator expansion" (Anderson 1958). This perturbative expansion converges well in this strong localization regime. Most eigenstates remain mostly on one site.

We do not have translational invariance, no exact degeneracies in ϵ_x's. Can have ϵ_x's random, or in a nonrandom, nonperiodic pattern (e.g. quasiperiodic).

Randomness is not important for Anderson localization.

~~Broken trans~~

Lack of translational invariance is important and "detuning": $|\epsilon_x - \epsilon_{x+1}| \gg t_x$

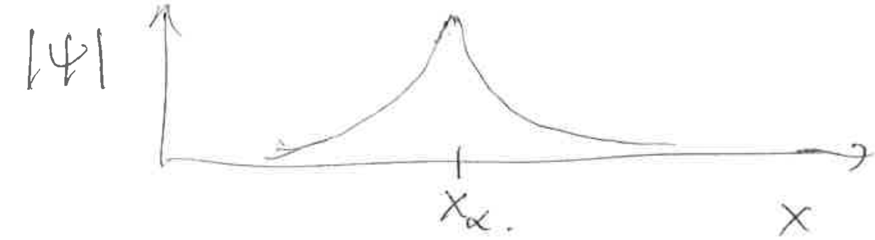
For all $t_x = 0$, the single-particle eigenstates of H are on each site, with energies ϵ_x.

Then treat t_x perturbatively: this makes each eigenstate have ~~an ex~~ "tails" in its eigenfunction, decaying exponentially away from site of maximum amplitude.

$$\psi_\alpha(x) \sim e^{-|x-x_\alpha|/\xi}$$

ψ_α: eigenfunction; x_α: "center" of its localization; ξ: localization length

single-particle eigenfunctions are localized in real space.



Using the basis $\{|\alpha\rangle\}$ of the single-particle eigenstates:

$$H = \sum_\alpha \epsilon_\alpha c^\dagger_\alpha c_\alpha$$

ϵ_α: single-particle eigenenergies. all $|\alpha\rangle$ localized.

Such a noninteracting localized H can occur in 2D or 3D, also.

$$H = \sum_{\alpha} \epsilon_\alpha c_\alpha^\dagger c_\alpha$$

Now consider this as a many-body system, with all $|\alpha\rangle$ possibly occupied. (fermions or bosons)

$n_\alpha = c_\alpha^\dagger c_\alpha$ is the occupation number of single-particle eigenstate α.

This H is a type of integrable system, with a complete set of localized commuting operators:

$$[H, n_\alpha] = 0 = [n_\alpha, n_\beta].$$

This is the structure of the MBL phase:

A complete set of localized commuting operators.

The many-body eigenfunctions are <u>not</u> localized in real space, since a typical eigenfunction has particles on or near every site.

It is the "eigenoperators" that are localized in real space.

There is also a more abstract localization in the many-body "Fock space" of <u>simultaneous</u> eigenstates of all the $n_x = c_x^\dagger c_x$. (A N-dimensional hypercube for spinless fermions on N sites.)