What is equilibrium and how do we get there?

An approach from isolated quantum systems

Hal Tasaki
collaborators: Sheldon Goldstein and Takashi Hara

YITP Workshop on Quantum Information Physics
August 5, 2014

main messages

message 1

A single quantum mechanical pure state can fully represent equilibrium state in a macroscopic system (and such pure states are TYPICAL)

message 2

Unitary time evolution in an isolated quantum system can describe the approach to equilibrium

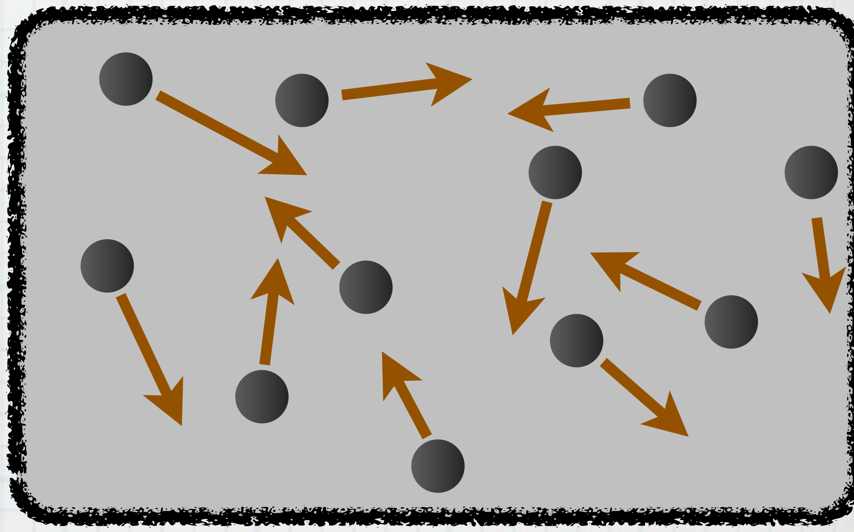
a pure state which represents equilibrium — an instructive example

Choose momenta $\boldsymbol{p}_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N$ randomly according to the Maxwell-Boltzmann distribution at temperature T, and fix them

Then, define a pure state by

$$\varphi_{\mathrm{ex}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \prod_{\ell=1}^{N} \exp\left[i \frac{\boldsymbol{p}_\ell \cdot \boldsymbol{r}_\ell}{\hbar}\right]$$

Can you distinguish $|\varphi_{\mathrm{ex}}\rangle$ from the equilibrium state of a dilute gas?



Usually, you CAN'T

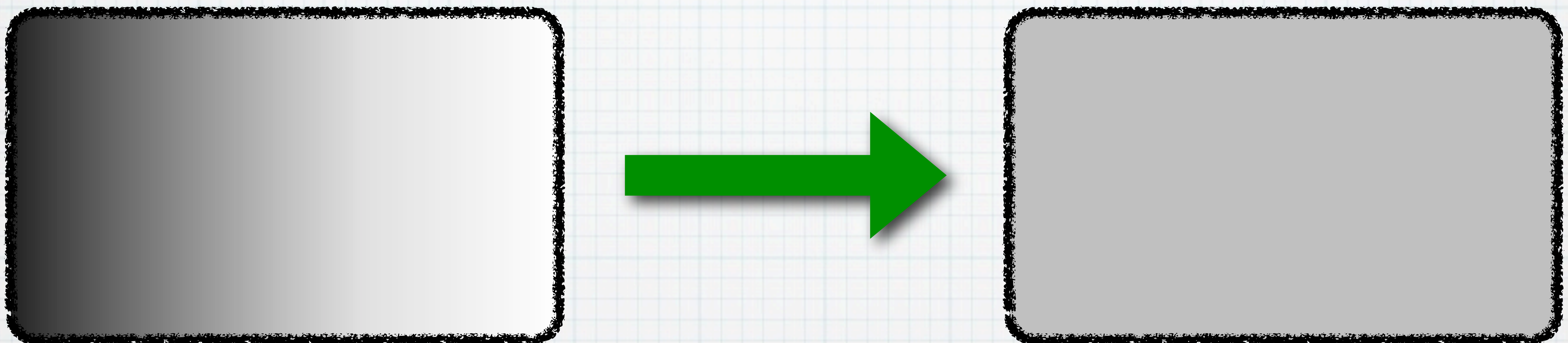
You CAN, IF you know and can measure the operator $|\varphi_{\mathrm{ex}}\rangle\langle\varphi_{\mathrm{ex}}|$

The state $|\varphi_{\mathrm{ex}}\rangle$ represents equilibrium!

General and heuristic pictures about equilibrium

Macroscopic view

Any macroscopic system settles to an equilibrium state after a sufficiently long time



a system consisting of a single substance

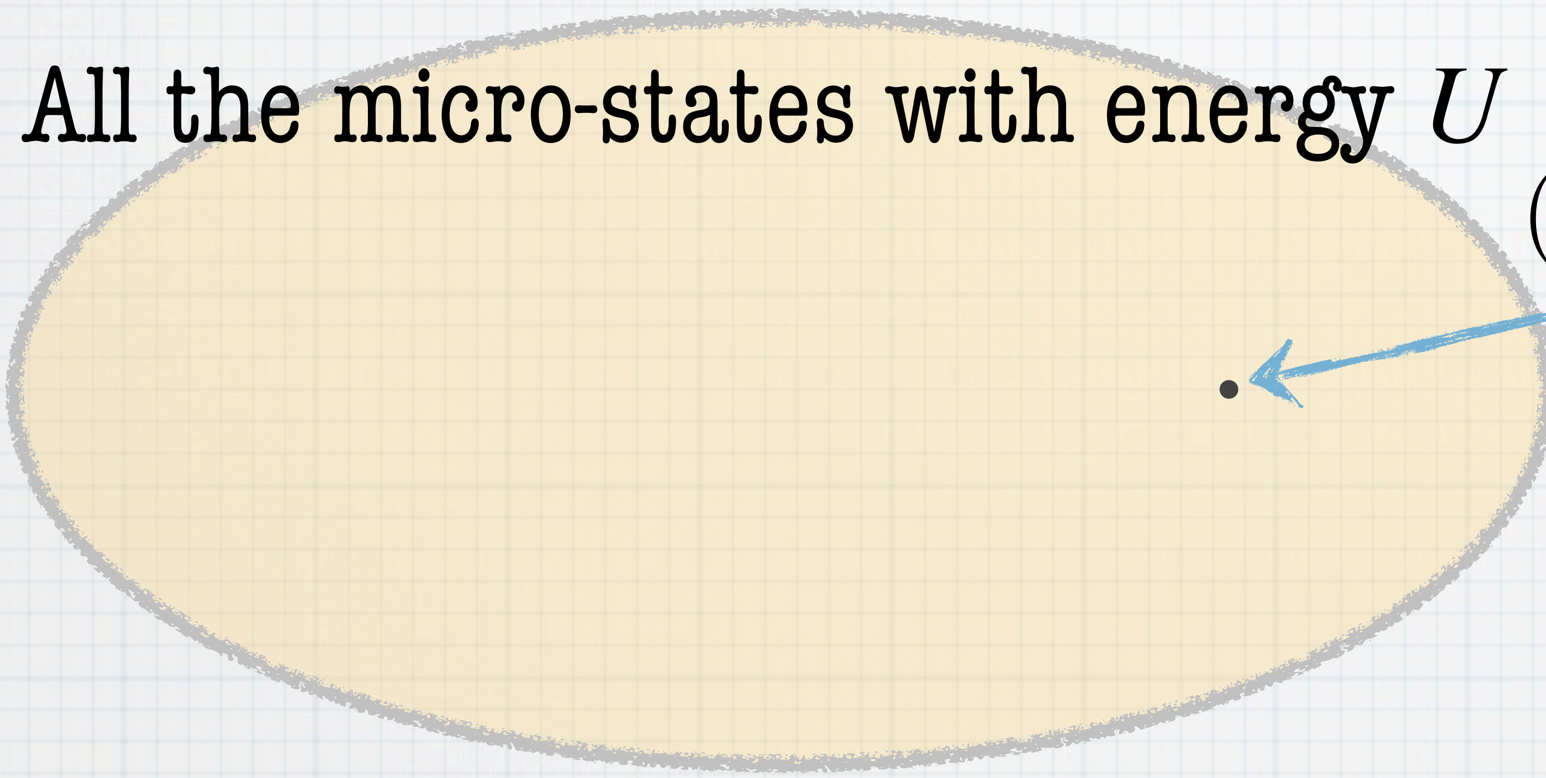
Equilibrium state

No macroscopic changes, no macroscopic flows

Uniquely determined by specifying only few macroscopic variables (i.e., the total energy U)
(V and N are fixed)

Microscopic view

Microscopically there are A LOT OF states with energy U



$(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N, p_1, \ldots, p_N)$

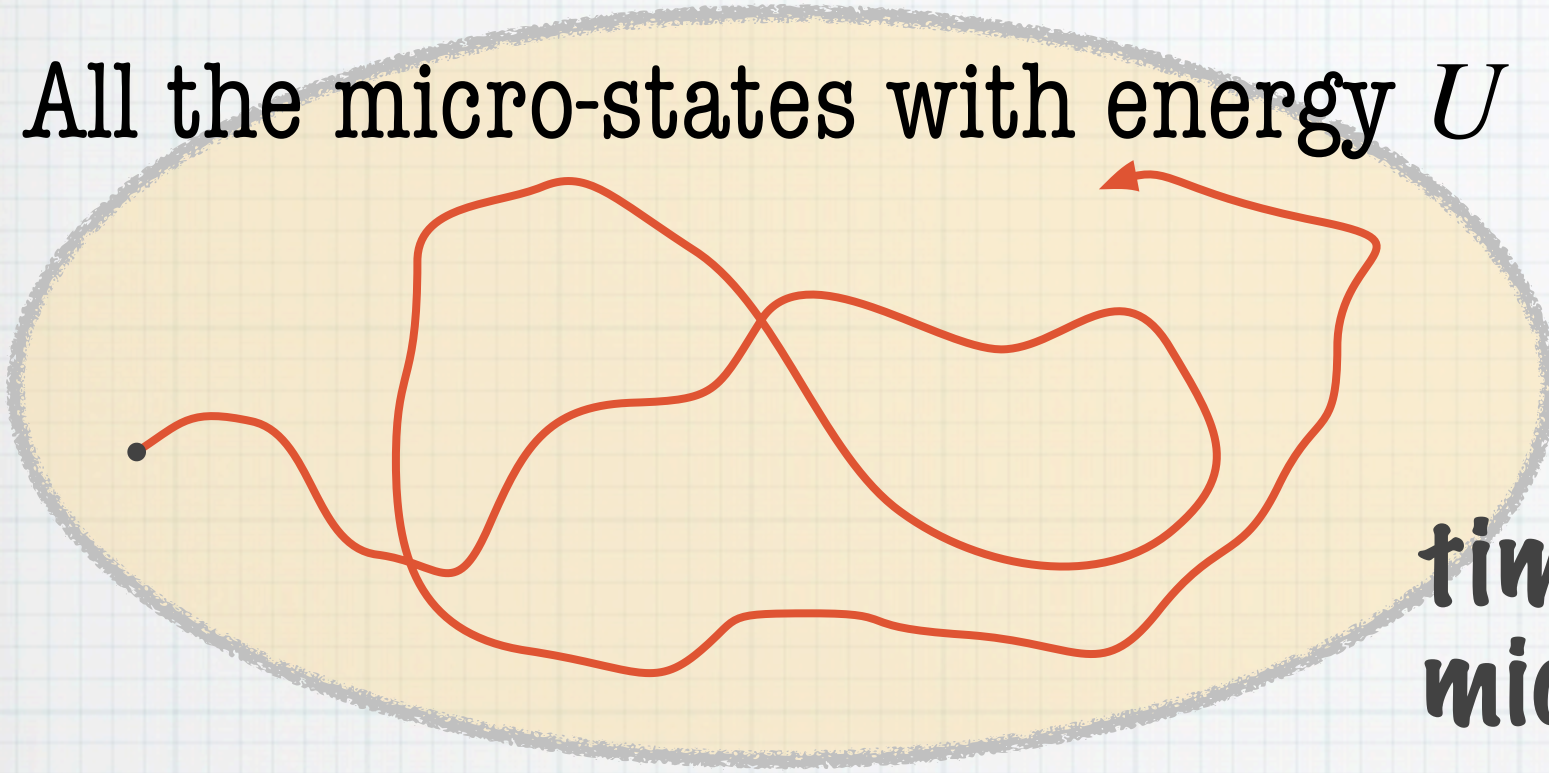
the positions and momenta of all the molecules

Standard procedure of statistical mechanics (principle of equal weights)

The microcanonical distribution (in which all the micro-states with U appear with the equal probabilities) describes equilibrium

Why does this work??

Ergodicity argument



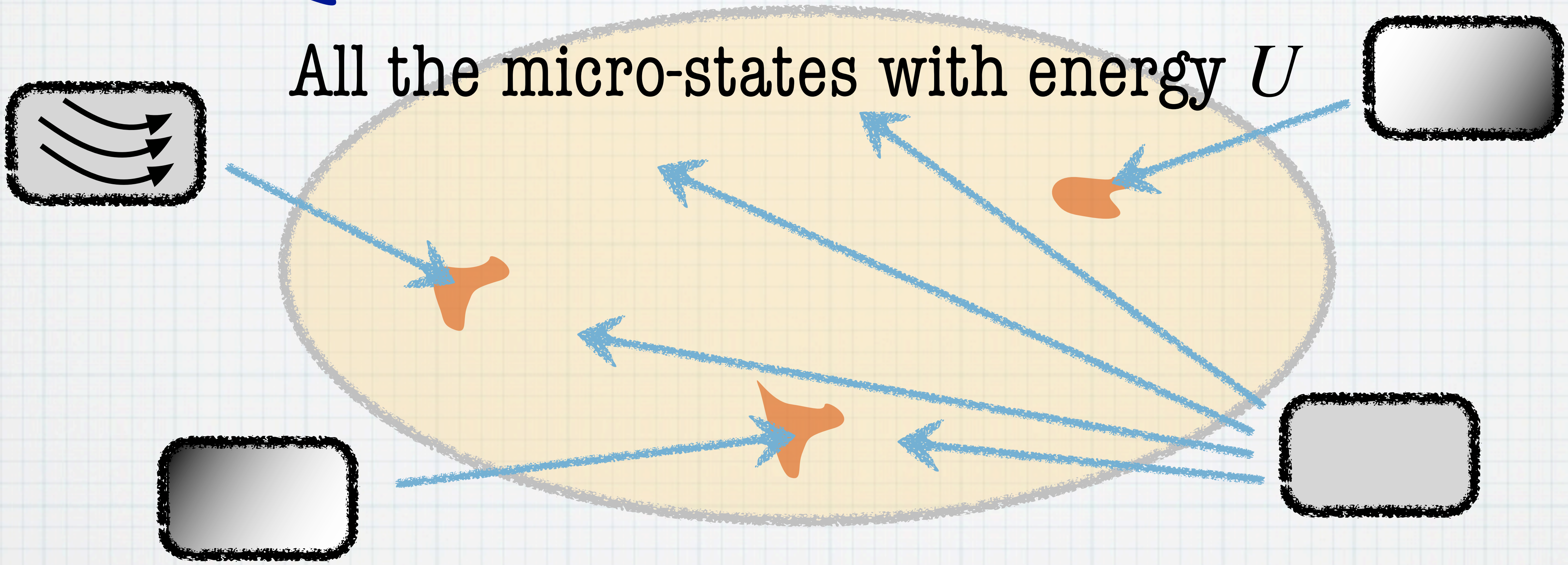
As time evolves, the state of the system visits most part of the phase space

time average leads to the microcanonical distribution

Very interesting idea that led to rich mathematical development; BUT misses the point as a physical mechanism of the approach to equilibrium

- ☑ It takes too long
- ☑ The idea becomes harder to realize in systems with higher degrees of freedom (but, stat mech is for systems with huge degrees of freedom!)

Typicality argument



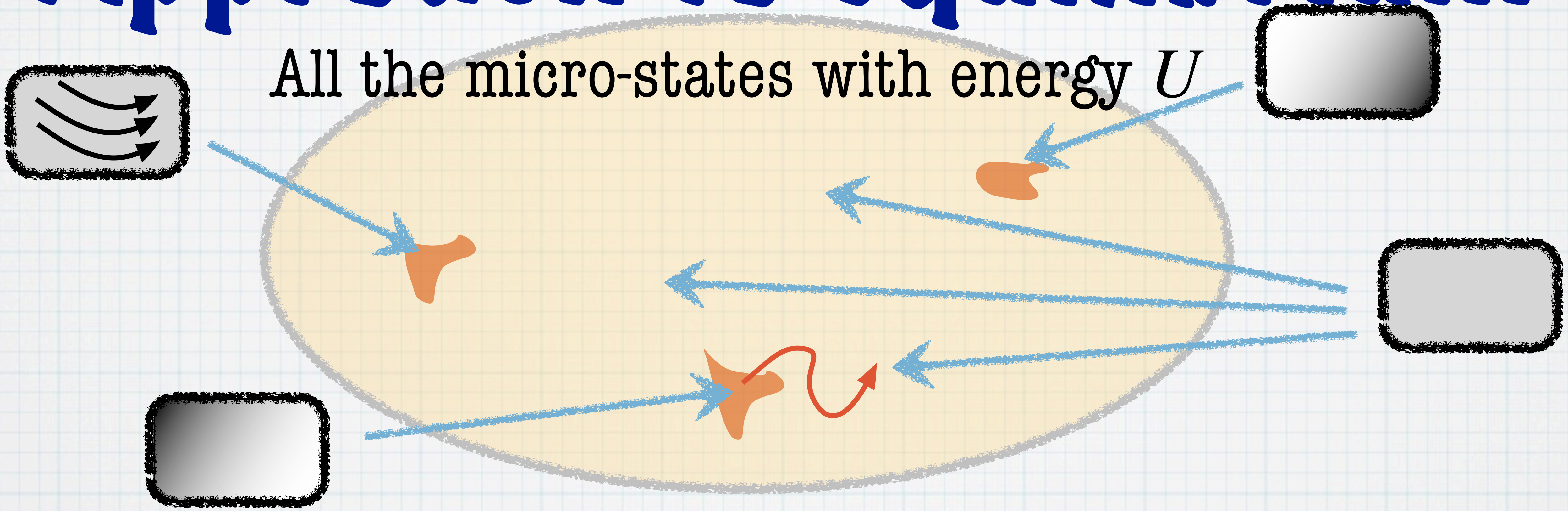
In a macroscopic system, a great majority of micro-states with energy U look identical (from macro point of view)

"Equilibrium" = the common properties shared by these almost identical micro-states

thus the microcanonical ensemble works

A single micro-state may represent equilibrium!

Approach to equilibrium



Non-equilibrium states:
minor atypical states

↓ relaxation

Equilibrium states:
typical states

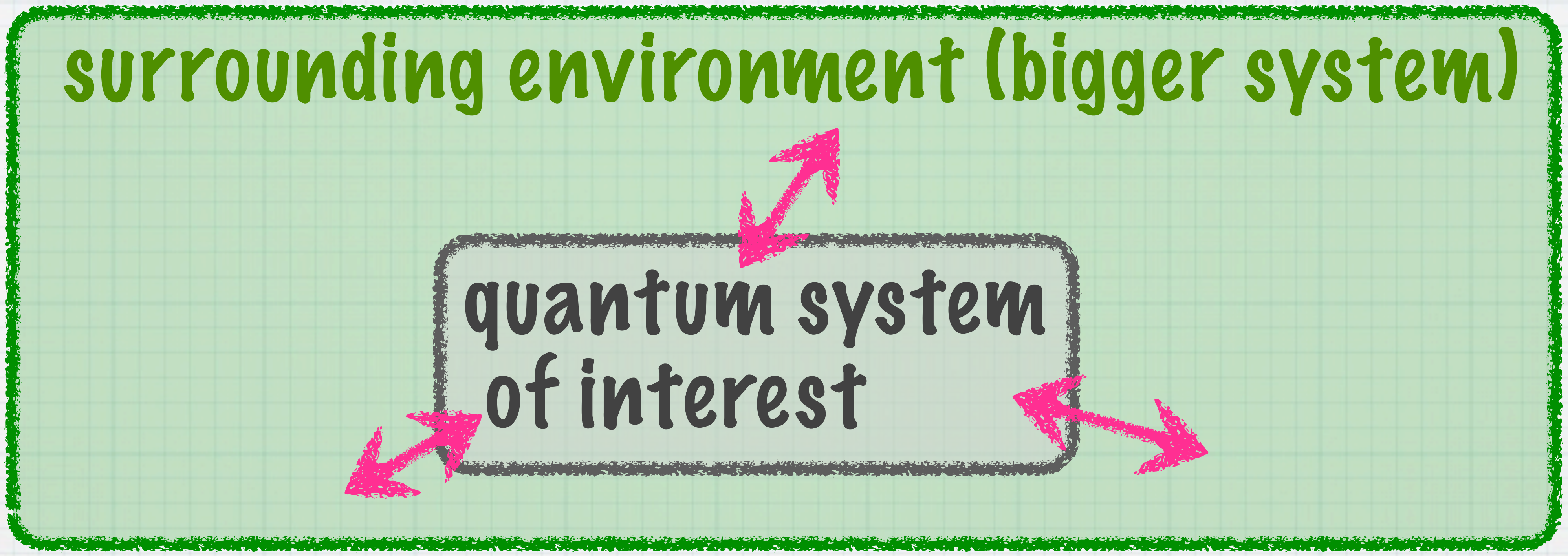
Humpty Dumpty sat on a wall,
Humpty Dumpty had a great fall.
All the king's horses and all the king's men
Couldn't put Humpty together again

the approach to equilibrium is quite a robust phenomenon

Isolated macroscopic quantum systems

Basic setting

Standard (and realistic) treatment



Our (obviously unrealistic) treatment

quantum system of interest

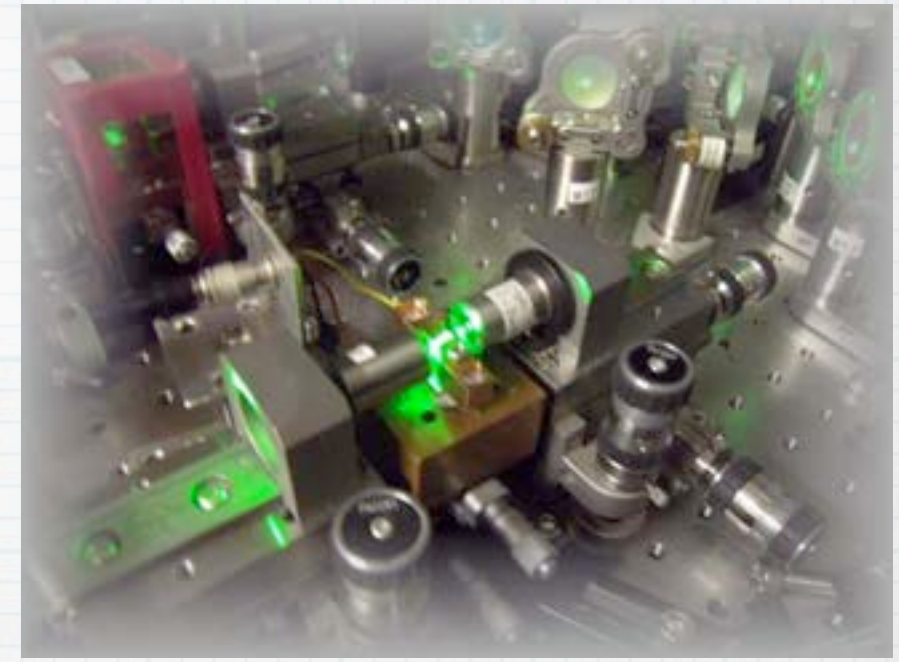
perfectly isolated from the outside world

Why isolated systems?

Standard (fashionable) answer

We can realize isolated quantum systems in ultra cold atoms

clean system of 10^7 atoms at 10^{-7} K



My (old-fashioned) answer

This is still a very fundamental study, very very far from practical applications

We wish to learn what isolated systems can do (e.g., whether they exhibit the approach to equilibrium)

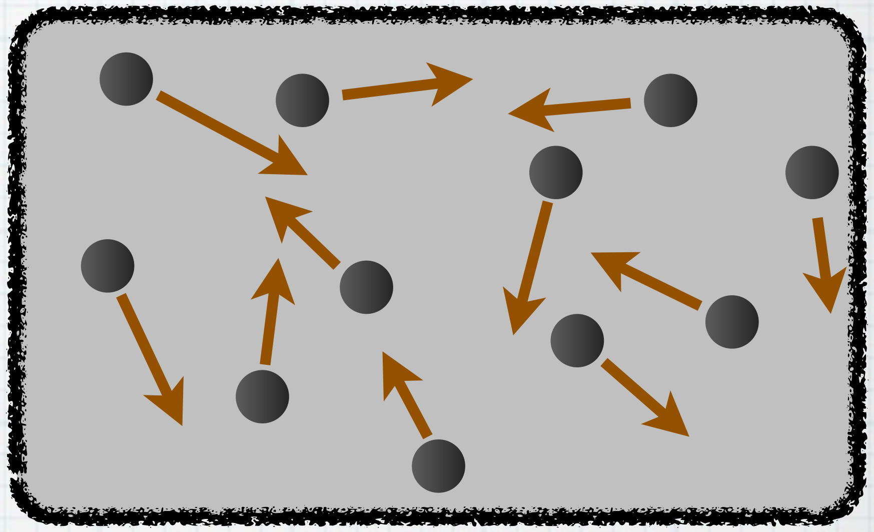
After that, we may study the effect played by the environment

Settings and assumptions

Macroscopic system

Quantum system in a large volume V

- Particle system with constant $\rho = N/V$
- Quantum spin system



Hilbert space $\mathcal{H}_{\mathrm{tot}}$

Hamiltonian $\hat{H}$

Energy eigenstate $\hat{H}|\psi_j\rangle = E_j|\psi_j\rangle$

$$\langle\psi_j|\psi_j\rangle = 1$$

The number of states

$\Omega_V(U) =$ (the number of j such that $E_j \le U$)

$$\sim \exp\big[\,V\,\sigma(U/V)\,\big]$$

entropy density $\sigma(\epsilon)$

inverse temperature $\beta(u) = \sigma'(u)$

Energy shell

Fix arbitrary u and small Δu, and consider the range of energy $u - \Delta u \le E_j/V \le u$ with $j = 1, \ldots, D$

we have relabeled j

$$D \sim e^{\sigma(u)\, V}$$

microcanonical average of an observable $\hat{O}$

$$\langle \hat{O} \rangle_{\mathrm{mc}} := \frac{1}{D} \sum_{j=1}^{D} \langle \psi_j | \hat{O} | \psi_j \rangle$$

microcanonical energy shell ~~$\mathcal{H}_{u-\Delta u, u}$~~ → $\mathcal{H}$

the space spanned by $|\psi_j\rangle$ with $j = 1, \ldots, D$

Pure state which represents equilibrium

Suppose that we are interested only in a SINGLE extensive physical quantity $\hat{A} = O(V)$

$\delta > 0$ precision for measuring $\hat{A}/V$

DEFINITION: A normalized pure state $|\varphi\rangle \in \mathcal{H}$ represents equilibrium if there is a constant $\alpha > 0$, and

$$\langle\varphi|\,\hat{P}\big[\,|\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}|/V \geq \delta\,\big]\,|\varphi\rangle \leq e^{-\alpha V}$$

projection

if we measure $\hat{A}$ in $|\varphi\rangle$, then

$$|A_{\mathrm{measured}} - \langle\hat{A}\rangle_{\mathrm{mc}}|/V \leq \delta$$

with probability $\geq 1 - e^{-\alpha V}$

one almost surely gets the equilibrium value!

Basic assumption

Extensive physical quantity of interest $\hat{A} = O(V)$

$\delta > 0$ precision for measuring $\hat{A}/V$

THERMODYNAMIC BOUND (TDB):

There is a constant $\gamma > 0$, and one has

$$\left\langle \hat{P}\left[\,|\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}| \geq V\delta\,\right]\right\rangle_{\mathrm{mc}} \leq e^{-\gamma V}$$

for any V

statement in statistical mechanics

simply says large fluctuation is exponentially rare
(a weak version of large deviation property)

expected to be valid for ANY (pure) equilibrium state, but has been proved (very recently) only in limited situations

a general proof seems to be extremely hard

Thermodynamic bound

THEOREM: Take a quantum system on a lattice with short-ranged Hamiltonian, and let $\hat{A} = \sum_x \hat{a}_x$, where $\hat{a}_x$ acts only on site x. Then for any δ there is γ and we have

$$\left\langle \hat{P}\big[\,|\hat{A} - \langle \hat{A} \rangle_{\mathrm{mc}}| \geq V\delta\,\big] \right\rangle_{\mathrm{mc}} \leq e^{-\gamma V}$$

provided that $\beta(u)$ is sufficiently small

THEOREM: For the Ising model under magnetic field in the x-direction, we have for any δ that

$$\left\langle \hat{P}\big[\,|\hat{S}_z^{\mathrm{tot}}| \geq V\delta\,\big] \right\rangle_{\mathrm{mc}} \leq \exp\Big[-\frac{\delta^2}{4\chi^{\mathrm{cl}}(\beta(u))}\,V\Big]$$

provided that $\beta(u) < \beta_{\mathrm{c}}^{\mathrm{cl}}$

works for any u in the one-dimensional model

Typicality of pure states which represent equilibrium

Average over $\mathcal{H}$

a state $\mathcal{H} \ni |\varphi\rangle = \sum_{j=1}^{D} \alpha_j \, |\psi_j\rangle$ with $\langle\varphi|\varphi\rangle = 1$

can be regarded as a point on the unit sphere of $\mathbb{C}^D$

a natural (basis independent) measure on $\mathcal{H}$ is the uniform measure on the unit sphere

corresponding average

$$\overline{(\cdots)} := \frac{\int d\alpha_1 \cdots d\alpha_D \, \delta\big(1 - \sum_{j=1}^{D} |\alpha_j|^2\big) \, (\cdots)}{\int d\alpha_1 \cdots d\alpha_D \, \delta\big(1 - \sum_{j=1}^{D} |\alpha_j|^2\big)}$$

$$d\alpha := d(\mathrm{Re}\alpha) \, d(\mathrm{Im}\alpha)$$

From the symmetry

$$\overline{\alpha_j^* \alpha_k} = \frac{1}{D} \, \delta_{j,k}$$

Average over $\mathcal{H}$ and mc-average

operator $\hat{O}$ normalized state $|\varphi\rangle = \sum_{j=1}^{D} \alpha_j \, |\psi_j\rangle$

quantum mechanical expectation value

$$\langle\varphi|\hat{O}|\varphi\rangle = \sum_{j,k=1}^{D} \alpha_j^* \alpha_k \, \langle\psi_j|\hat{O}|\psi_k\rangle$$

average over $\mathcal{H}$

$$\overline{\langle\varphi|\hat{O}|\varphi\rangle} = \sum_{j,k} \overline{\alpha_j^* \alpha_k} \, \langle\psi_j|\hat{O}|\psi_k\rangle$$

$$= \frac{1}{D} \sum_{j=1}^{D} \langle\psi_j|\hat{O}|\psi_j\rangle = \langle\hat{O}\rangle_{\mathrm{mc}}$$

average over infinitely many states in the shell

average over D energy eigenstates

Another way of looking at the microcanonical average

Typicality of equilibrium

provable for some models

Assume Thermodynamic bound (TDB)

$$\left\langle \hat{P}\left[\,|\hat{A}-\langle\hat{A}\rangle_{\rm mc}|/V \ge \delta\,\right]\right\rangle_{\rm mc} \le e^{-\gamma V}$$

THEOREM: Choose a normalized $|\varphi\rangle \in \mathcal{H}$ randomly.
Then with probability $\ge 1-e^{-(\gamma-\alpha)V}$

$$\langle\varphi|\,\hat{P}\left[\,|\hat{A}-\langle\hat{A}\rangle_{\rm mc}|/V \ge \delta\,\right]|\varphi\rangle \le e^{-\alpha V}$$

PROOF (easy) write $\hat{P}_\ge = \hat{P}\left[\,|\hat{A}-\langle\hat{A}\rangle_{\rm mc}|/V \ge \delta\,\right]$

$$e^{-\alpha V}\,{\rm Prob}\left[\,\langle\varphi|\hat{P}_\ge|\varphi\rangle \ge e^{-\alpha V}\,\right] \le \overline{\langle\varphi|\hat{P}_\ge|\varphi\rangle} = \langle\hat{P}_\ge\rangle_{\rm mc} \le e^{-\gamma V}$$

$${\rm Prob}\left[\,\langle\varphi|\hat{P}_\ge|\varphi\rangle \ge e^{-\alpha V}\,\right] \le e^{-(\gamma-\alpha)V}$$

one can prove stronger estimate (use Sugita's result)

message 1

Almost all pure state $|\varphi\rangle$ represents equilibrium!!

The approach to equilibrium

Next question

initial state $|\varphi(0)\rangle \in \mathcal{H}$ $\qquad |\varphi(t)\rangle = e^{-i\hat{H}t}|\varphi(0)\rangle$

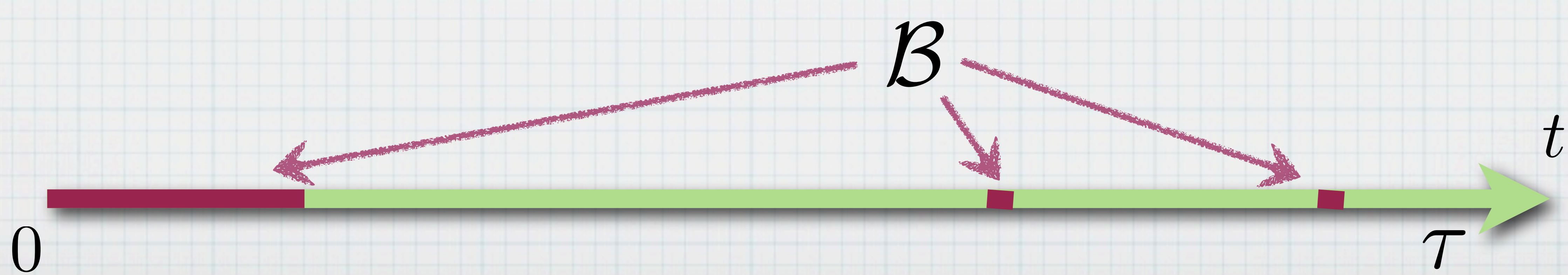
under suitable conditions we shall prove that

$|\varphi(t)\rangle$ represents equilibrium for most t in the long run

↕ the approach to equilibrium!

there exist a (large) constant τ and a subset $\mathcal{B} \subset [0,\tau]$ with $|\mathcal{B}|/\tau \le e^{-\alpha V}$ such that for any $t \in [0,\tau]\backslash\mathcal{B}$

$$\langle\varphi(t)|\,\hat{P}\big[\,|\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}|/V \ge \delta\,\big]\,|\varphi(t)\rangle \le e^{-\alpha V}$$



Two strategies

STRATEGY 1: based on an assumption on the initial state

Tasaki 1998, Reimann 2008
Linden, Popescu, Short, Winter 2009
and many others

STRATEGY 2: based on "eigenstate thermalization"

First strategy

Expand the initial state as $|\varphi(0)\rangle = \sum_{j=1}^{D} c_j \, |\psi_j\rangle$

$$\sum_{j=1}^{D} |c_j|^2 = 1$$

ASSUMPTIONS:

- ☑ coefficients are not too sharply concentrated

$$|c_j|^2 \leq e^{\kappa V}/D \qquad 0 < \kappa < \gamma - 2\alpha$$

- ☑ thermodynamic bound (TDB)
- ☑ no degeneracy $\quad j \neq j' \Rightarrow E_j \neq E_{j'}$

provable for some models

THEOREM: For any $|\varphi(0)\rangle \in \mathcal{H}$ satisfying the above, $|\varphi(t)\rangle$ represents equilibrium for most t in the long run

First strategy

Expand the initial state as $|\varphi(0)\rangle = \sum_{j=1}^{D} c_j \, |\psi_j\rangle$

☑ coefficients are not too sharply concentrated

$$|c_j|^2 \leq e^{\kappa V}/D$$

is this reasonable?

YES, if an experimentalist innocently prepares an initial state, it is very very likely that this is satisfied

WHO KNOWS? we don't know almost anything about state preparation in macroscopic systems

most works on equilibration and thermalization in isolated quantum systems are based on similar assumption about the "lack of sharp concentration"

proof 1/2

initial state $|\varphi(0)\rangle = \sum_{j=1}^{D} c_j \, |\psi_j\rangle$

time-evolution $|\varphi(t)\rangle = \sum_{j=1}^{D} c_j \, e^{-iE_j t} \, |\psi_j\rangle$

$$\langle\varphi(t)|\hat{P}_{\geq}|\varphi(t)\rangle = \sum_{j,k} c_j^* c_k \, \boxed{e^{i(E_j - E_k)t}} \langle\psi_j|\hat{P}_{\geq}|\psi_k\rangle$$

oscillates

long-time average

$$\lim_{\tau\uparrow\infty} \frac{1}{\tau}\int_0^\tau dt \langle\varphi(t)|\hat{P}_{\geq}|\varphi(t)\rangle = \sum_j \boxed{|c_j|^2} \langle\psi_j|\hat{P}_{\geq}|\psi_j\rangle$$

$$\leq \boxed{\frac{e^{\kappa V}}{D}} \sum_{j=1}^{D} \langle\psi_j|\hat{P}_{\geq}|\psi_j\rangle = e^{\kappa V} \, \langle\hat{P}_{\geq}\rangle_{\mathrm{mc}}$$

$$\leq e^{-(\gamma-\kappa)V} \leq e^{-2\alpha V}/2$$

proof 2/2

for long-time average

$$\lim_{\tau\uparrow\infty}\frac{1}{\tau}\int_0^\tau dt\langle\varphi(t)|\hat{P}_\geq|\varphi(t)\rangle \leq e^{-2\alpha V}/2$$

for sufficiently large τ

$$\frac{1}{\tau}\int_0^\tau dt\langle\varphi(t)|\hat{P}_\geq|\varphi(t)\rangle \leq e^{-2\alpha V}$$

define the "bad" set as

$$\mathcal{B} = \left\{ t \in [0,\tau] \,\middle|\, \langle\varphi(t)|\hat{P}_\geq|\varphi(t)\rangle \geq e^{-\alpha V} \right\}$$

then obviously $\displaystyle \frac{1}{\tau}\int_0^\tau dt\langle\varphi(t)|\hat{P}_\geq|\varphi(t)\rangle \geq \frac{|\mathcal{B}|}{\tau}e^{-\alpha V}$

we thus find $|\mathcal{B}|/\tau \leq e^{-\alpha V}$

Two strategies

STRATEGY 1: based on an assumption on the initial state

Tasaki 1998, Reimann 2008
Linden, Popescu, Short, Winter 2009
and many others

STRATEGY 2: based on "eigenstate thermalization"

arXiv:1003.2133 *(Submitted on 10 Mar 2010 (v1), last revised 2 Sep 2010 (this version, v2))*

Proof of the Ergodic Theorem and the H-Theorem in Quantum Mechanics

John von Neumann

Zeitschrift fuer Physik 57: 30-70 (1929)

Goldstein, Lebowitz, Mastrodonato, Tumulka, Zanghi 2010

second strategy

ASSUMPTIONS:

☑ no degeneracy $j \neq j' \Rightarrow E_j \neq E_{j'}$

☑ $\langle\psi_j|\,\hat{P}\big[\,|\hat{A} - \langle\hat{A}\rangle_{\rm mc}|/V \geq \delta\,\big]\,|\psi_j\rangle \leq e^{-\gamma\,V}$

for each $j = 1, \ldots, D$ $\qquad \gamma > 2\alpha$

Each $|\psi_j\rangle$ represents equilibrium

"energy eigenstate thermalization"

suggested (but not guaranteed) by the typicality of equilibrium

THEOREM: For ANY $|\varphi(0)\rangle \in \mathcal{H}$,
$|\varphi(t)\rangle$ represents equilibrium for most t in the long run

proof

initial state $|\varphi(0)\rangle = \sum_{j=1}^{D} c_j \, |\psi_j\rangle$

time-evolution $|\varphi(t)\rangle = \sum_{j=1}^{D} c_j \, e^{-iE_j t} \, |\psi_j\rangle$

$$\langle\varphi(t)|\hat{P}_{\geq}|\varphi(t)\rangle = \sum_{j,k} c_j^* c_k \, e^{i(E_j - E_k)t} \langle\psi_j|\hat{P}_{\geq}|\psi_k\rangle$$

long-time average

$$\lim_{\tau\uparrow\infty} \frac{1}{\tau} \int_0^\tau dt \langle\varphi(t)|\hat{P}_{\geq}|\varphi(t)\rangle = \sum_j |c_j|^2 \boxed{\langle\psi_j|\hat{P}_{\geq}|\psi_j\rangle}$$

$$\leq \boxed{e^{-\gamma V}} \sum_j |c_j|^2 = e^{-\gamma V} \leq e^{-2\alpha V}/2$$

the rest is exactly the same

Comparison of the two theorems about thermalization

initial state $|\varphi(0)\rangle \in \mathcal{H}$ $\qquad |\varphi(t)\rangle = e^{-i\hat{H}t}|\varphi(0)\rangle$

$|\varphi(t)\rangle$ represents equilibrium for most t in the long run

the approach to equilibrium!

FIRST THEOREM:

requires the assumption about the "lack of sharp concentration" in the initial state

the other conditions (TDB and non-degeneracy) are verified in concrete models

message 2

SECOND THEOREM:

works for an ARBITRARY initial state

the "energy eigenstate thermalization" is not yet proved in any nontrivial concrete systems

Results for typical projections

Motivation

REMAINING ESSENTIAL ISSUES

☑ Is the energy eigenstate thermalization true?

$$\langle\psi_j|\hat{P}_{\geq}|\psi_j\rangle \ll 1 \qquad j = 1,\ldots,D$$

☑ What is the time-scale τ necessary for thermalization?

It is extremely difficult to solve these issues for a concrete

$$\hat{P}_{\geq} = \hat{P}\left[\,|\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}|/V \geq \delta\,\right]$$

Study the projection $\hat{P}_{\geq}$ onto a random d dimensional subspace of the energy shell $\mathcal{H}$ $\qquad d \ll D$

we might understand certain "generic" features

philosophy of random matrix for nuclear physics

Energy eigenstate thermalization

THEOREM: Let $\hat{P}_{\geq}$ be the projection operator onto a random d dimensional subspace of $\mathcal{H}$, where $d \ll D$. Then with probability close to 1, we have

$$\langle \psi_j | \hat{P}_{\geq} | \psi_j \rangle \ll 1$$

uniformly in $j = 1, \ldots, D$

von Neumann (1929)
Goldstein, Lebowitz, Mastrodonato, Tumulka, Zanghi (2010)

energy eigenstate thermalization is typically valid

this does not prove "energy eigenstate thermalization" for a given concrete system, but suggests that it is likely

Time scale for thermalization

THEOREM: Let $\hat{P}_{\geq}$ be the projection operator onto a random d dimensional subspace of $\mathcal{H}$, where $d \ll D$. Then with probability close to 1, the following is true.

For ANY initial state $|\varphi(0)\rangle \in \mathcal{H}$, and any τ, we have

$$\frac{1}{\tau}\int_0^\tau dt \langle \varphi(t)|\hat{P}_{\geq}|\varphi(t)\rangle \lesssim \frac{\tau_B}{\tau}$$

where $\tau_B := h/(k_B T)$ is the Boltzmann time

Goldstein, Hara, Tasaki (2014)

$$k_B T = 1/\sigma'(u)$$

any initial state thermalizes in the time-scale $\tau \gg \tau_B$

Extremely quick thermalization

any initial state thermalizes in the time-scale $\tau \gg \tau_B$

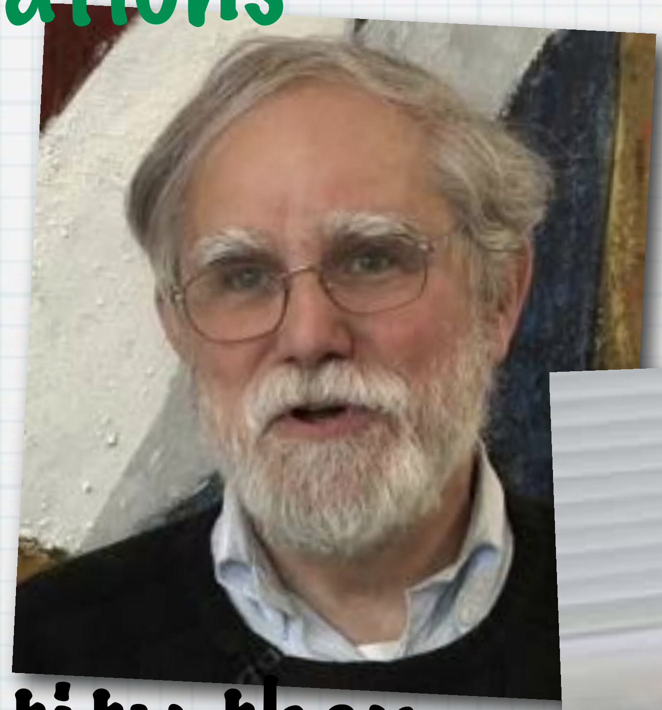
$$T \sim 300\ \mathrm{K} \longrightarrow \tau_B \sim 10^{-13}\ \mathrm{s}$$

THEOREM: EVERYTHING THERMALIZES WITHIN A MICROSECOND!! ?

Goldstein, Hara, Tasaki (2014)

one encounters such quick relaxations in several physical contexts

but this is certainly highly unrealistic in general!



THEOREM: If $\hat{H}$ is local and there is a local conserved quantity then the relaxation time can be $\geq O(L)$

The limit of the typicality approach

THE METHOD OF APPEAL TO TYPICALITY

show that

"property A is true of most B"

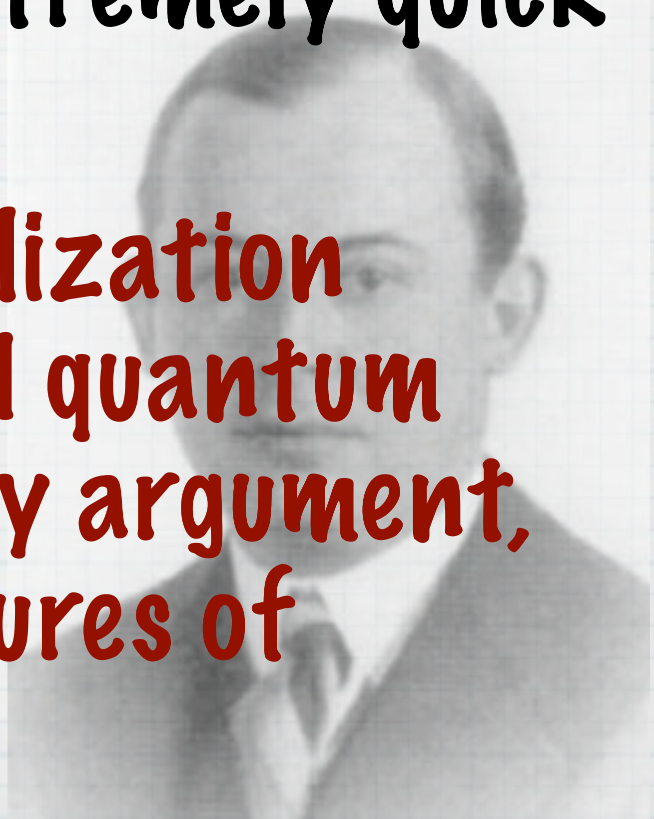
this suggests that

"property A is true of a concrete given B"

(unless there are reasons to expect otherwise)

we have (unfortunately) shown that "extremely quick decay is true of most $\hat{P}_{\geq}$"

To develop a satisfactory theory of thermalization (including the issue of time-scale) in isolated quantum systems , we can no longer rely on typicality argument, but should take into account essential features of realistic quantum systems



Summary

- ☑ In a macroscopic quantum system, a typical state (with almost fixed energy) represents equilibrium

- ☑ With suitable assumptions, one can show that a purely quantum mechanical time-evolution in an isolated system brings the system towards equilibrium

- ☑ To understand the important issue of time-scale, we need to go beyond the philosophy of appeal to typicality