Typicality and thermalization in isolated quantum systems

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will be revised soon!

arXiv:1507.06479

about the talk

- ☑ Foundation of equilibrium statistical mechanics based on pure quantum mechanical states in macroscopic isolated quantum systems

  von Neumann 1929, Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi 2010

- ☑ Main messages
  - a pure quantum mechanical state can fully represent thermal equilibrium
  - the unitary time evolution in an isolated quantum system can describe thermalization

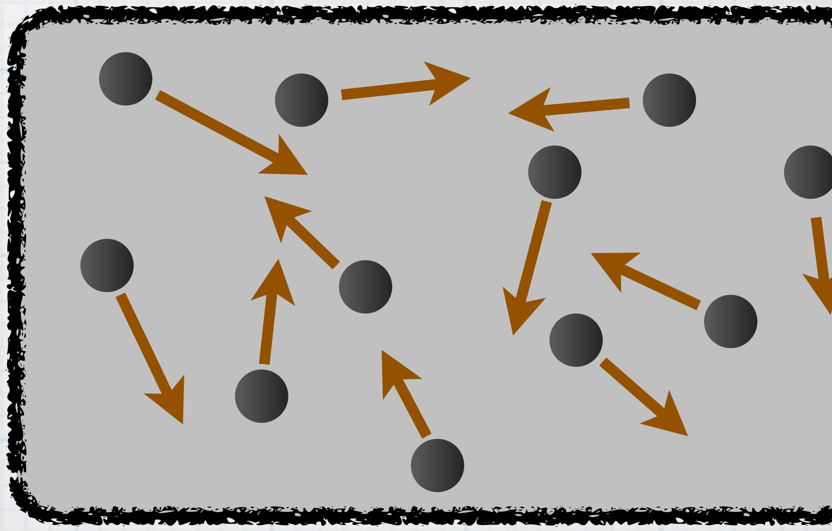
a pure state which represents thermal equilibrium: an instructive example

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 experimentally distinguish $|\varphi_{\mathrm{ex}}\rangle$ from the canonical distribution of a dilute gas?



Usually, you CAN'T

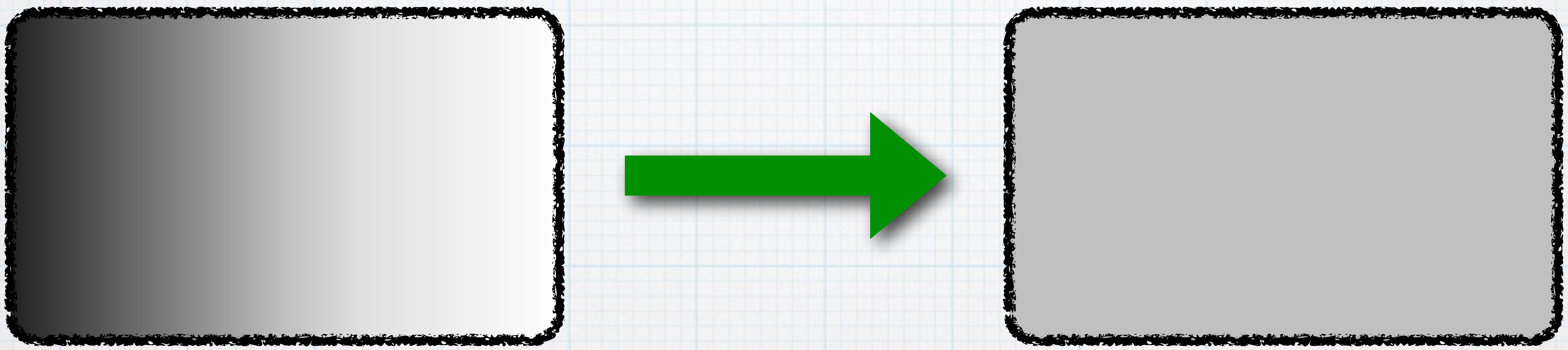
You CAN, IF you know and can measure the operator $|\varphi_{\mathrm{ex}}\rangle\langle\varphi_{\mathrm{ex}}|$

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

Heuristic pictures about thermal equilibrium

Macroscopic view

An isolated macroscopic system always settles to thermal equilibrium state after a sufficiently long time



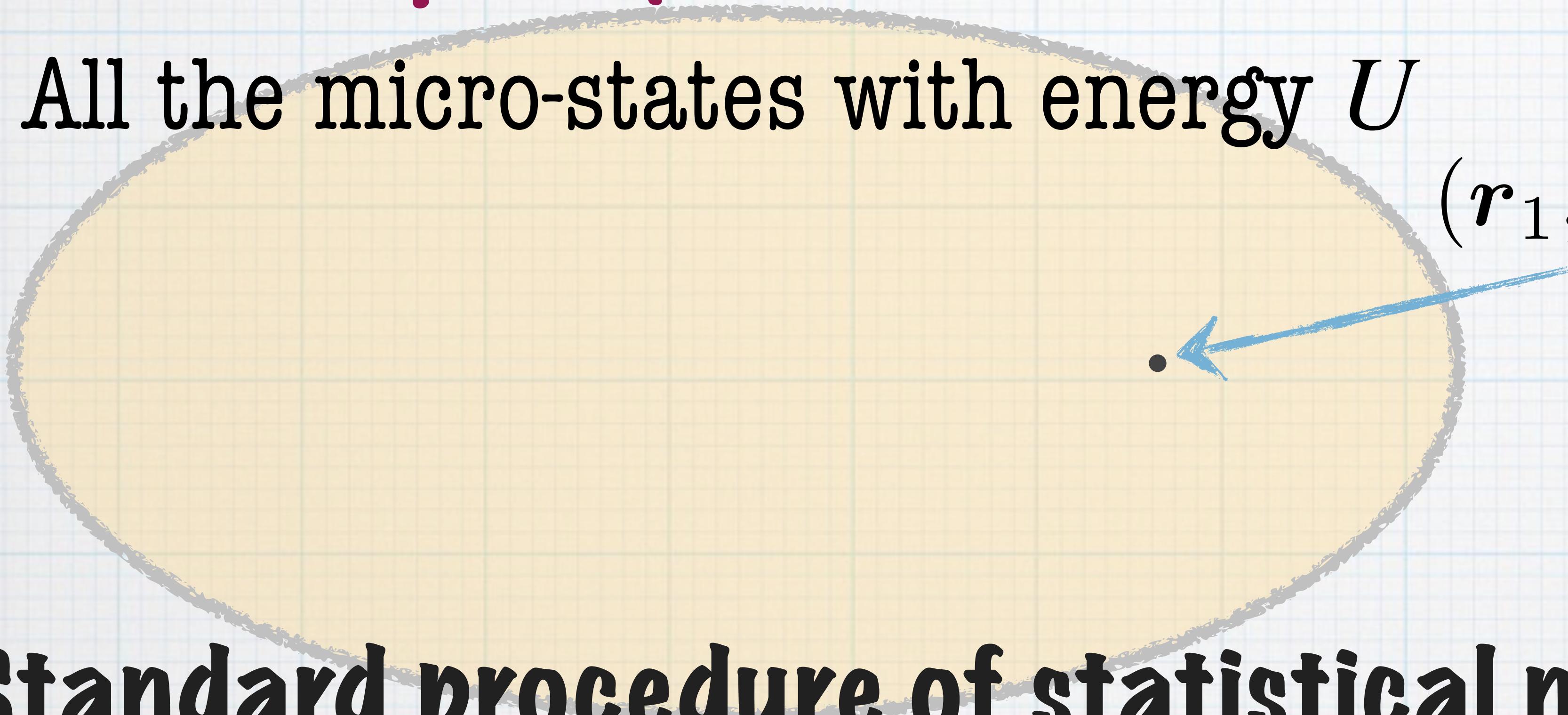
Thermal equilibrium

- No macroscopic changes, no macroscopic flows
- Uniquely determined by specifying only few macroscopic variables
  (e.g., the total energy U, in a system consisting of a single substance when V and N are fixed)

Microscopic view

Microscopically there are A LOT OF states with energy U

All the micro-states with energy U



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

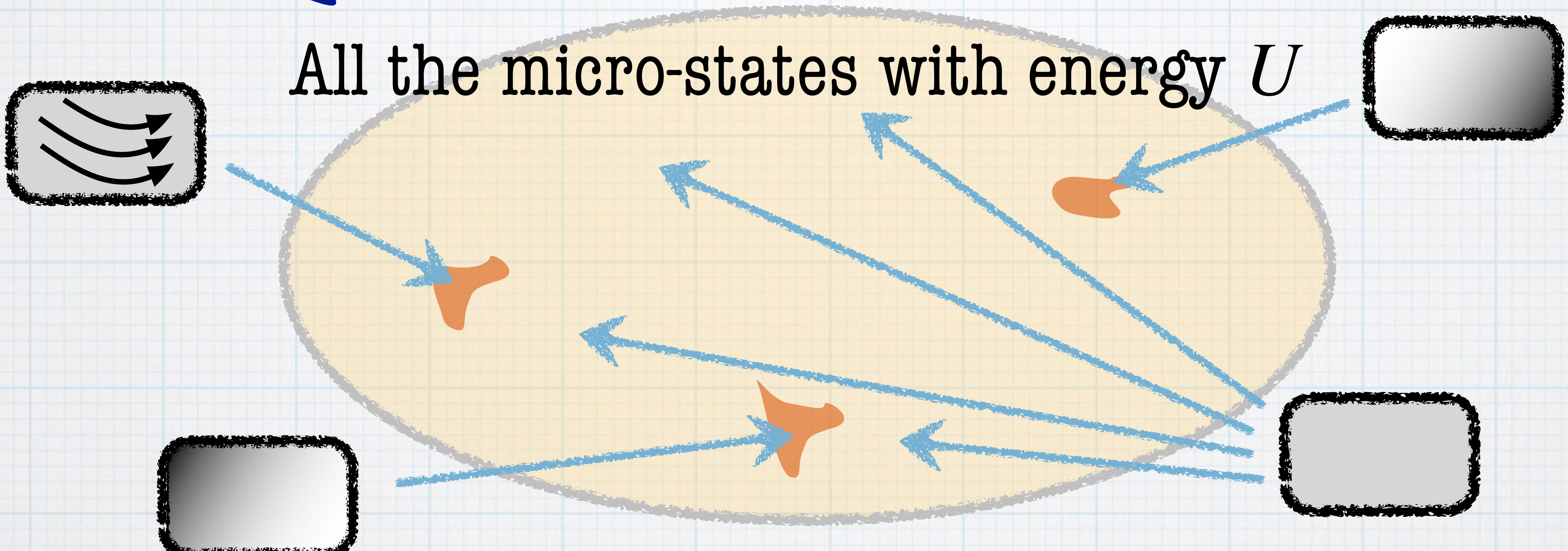
the positions and momenta of all the molecules

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 thermal equilibrium

Why does this work??
What is the underlying picture?

Typicality argument



FACT: In a macroscopic system, a great majority of microscopic states with energy U look identical from the macroscopic point of view

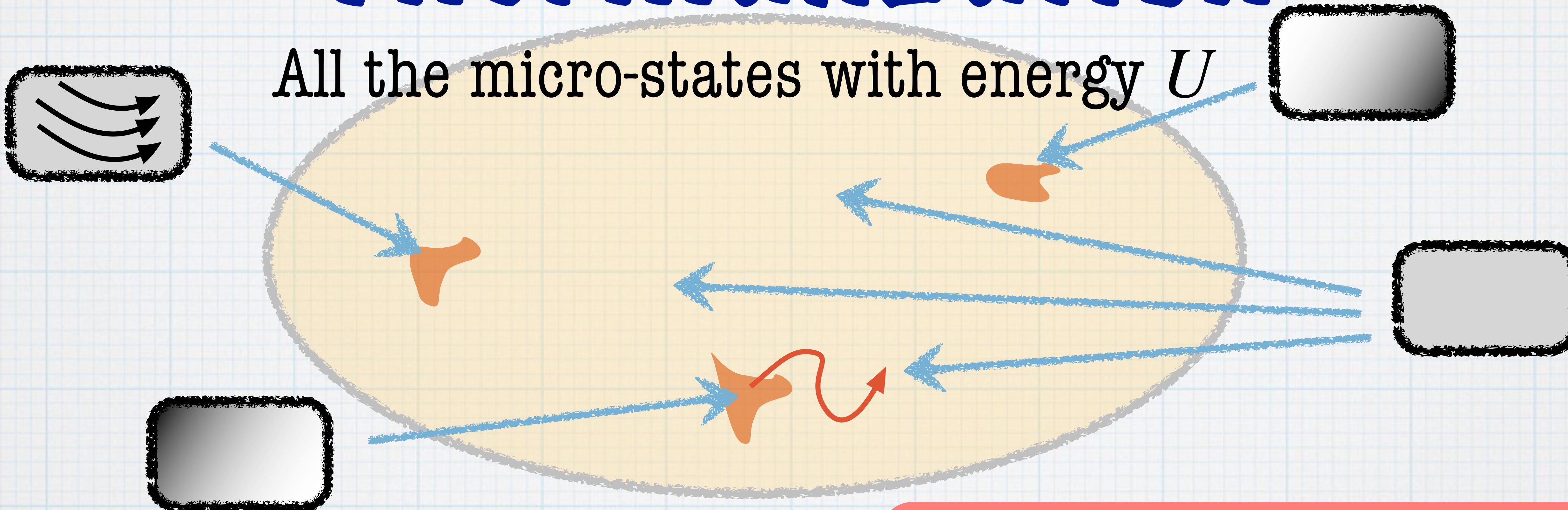
we shall prove this

POSTULATE: "thermal equilibrium" = common properties shared by these majority of states

thus the microcanonical ensemble works

A single microscopic state may fully represent thermal equilibrium!

Thermalization



we shall partially prove this

Non-equilibrium states: exceptional

thermalization

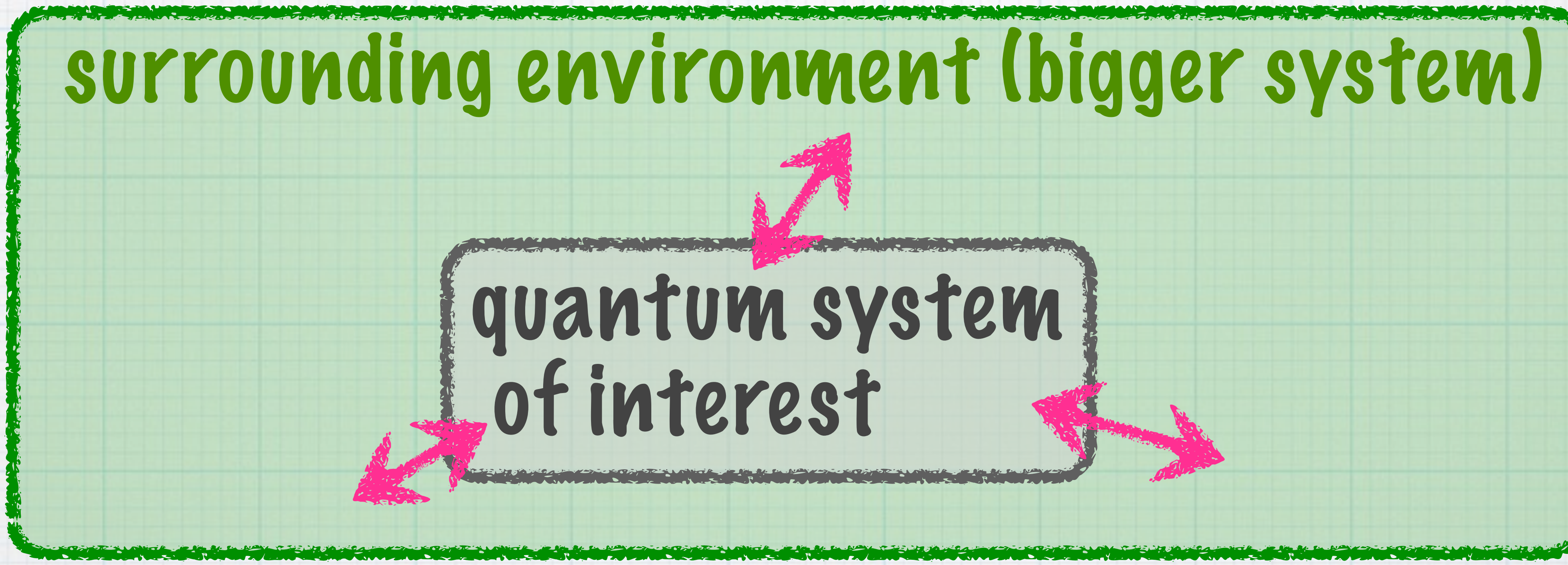
states in the overwhelming majority (thermal equilibrium)

Thermalization (= the approach to thermal equilibrium) is quite a robust phenomenon

Some remarks about the basic setting

Basic setting

Standard (and realistic) treatment



Our (obviously unrealistic) treatment

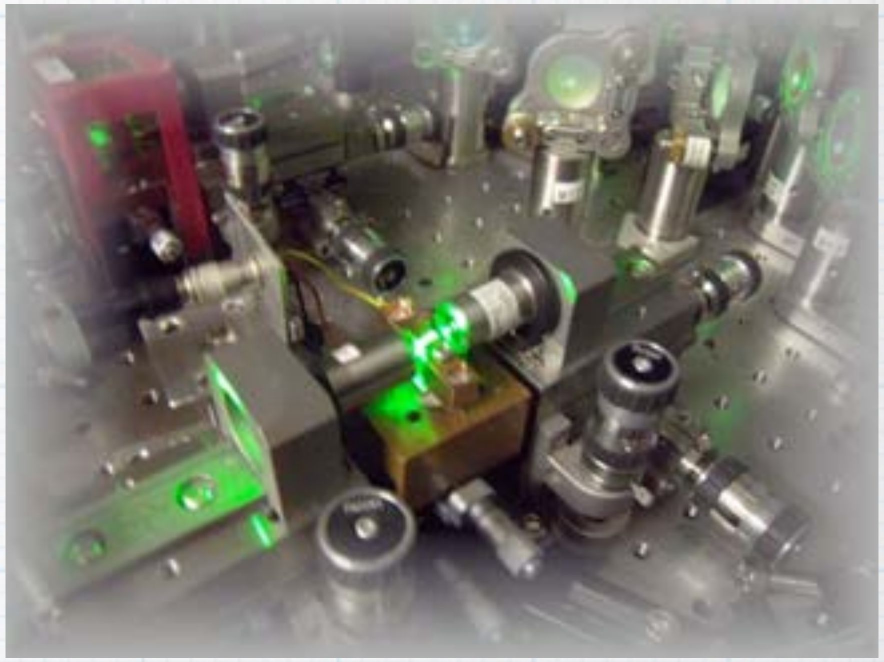
perfectly isolated from the outside world

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 can thermalize)

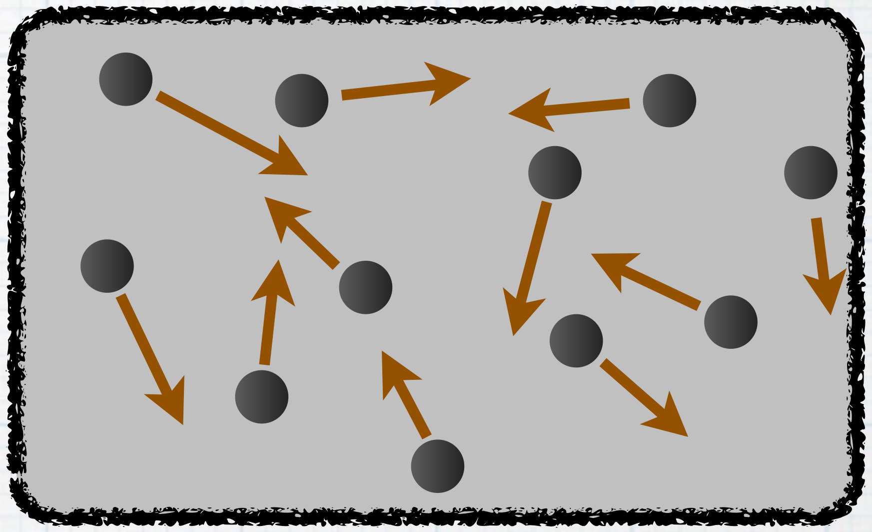
After that, we may study the effect played by the environment

Settings and main assumptions

The system

Isolated 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 eigenvalue and the normalized energy eigenstate

$$\hat{H}|\psi_j\rangle = E_j|\psi_j\rangle \qquad \langle\psi_j|\psi_j\rangle = 1$$

Suppose that one is interested (only) in n extensive quantities $\hat{M}_1, \ldots, \hat{M}_n$

independent of V

Microcanonical energy shell

Fix arbitrary u and small Δu, and consider the energy eigeneigenvalues such that

$$u - \Delta u \leq E_j/V \leq u$$

relabel j so that this corresponds to $j = 1, \ldots, D$

$$D \sim e^{\sigma_0 V}$$

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 $\mathcal{H}_{\mathrm{sh}}$

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

Pure state which represents thermal equilibrium

Extensive quantities $\hat{M}_1, \ldots, \hat{M}_n$

equilibrium value $m_i := \lim_{V\uparrow\infty} \dfrac{1}{V} \langle \hat{M}_i \rangle_{\mathrm{mc}}$

DEFINITION: A normalized pure state $|\varphi\rangle \in \mathcal{H}_{\mathrm{sh}}$, for some $V > 0$, represents thermal equilibrium if

$$\langle\varphi|\, \hat{P}\big[\, \big|\hat{M}_i/V - m_i\big| \ge \delta_i \,\big]\, |\varphi\rangle \le e^{-\alpha V}$$

for all $i = 1, \ldots, n$

projection

fixed const. (precision)

fixed const.

if one measures $\hat{M}_i/V$ in such $|\varphi\rangle$, then

$$\big|(\text{measurement result}) - m_i\big| \le \delta_i$$

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

Pure state which represents thermal equilibrium

Extensive quantities $\hat{M}_1, \ldots, \hat{M}_n$

equilibrium value $m_i := \lim_{V\uparrow\infty} \frac{1}{V} \langle \hat{M}_i \rangle_{\mathrm{mc}}$

if one measures $\hat{M}_i/V$ in such $|\varphi\rangle$, then

$$\big|(\text{measurement result}) - m_i\big| \le \delta_i$$

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

we almost certainly get the equilibrium value!

From $|\varphi\rangle$ we get complete information about the thermal equilibrium

$\boxed{|\varphi\rangle \text{ represents thermal equilibrium!}}$

Basic assumption

guarantees that the system is "healthy"

Extensive quantities $\hat{M}_i$ equilibrium value m_i precision δ_i

statement in statistical mechanics

THERMODYNAMIC BOUND (TDB):

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

$$\sum_{i=1}^{n} \Big\langle \hat{P}\big[\,|\hat{M}_i/V - m_i| \geq \delta_i\,\big] \Big\rangle_{\mathrm{mc}} \leq e^{-\gamma V}$$

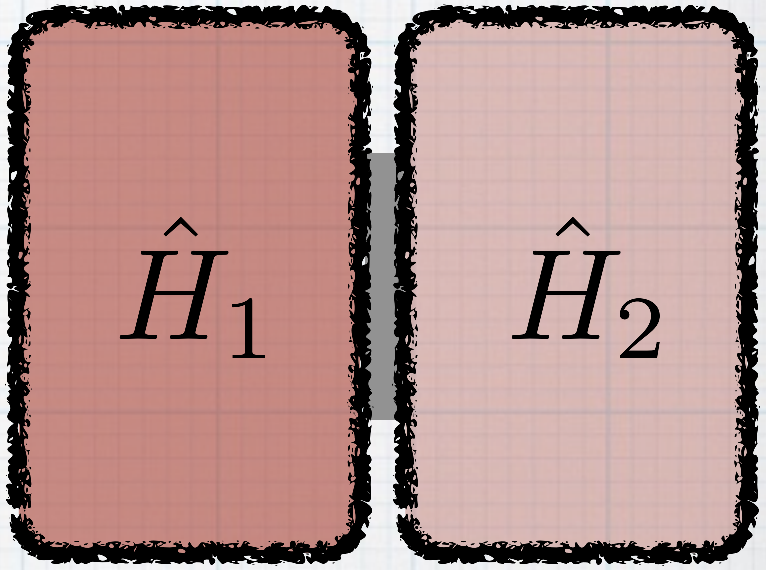
simply says large fluctuation is exponentially rare in the MC ensemble (large deviation upper bound)

expected to be valid in ANY uniform thermodynamic phase, but has been proved in limited situations

Example of TDB (1)

Two identical bodies in thermal contact

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{int}}$$



we focus on the energy difference

$$n = 1 \qquad \hat{M} = \hat{H}_1 - \hat{H}_2$$

THEOEM: Suppose that the system is not at the triple point. Then one has for any $\delta > 0$ that

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

with $\gamma \simeq \dfrac{\delta^2}{2k_{\text{B}}T^2 c(T)}$

proof: elementary method in the large deviation theory

Example of TDB (2)

General quantum spin chain

translation invariant short-range Hamiltonian and observables

$$\hat{H} = \sum_x \hat{h}_x \qquad \hat{M}_i = \sum_x \hat{m}_x^{(i)}$$

THEOEM: For any u and any $\delta_1, \ldots, \delta_n > 0$ there exists $\gamma > 0$ and one has

$$\sum_{i=1}^{n} \Big\langle \hat{P}\big[\,|\hat{M}_i/V - m_i| \ge \delta_i\,\big] \Big\rangle_{\mathrm{mc}} \le e^{-\gamma V}$$

for any V

corollary of the general theory of Y. Ogata's

Typicality of pure states which represent thermal equilibrium

Typicality of thermal equilibrium

overwhelming majority of states in the energy shell $\mathcal{H}_{\rm sh}$ represent thermal equilibrium (in a certain sense)

von Neumann 1929

Bocchieri, Loinger 1959

Llyoid 1988

Sugita 2006

Popescu, Short, Winter 2006

Goldstein, Lebowitz, Tunulkam Zanghi 2006

Reimann 2007

we shall formulate our version

Measure on $\mathcal{H}_{\rm sh}$

a state $\mathcal{H}_{\rm sh} \ni |\varphi\rangle = \sum_{j=1}^{D} \alpha_j \, |\psi_j\rangle$ with $\sum_{j=1}^{D} |\alpha_j|^2 = 1$

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

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

corresponding average

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

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

From the symmetry

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

Average over $\mathcal{H}_{\rm sh}$ 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 $\mathcal{H}_{\rm sh}$

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

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

average over infinitely many states in the shell

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

average over D energy eigenstates

Another way of looking at the microcanonical average

Typicality of thermal equilibrium

Assume Thermodynamic bound (TDB)

provable for some models

$$\langle\varphi|\,\hat{P}\big[\,\big|\hat{M}_i/V - m_i\big| \ge \delta_i\,\big]\,|\varphi\rangle =$$

$$= \Big\langle\,\hat{P}\big[\,\big|\hat{M}_i/V - m_i\big| \ge \delta_i\,\big]\,\Big\rangle_{\mathrm{mc}} \le e^{-\gamma V}$$

THEOREM: Choose a normalized $|\varphi\rangle \in \mathcal{H}_{\mathrm{sh}}$ randomly according to the uniform measure on the unit sphere. Then with probability $\ge 1 - e^{-(\gamma-\alpha)V}$

$$\langle\varphi|\,\hat{P}\big[\,\big|\hat{M}_i/V - m_i\big| \ge \delta_i\,\big]\,|\varphi\rangle \le e^{-\alpha V}$$

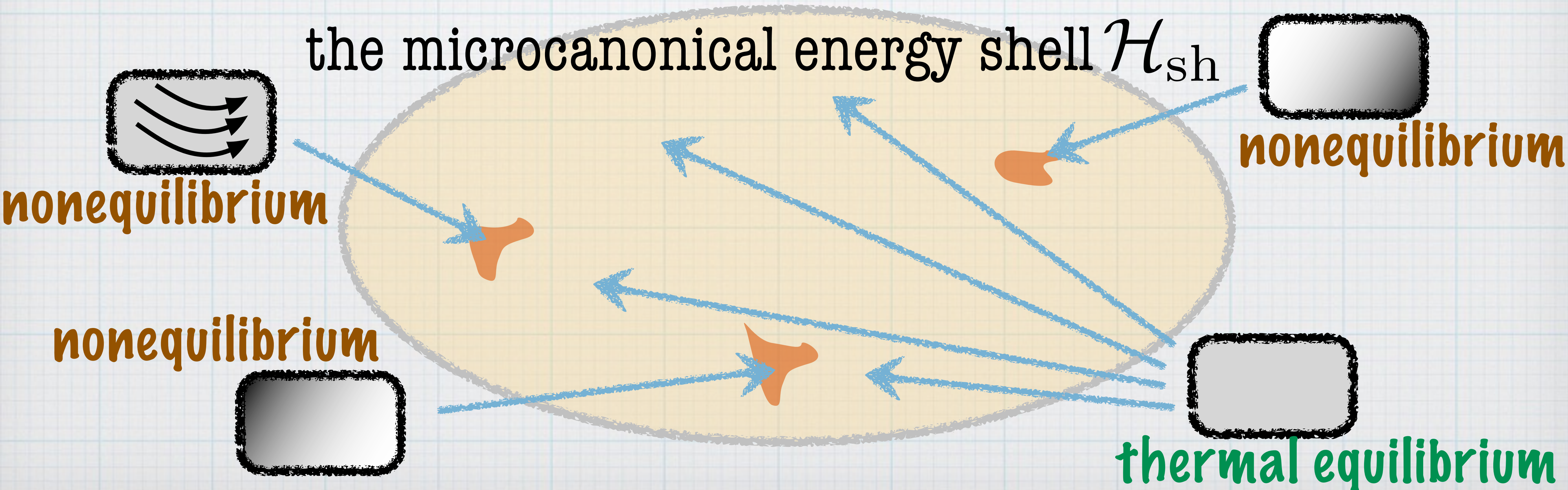
for each $i = 1, \ldots, n$

Almost all pure states $|\varphi\rangle \in \mathcal{H}_{\mathrm{sh}}$ represent thermal equilibrium!!

Typicality of thermal equilibrium

Almost all pure states $|\varphi\rangle \in \mathcal{H}_{\rm sh}$ represent thermal equilibrium!!

FACT: macroscopically, a great majority of states with the same energy look identical
POSTULATE: they correspond to thermal equilibrium



Thermalization
or
the approach to thermal equilibrium

Question

initial state $|\varphi(0)\rangle \in \mathcal{H}_{\rm sh}$

unitary time-evolution $|\varphi(t)\rangle = e^{-i\hat{H}t}|\varphi(0)\rangle$

Does $|\varphi(t)\rangle$ approach thermal equilibrium?

numerical

Jensen, Shanker 1985

Satio, Takesue, Miyashita 1996

many recent works

mathematical

von Neumann 1929

Tasaki 1998

Reimann 2008

Linden, Popescu, Short, Winter 2009

Goldstein, Lebowitz, Mastrodonato, Tumulka, Zanghi 2010

many recent works

we shall formulate our version

Basic idea

initial state $\mathcal{H}_{\rm sh} \ni |\varphi(0)\rangle = \sum_{j=1}^{D} c_j\,|\psi_j\rangle$

time-evolution

$$|\varphi(t)\rangle = e^{-i\hat{H}t}|\varphi(0)\rangle = \sum_{j=1}^{D} c_j\, e^{-iE_j t}\,|\psi_j\rangle$$

expectation value of the projection $\hat{P}_{\geq} = \hat{P}\big[\,|\hat{M}_i/V - m_i| \geq \delta_i\,\big]$

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

oscillates (assume no degeneracy)

long-time average

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

related to $\langle\hat{P}_{\geq}\rangle_{\rm mc}$ and very small?

Assumptions

provable for some models

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

☑ thermodynamic bound (TDB) $\sum_{i=1}^{n} \left\langle \hat{P}\left[\,|\hat{M}_i/V - m_i| \geq \delta_i\,\right] \right\rangle_{\mathrm{mc}} \leq e^{-\gamma V}$

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

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

☑ coefficients are mildly distributed in the sense that

$$D_{\mathrm{eff}} := \left(\sum_{j=1}^{D} |c_j|^4\right)^{-1} \geq e^{-\eta V} D$$

with $0 < \eta < \gamma$

the effective number of contributing levels

in general $D \geq D_{\mathrm{eff}} \geq 1$

There are plenty of $|\varphi(0)\rangle$ satisfying the condition

Main theorem

provable for some models

- ☑ no degeneracy $j \neq j' \Rightarrow E_j \neq E_{j'}$
- ☑ thermodynamic bound (TDB) $\sum_{i=1}^{n} \Bigl\langle \hat{P}\bigl[\,|\hat{M}_i/V - m_i| \geq \delta_i\,\bigr] \Bigr\rangle_{\mathrm{mc}} \leq e^{-\gamma V}$
- ☑ coefficients are mildly distributed in the sense that

$$D_{\mathrm{eff}} := \Bigl(\sum_{j=1}^{D} |c_j|^4\Bigr)^{-1} \geq e^{-\eta V} D$$

with $0 < \eta < \gamma$

THEOREM: For any initial state $|\varphi(0)\rangle$ satisfying the above condition, $|\varphi(t)\rangle$ represents thermal equilibrium for most t in the long run

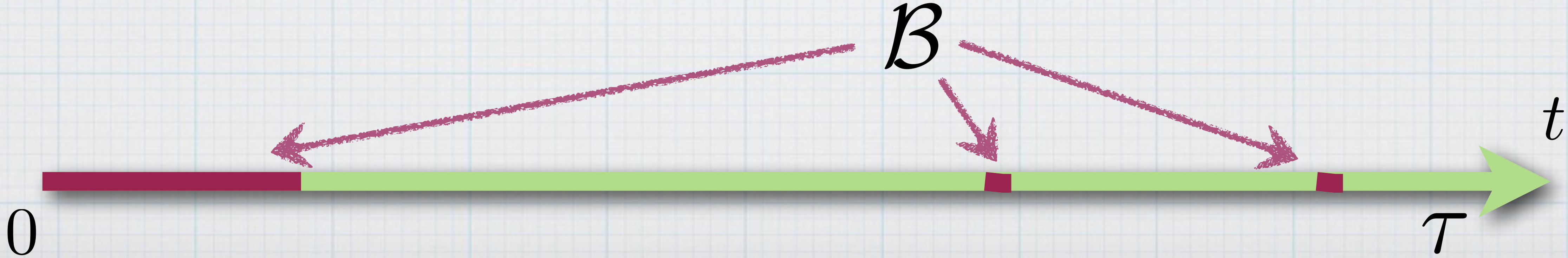
“for most t in the long run”

THEOREM: For any initial state $|\varphi(0)\rangle$ satisfying the above condition, $|\varphi(t)\rangle$ represents thermal equilibrium for most t in the long run

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

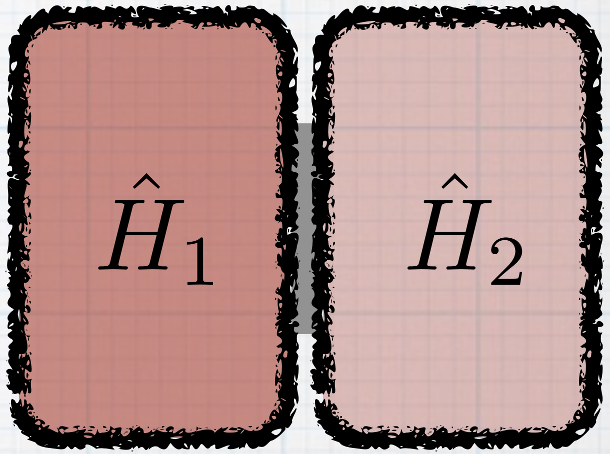
$$\langle\varphi(t)|\, \hat{P}\Big[\, \big|\hat{M}_i/V - m_i\big| \geq \delta_i \,\Big]\, |\varphi(t)\rangle \leq e^{-\alpha V}$$

for each $i = 1, \ldots, n$

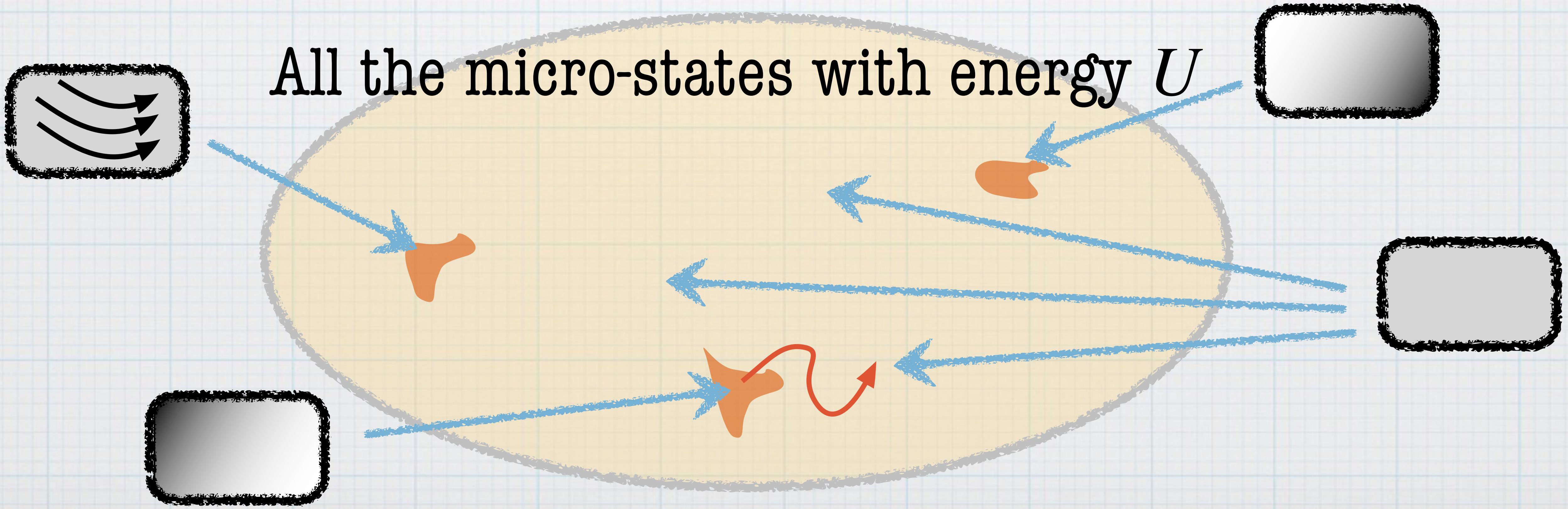


Thermalization

Thermalization (based only on the unitary time evolution) has been established for a class of initial states in concrete models!



Conjecture: "realistic" (noneq.) initial states satisfy the condition for the theorem (not yet proven!)



Summary

- ☑ We have defined the notion of pure states representing thermal equilibrium
- ☑ TYPICALITY: In a macroscopic quantum system, an overwhelming majority of pure states (in the energy shell) represent thermal equilibrium
- ☑ THERMALIZATION: With suitable assumptions, one can show that a purely quantum mechanical time-evolution in an isolated system brings the system towards thermal equilibrium

Remaining issues

- ☑ Show that "realistic" noneq. initial states in concrete models satisfy the condition for the theorem
- ☑ Time scale of thermalization