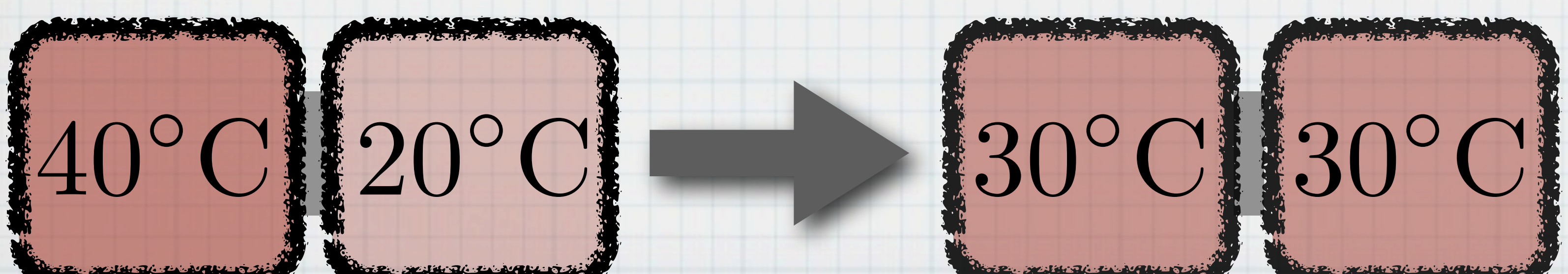
What is thermal equilibrium and how do we get there?

Hal Tasaki

QMath 13, Oct. 9, 2016, Atlanta



arXiv:1507.06479 and more

about the talk

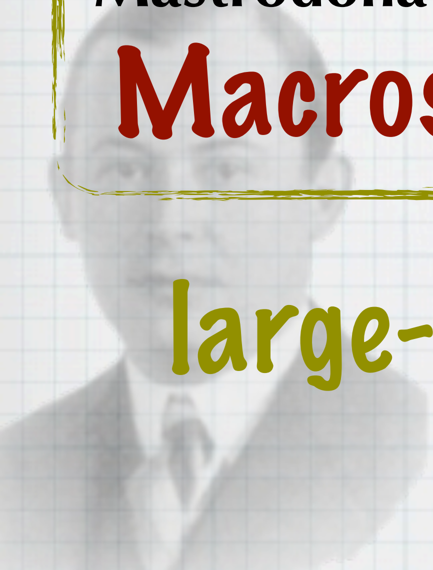
☑ Foundation of equilibrium statistical mechanics based on pure quantum mechanical states in macroscopic isolated quantum systems

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

Macroscopic view point

Tasaki 1998
Reimann 2008
Linden, Popescu, Short, Winter 2009

Equilibration from large "effective dimension"

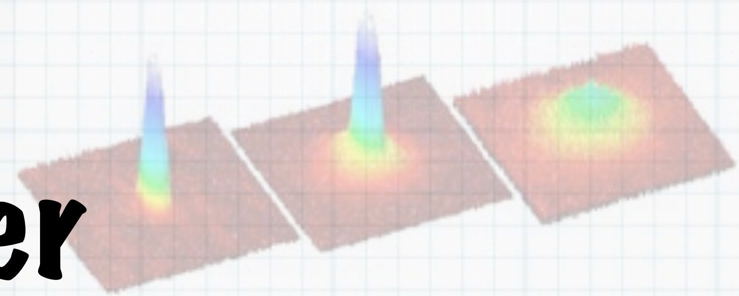


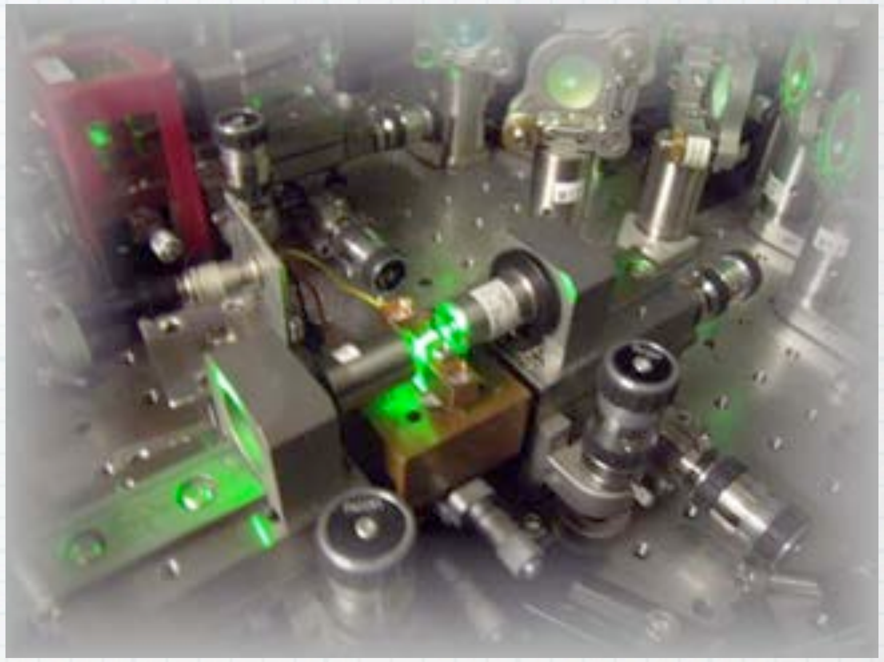
large-deviation theory

☑ (Hopefully) the simplest picture for thermalization (approach to thermal equilibrium)

we do not use ETH (energy eigenstate thermalization hypothesis)

Why isolated quantum systems?





Fashionable answer

We can realize isolated quantum systems in ultra cold atoms

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

Old-fashioned answer

This is still a very fundamental study

We wish to learn what isolated systems can do (e.g., whether they can thermalize)

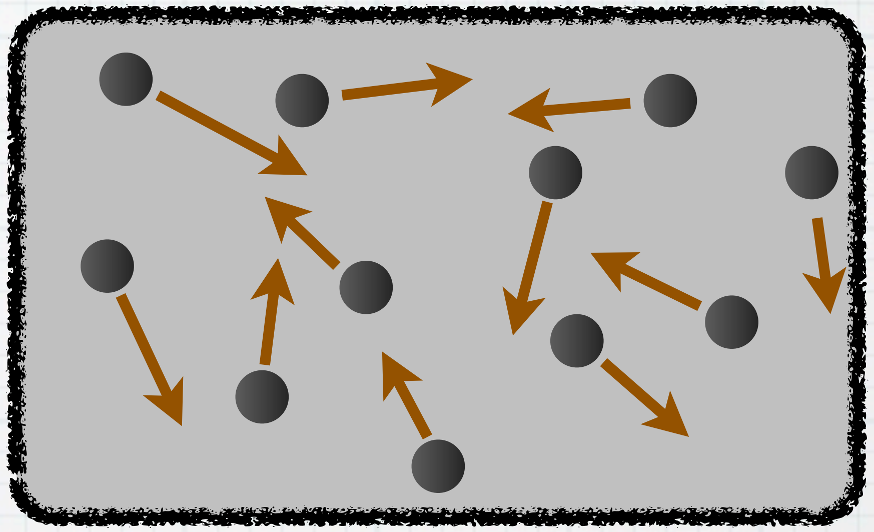
After that, we may study the effect played by the environment

Settings and main assumptions

The system

Isolated quantum system in a large volume V

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



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

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 in a single extensive quantity $\hat{M}$ with $[\hat{M}, \hat{H}] \neq 0$ in general

extension to n quantities $\hat{M}_1, \ldots, \hat{M}_n$ is easy

Examples

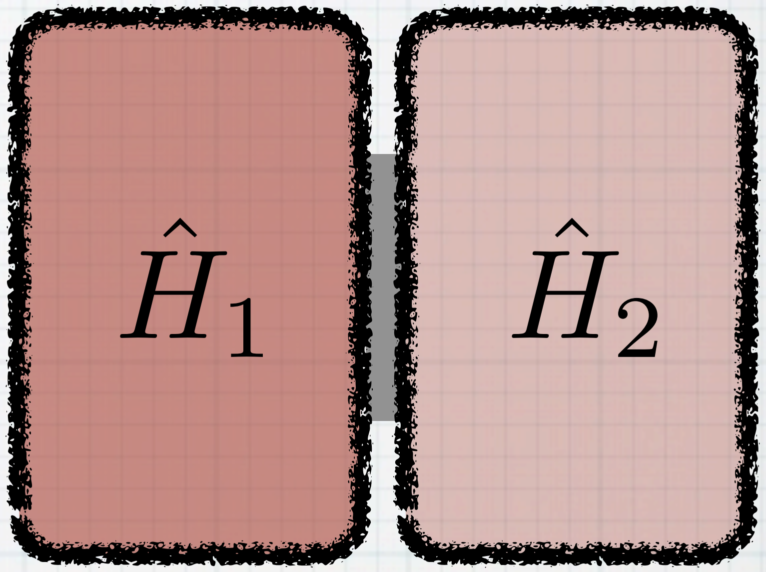
Two identical bodies in thermal contact

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

acts on the boundary

the energy difference

$$\hat{M} = \hat{H}_1 - \hat{H}_2$$



General quantum spin chain

translationally invariant short-range Hamiltonian and an observable

$$\hat{H} = \sum_{i=1}^{L} \hat{h}_i \qquad \hat{M} = \sum_{i=1}^{L} \hat{m}_i$$

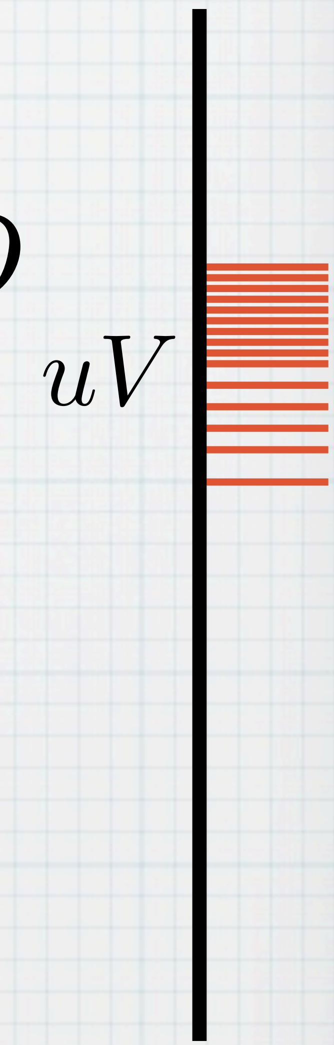
Microcanonical energy shell

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

$$u - \Delta u \le E_j/V \le u + \Delta u$$

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

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



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

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

microcanonical energy shell $\mathcal{H}_{\mathrm{sh}}$

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

A pure state which represents thermal equilibrium

extensive quantity of interest $\hat{M}$

equilibrium value $m := \lim_{V\uparrow\infty} \langle \hat{M}/V \rangle^u_{\mathrm{mc}}$

projection onto "nonequilibrium part" (in $\mathcal{H}_{\mathrm{tot}}$)

fixed const. (precision)

$$\hat{P}_{\mathrm{neq}} := \hat{P}\big[\,|\hat{M}/V - m| \ge \delta\,\big]$$

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

$$\langle\varphi|\,\hat{P}_{\mathrm{neq}}\,|\varphi\rangle \le e^{-\alpha V}$$

fixed const.

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

$$\big|(\text{measurement result}) - m\big| \le \delta$$

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

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

Basic assumption

which guarantees that the system is "healthy"

$\hat{P}_{\mathrm{neq}}$ projection onto "nonequilibrium part"

statement in statistical mechanics

THERMODYNAMIC BOUND (TDB):
There is a constant $\gamma > 0$, and one has, for any V

$$\langle \hat{P}_{\mathrm{neq}} \rangle^{u}_{\mathrm{mc}} \le e^{-\gamma V}$$

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

expected to be valid in ANY uniform thermodynamic phase, and can be proven in many cases including the two examples

Examples

Two identical bodies in thermal contact

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

acts on the boundary

the energy difference

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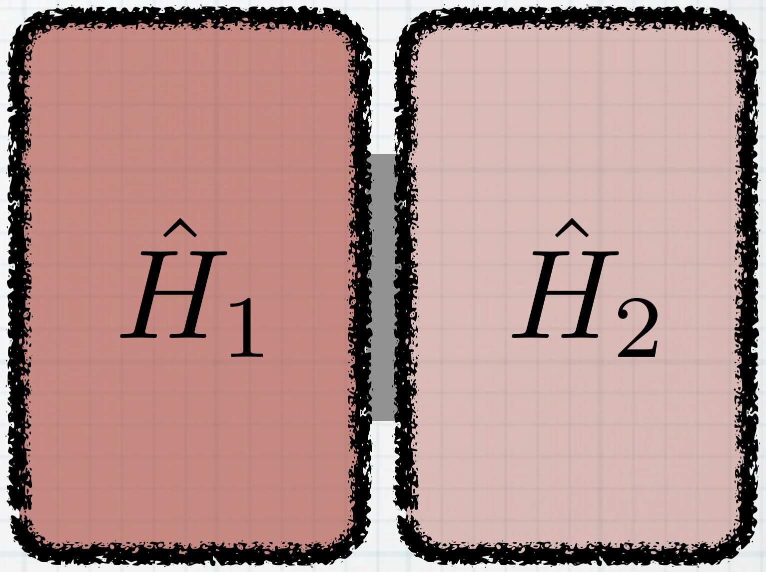

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translationally invariant short-range Hamiltonian and an observable

$$\hat{H} = \sum_{i=1}^{L} \hat{h}_i \qquad \hat{M} = \sum_{i=1}^{L} \hat{m}_i$$

Examples

Two identical bodies in thermal contact

$$\langle \hat{P}[\,|(\hat{H}_1 - \hat{H}_2)/V| \geq \delta\,]\rangle_{\mathrm{mc}}^{u} \leq e^{-\gamma V}$$

the e

$$\hat{M} = \hat{H}_1$$

thermodynamic bound can be proved easily (except at the triple point) using classical techniques

General quantum spin chain

translationally invariant short-range Hamiltonian

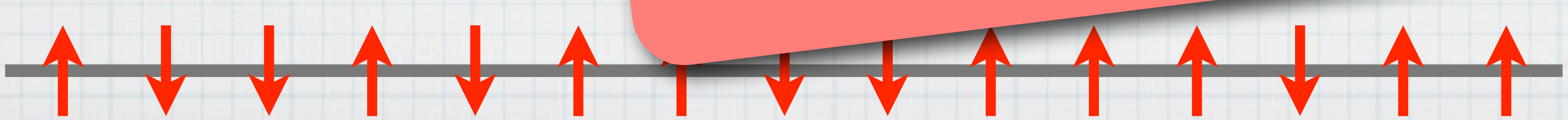
and an observable

$$\langle \hat{P}[\,|(\hat{M}/V) - m| \geq \delta\,]\rangle_{\mathrm{mc}}^{u} \leq e^{-\gamma V}$$

$$\hat{H} = \sum$$

$$i=1$$

thermodynamic bound follows as a corollary of the general theory of Ogata 2010



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
Llyoid 1988
Sugita 2006
Popescu, Short, Winter 2006
Goldstein, Lebowitz, Tunulkam Zanghi 2006
Reimann 2007

we shall formulate our version
(proof is standard and trivial)

Haar 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

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

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

From the symmetry $\quad \overline{\alpha_j^* \alpha_k} = \dfrac{1}{D} \, \delta_{j,k}$

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

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

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

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

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

average over infinitely many states in the shell

average over D energy eigenstates

Another way of looking at the microcanonical average

Typicality of thermal equilibrium

Assume Thermodynamic bound (TDB)

provable for many models

$$\overline{\langle\varphi|\hat{P}_{\rm neq}|\varphi\rangle} = \langle\hat{P}_{\rm neq}\rangle^{u}_{\rm mc} \le e^{-\gamma\,V}$$

Markov inequality

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

$$\langle\varphi|\,\hat{P}_{\rm neq}\,|\varphi\rangle \le e^{-\alpha\,V}$$

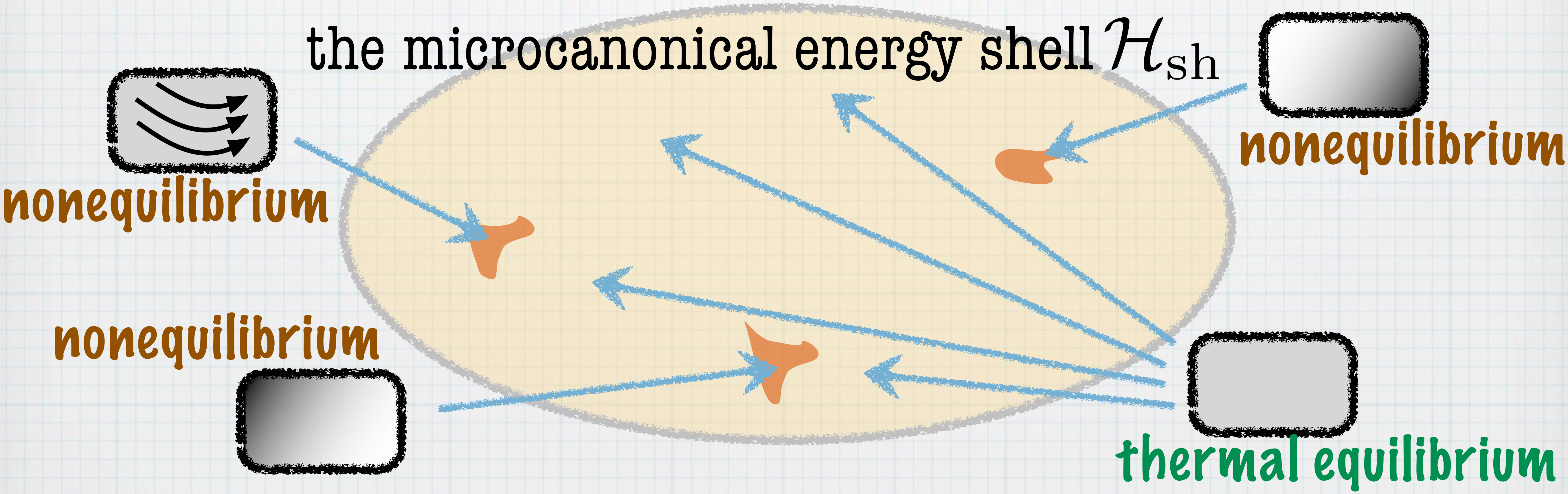
the pure state $|\varphi\rangle$ represents thermal equilibrium

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

What is thermal equilibrium?

Thermal equilibrium is a typical property shared by the majority of (pure) states in the energy shell

Almost all pure states (with respect to the Haar measure) $|\varphi\rangle \in \mathcal{H}_{\rm sh}$ represent thermal equilibrium



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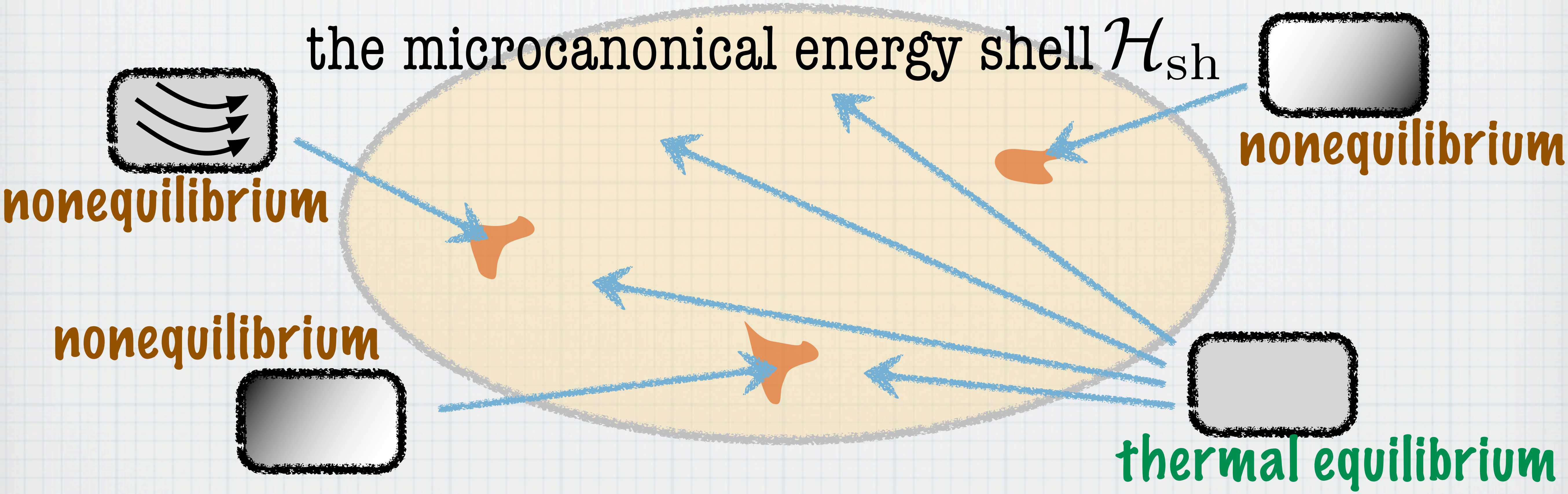


How do we get there?

Thermalization
or
the approach to thermal equilibrium

Question

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

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
Rigol, Dunjko, Olshanni 2008

many 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 possibly the simplest version which is directly related to macroscopic physics

Derivation (easy)

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

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 on nonequilibrium

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

oscillates (assume no degeneracy)

long-time average

"diagonal ensemble"

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

$$\leq \sqrt{\sum_j |c_j|^4 \sum_j \langle\psi_j|\hat{P}_{\mathrm{neq}}|\psi_j\rangle^2} \leq \sqrt{\sum_j |c_j|^4 \, \mathrm{Tr}_{\mathcal{H}_{\mathrm{sh}}}[\hat{P}_{\mathrm{neq}}]}$$

$$\lim_{\tau\uparrow\infty}\frac{1}{\tau}\int_0^\tau dt\langle\varphi(t)|\hat{P}_{\rm neq}|\varphi(t)\rangle \le \sqrt{\sum_j |c_j|^4\,\mathrm{Tr}_{\mathcal{H}_{\rm sh}}[\hat{P}_{\rm neq}]}$$

effective dimension

of $|\varphi(0)\rangle$ with respect to $\hat{H}$

$$D_{\rm eff} := \Big(\sum_{j=1}^{D}|c_j|^4\Big)^{-1}$$

Reimann 2008, Linden, Popescu, Short, Winter 2009

the effective number of energy eigenstates contributing to the expansion $|\varphi(0)\rangle = \sum_{j=1}^{D} c_j\,|\psi_j\rangle$

$$1 \le D_{\rm eff} \le D$$

thermodynamic bound

$$\frac{1}{D}\mathrm{Tr}_{\mathcal{H}_{\rm sh}}[\hat{P}_{\rm neq}] = \langle\hat{P}_{\rm neq}\rangle^{u}_{\rm mc} \le e^{-\gamma V}$$

$$\lim_{\tau\uparrow\infty}\frac{1}{\tau}\int_0^\tau dt\langle\varphi(t)|\hat{P}_{\rm neq}|\varphi(t)\rangle \le \Big(\frac{D}{D_{\rm eff}}\Big)^{1/2} e^{-\gamma V/2}$$

exponentially small if $D_{\rm eff}$ is large enough

Thermalization

provable for many models

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

☑ thermodynamic bound (TDB) $\langle \hat{P}_{\mathrm{neq}} \rangle^{u}_{\mathrm{mc}} \leq e^{-\gamma V}$

☑ "effective dimension" is large enough

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

with small $\eta > 0$

coefficients in the expansion $|\varphi(0)\rangle = \sum_{j=1}^{D} c_j \, |\psi_j\rangle$ are mildly distributed

essential assumption!

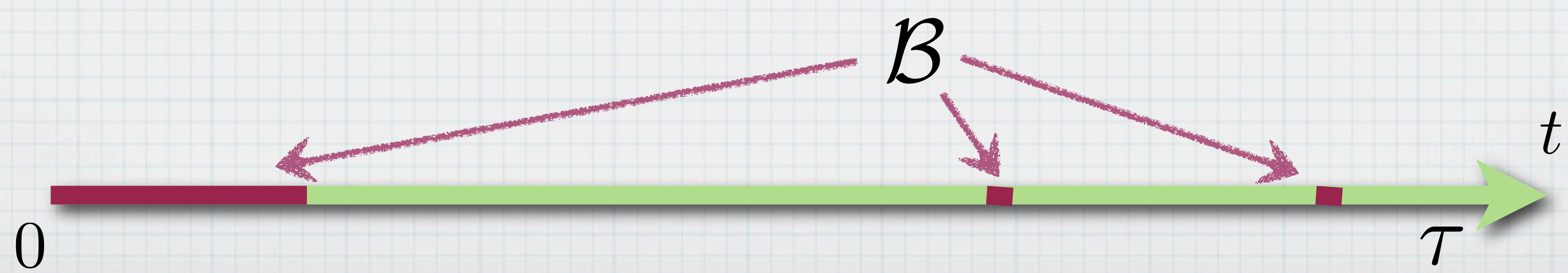
THEOREM: For any initial state $|\varphi(0)\rangle$ satisfying the above condition, $|\varphi(t)\rangle$ represents thermal equilibrium for most t in the long run

"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 $|\mathcal{B}|/\tau \le e^{-\nu V}$ such that for any $t \in [0, \tau] \backslash \mathcal{B}$

$$\langle \varphi(t)| \hat{P}_{\mathrm{neq}} |\varphi(t)\rangle \le e^{-\alpha V}$$

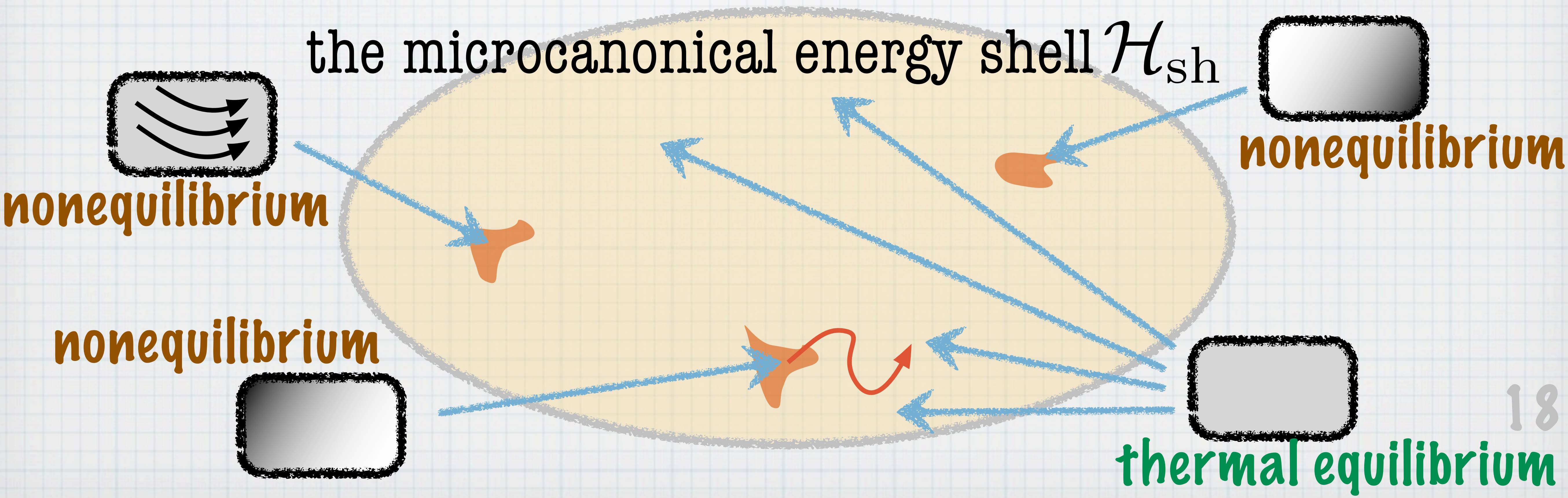


How do we get there?

A pure state evolving under the unitary time evolution thermalizes, i.e., represents thermal equilibrium for most t in the long run

The main assumption is that the effective dimension of the initial state is large enough

(exactly the same conclusion for mixed initial states)



On the effective dimension of “easily preparable” initial states

Conjecture

CONJECTURE: For most realistic Hamiltonian of a macroscopic system, most "easily preparable" initial state (with energy density u) has an effective dimension D_{eff} not much smaller than the dimension D of the energy shell, and hence thermalizes.

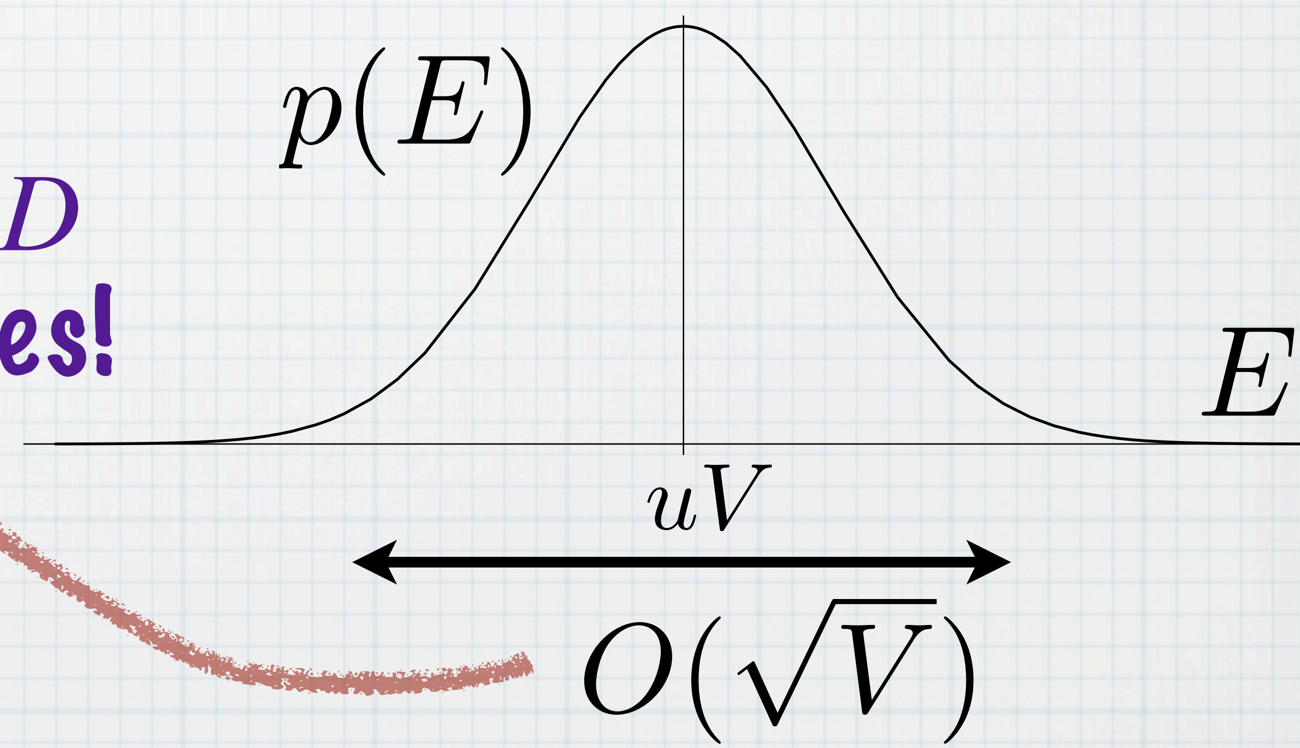
we still don't know how to characterize "easily preparable" states

but product states, Gibbs states of a different Hamiltonian, FCS=MPS, ... are easily preparable

A theoretical support for large D_{eff}

- ☑ Let the initial state $\hat{\rho}(0)$ be a sufficiently disordered state , e.g., a product state or a Gibbs state (of a different Hamiltonian) at high enough temperatures
- ☑ Quantum Central Limit Theorem : In such a state $\hat{\rho}(0)$, the probability distribution of the energy (eigenvalues of $\hat{H}$) converges to the Gaussian distribution as $V \uparrow \infty$

there are almost D energy eigenstates!



We expect $D_{\mathrm{eff}} \sim D$

$$D_{\mathrm{eff}} := \left(\sum_{j=1}^{D} \langle \psi_j | \hat{\rho}(0) | \psi_j \rangle^2 \right)^{-1}$$

Integrable vs non-integrable Hamiltonians

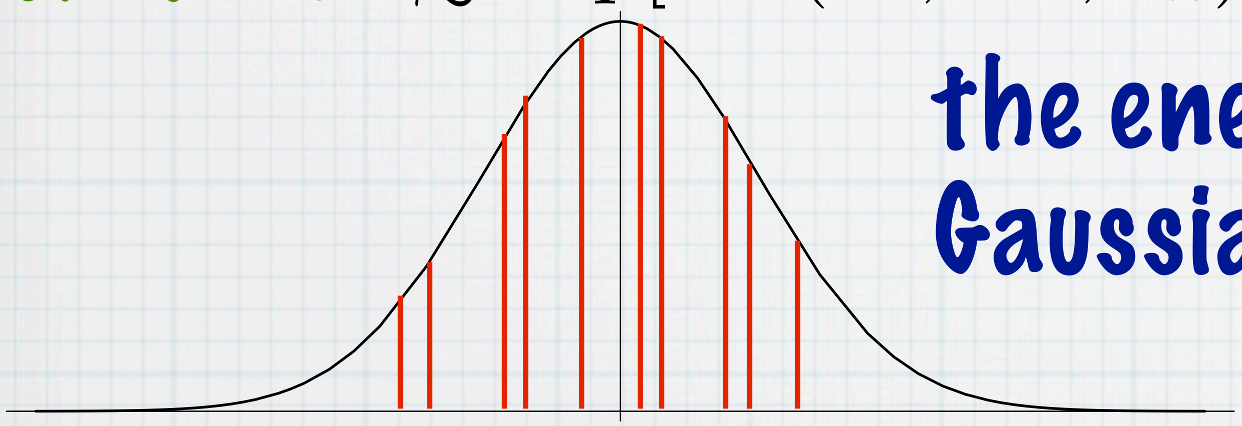
Rigol 2016

☑ If the Hamiltonian $\hat{H}$ is integrable, one has $D_{\text{eff}} \ll D$ for most sufficiently disordered initial states (there is equilibration, but not to thermal equilibrium)

conserved extensive quantities $\hat{A}_1, \hat{A}_2, \ldots, \hat{A}_n$

$\hat{A}_i/V \simeq \bar{a}_i$ in the initial state (QCT or Q Large-Deviation)

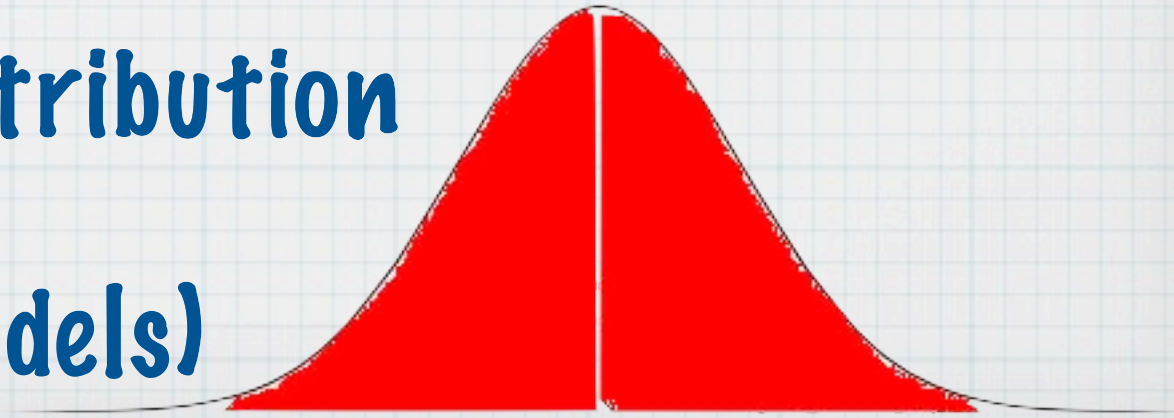
then $D_{\text{eff}} \lesssim \exp[V\sigma(\bar{a}_1, \ldots, \bar{a}_n)] \ll \exp[V \max_{a_1,\ldots,a_n} \sigma(a_1, \ldots, a_n)] \sim D$



the energy distribution converges to Gaussian, but is extremely sparse

similar situation is expected for many-body localization

☑ If $\hat{H}$ is non-integrable, the distribution is dense, and one has $D_{\text{eff}} \sim D$ (at least numerically, for some models)



Conjecture (refined)

CONJECTURE: For a non-random non-integrable Hamiltonian of a macroscopic system, most "easily preparable" initial state (with energy density u) has an effective dimension D_{eff} not much smaller than the dimension D of the energy shell, and hence thermalizes.

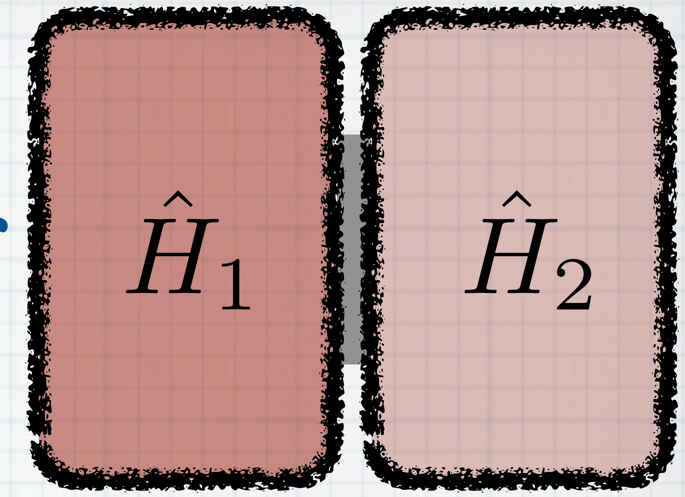
$$D_{\mathrm{eff}} := \Big(\sum_{j=1}^{D} \langle\psi_j|\hat{\rho}(0)|\psi_j\rangle^2\Big)^{-1} \quad D_{\mathrm{eff}} := \Big(\sum_{j=1}^{D} |c_j|^4\Big)^{-1}$$

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

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

- ☐ Is this true?? (Numerical works are not yet conclusive)
- ☐ It must be extremely difficult to justify this rigorously (we only have very artificial and simple examples)

Example



Toy model for two identical bodies in contact

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

$$\hat{H}_1|\xi_k\rangle = \epsilon_k|\xi_k\rangle \quad \hat{H}_2|\eta_\ell\rangle = \epsilon_\ell|\eta_\ell\rangle$$

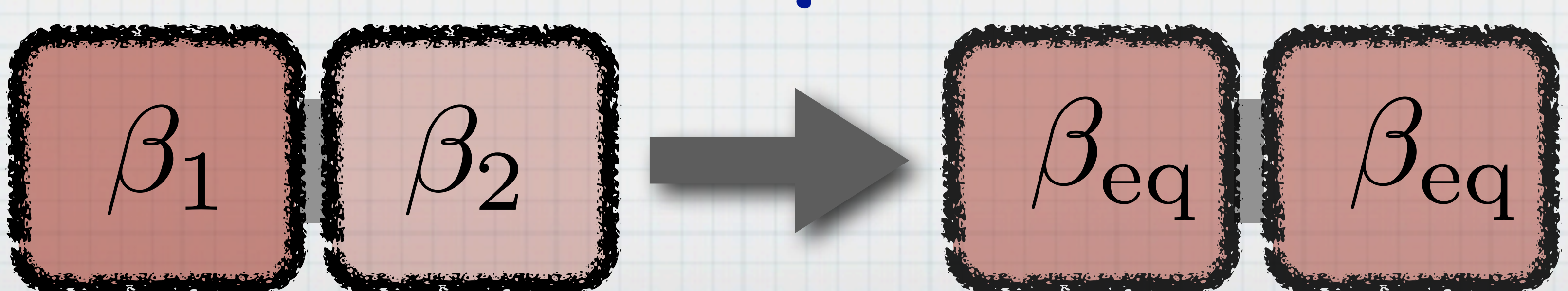
$$\hat{H}_{\rm int}|\xi_k\rangle|\eta_\ell\rangle = \varepsilon \sum_{\tau,\tau'=\pm 1} |\xi_{k+\tau}\rangle|\eta_{\ell+\tau'}\rangle$$

$|\psi_j\rangle = \sum_{k,\ell} c_{j;k,\ell}|\xi_k\rangle|\eta_\ell\rangle$ **where** $|c_{j;k,\ell}|$ **are dominant and comparable for** k, ℓ **with** $|E_j - (\epsilon_k + \epsilon_\ell)| \lesssim \varepsilon$

We can show $D_{\rm eff} \sim D$ **for** $\hat{\rho}(0) = \hat{\rho}^{\rm Gibbs}_{\beta_1} \otimes \hat{\rho}^{\rm Gibbs}_{\beta_2}$

an easily preparable initial state

We can shown that the system thermalizes!



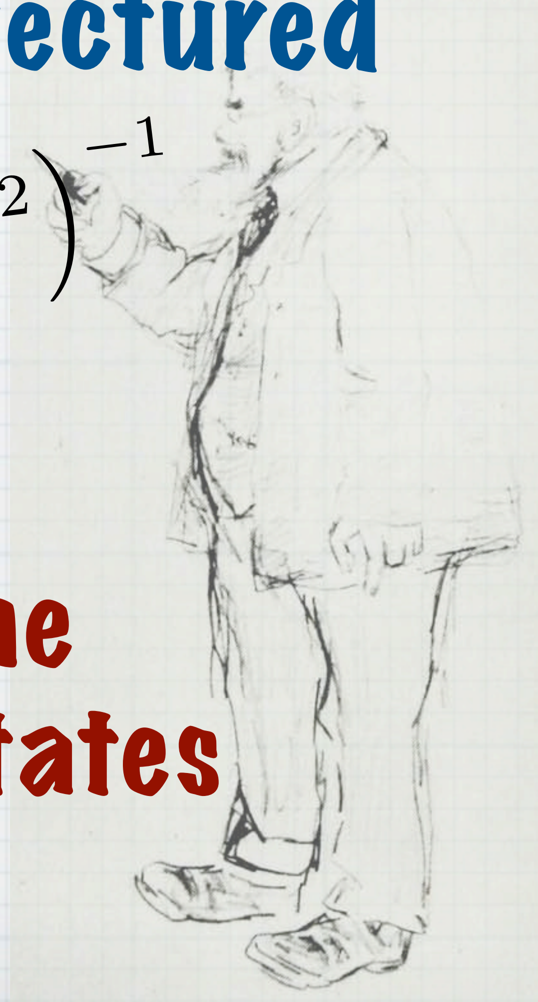
What is thermal equilibrium?

- ☑ Typical property of states in the energy shell
- ☑ Most pure states represent thermal equilibrium

How do we get there?

- ☑ Initial states with large effective dimension thermalizes only by unitary time evolution
- ☐ "Easily preparable" initial states are conjectured to have large effective dimension

$$D_{\mathrm{eff}} := \left(\sum_{j=1}^{D} \langle \psi_j | \hat{\rho}(0) | \psi_j \rangle^2 \right)^{-1}$$



Remaining issues

- ☐ Verify (partially) the conjecture about the effective dimension of "easily preparable" states
- ☐ Time scale of thermalization

related issues: 1

Energy Eigenstate Thermalization Hypothesis (ETH)

$\langle\psi_j|\hat{P}_{\rm neq}|\psi_j\rangle \le e^{-\kappa V}$ for any $j = 1, \ldots, D$

each energy eigenstate $|\psi_j\rangle$ represents thermal equilibrium

von Neumann 1929, Deutsch 1991, Srednicki 1994, and many more

THEOREM: For **ANY** initial state $|\varphi(0)\rangle \in \mathcal{H}_{\rm sh}$, $|\varphi(t)\rangle$ represents thermal equilibrium for most t in the long run

- ☑ The result is strong but probably it is not necessary to cover ANY initial states
- ☑ It is extremely difficult to verify the assumption in nontrivial quantum many body systems

related issues: 2

Time scale of thermalization: first step

von Neumann's random Hamiltonian $\hat{H}=\hat{U}\hat{H}_0\hat{U}^\dagger$

$\hat{H}_0$ fixed Hamiltonian $\hat{U}$ random unitary on $\mathcal{H}_{\rm sh}$

THEOREM: With probability close to 1, for ANY initial state $|\varphi(0)\rangle\in\mathcal{H}_{\rm sh}$ and any τ, we have

$$\tau^{-1}\int_0^\tau dt\langle\varphi(t)|\hat{P}_{\rm neq}|\varphi(t)\rangle\lesssim\beta/\tau$$

Goldstein, Hara, Tasaki 2015

Out-of-Time-Ordered (OTO) correlator in the MC ensemble

$$\overline{\langle W(t)VW(t)V\rangle}=|\phi(t)|^4\langle WVWV\rangle+2\{\phi(2t)\{\phi(-t)\}^2+\phi(-2t)\{\phi(t)\}^2-2|\phi(t)|^4\}\langle WV\rangle^2$$

$$\phi(t)=D^{-1}\sum_{j=1}^{D}e^{iE_jt}\qquad|\phi(t)|^2=\{1+(t/\beta)^2\}^{-1}$$

- ☑ The only time scale is the Boltzmann time $h/(k_{\rm B}T)$
- ☑ Only limited aspect of time-dependence in many-body quantum systems is captured in this approach

Reimann 2016

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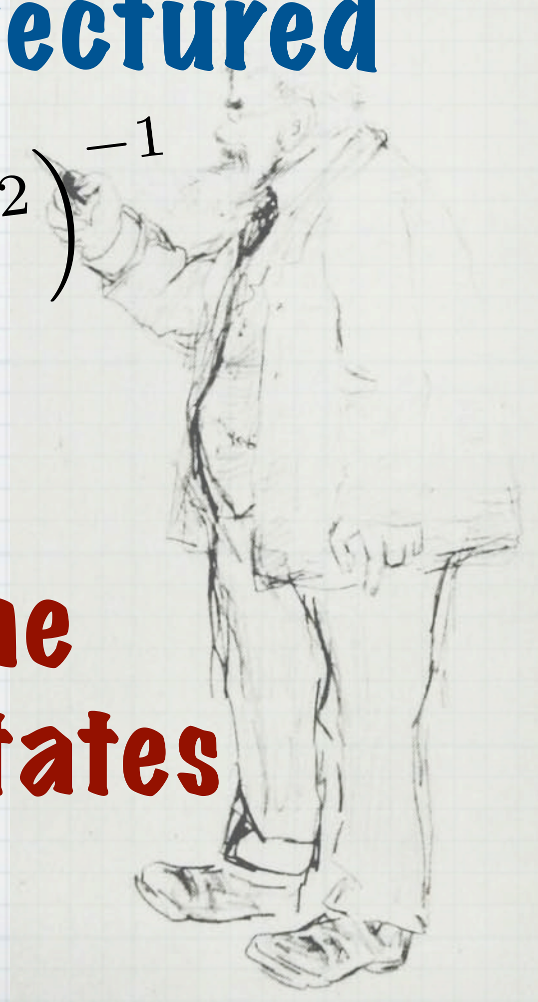

Remaining issues

- ☐ Verify (partially) the conjecture about the effective dimension of "easily preparable" states
- ☐ Time scale of thermalization