illustration by いらすとや

Nature abhors a vacuum

A simple rigorous example of thermalization in an isolated macroscopic quantum system

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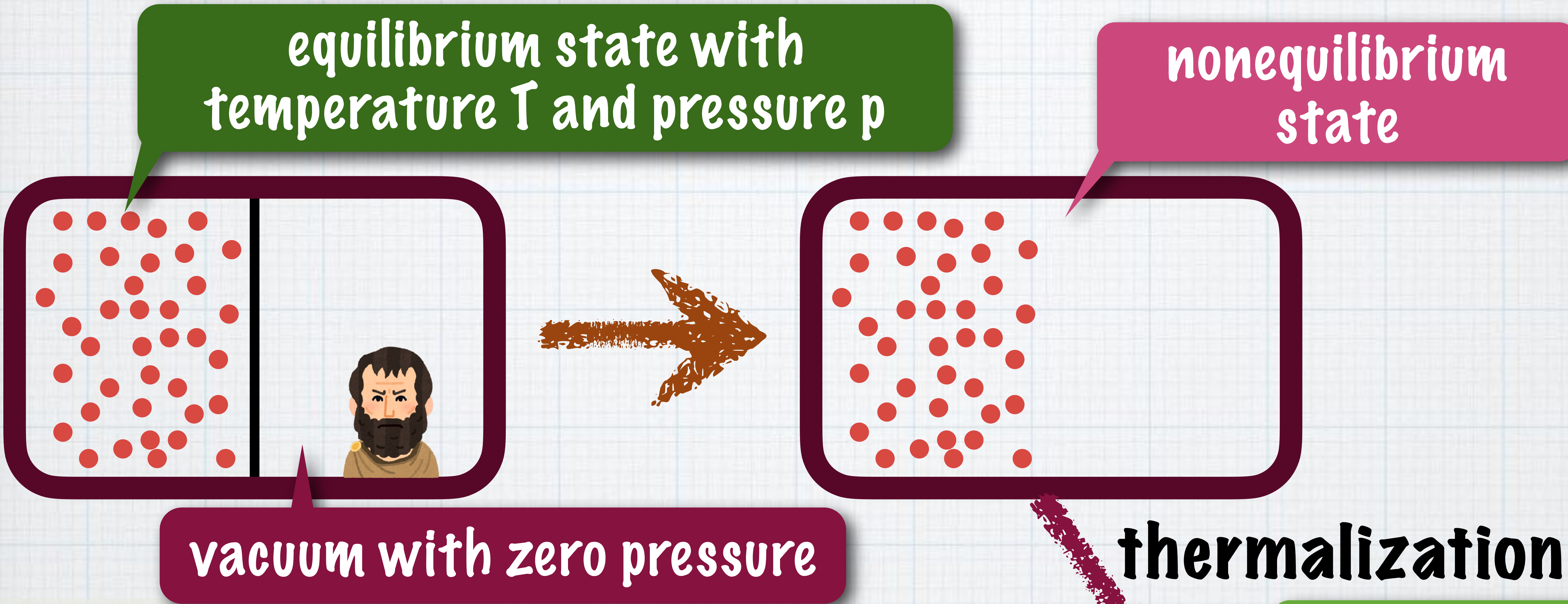
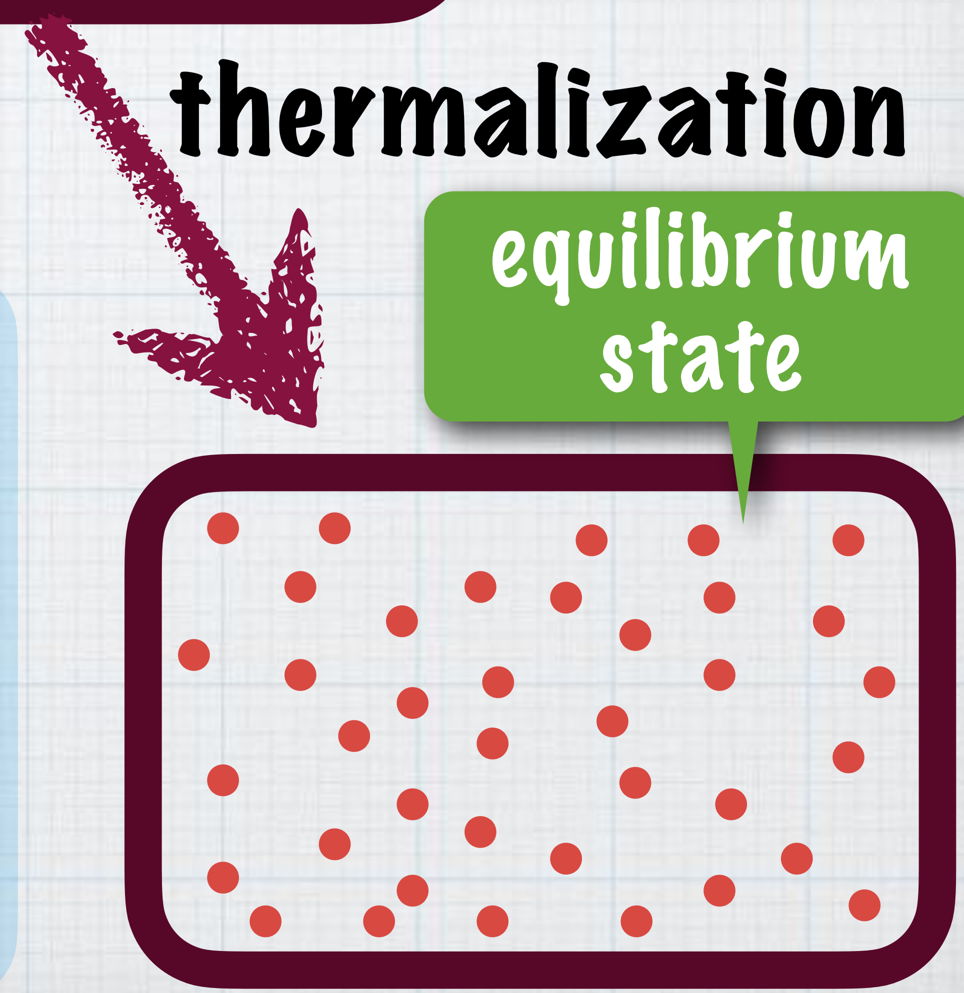
webinar @ YouTube / 2023

a typical process of thermalization





we prove that this process takes place in a dilute ideal gas of fermions on a chain evolving only by quantum-mechanical time-evolution (we treat the case $T = \infty$)

motivation

main result

frequently asked questions

essence of the proof

what is the origin of thermalization?

approach to thermal equilibrium

foundation of equilibrium statistical mechanics

question: does an isolated macroscopic quantum system thermalize only by means of quantum mechanical time-evolution? $|\Phi(t)\rangle = e^{-i\hat{H}t}|\Phi(0)\rangle$

YES! supported by numerous theoretical arguments, numerical simulations, and experiments in cold atoms

BUT, there were no concrete (and "realistic") examples in which the presence of thermalization was established without relying on any unproven assumptions

we prove the presence of thermalization (in a restricted sense) for low-density non-interacting fermions on a chain

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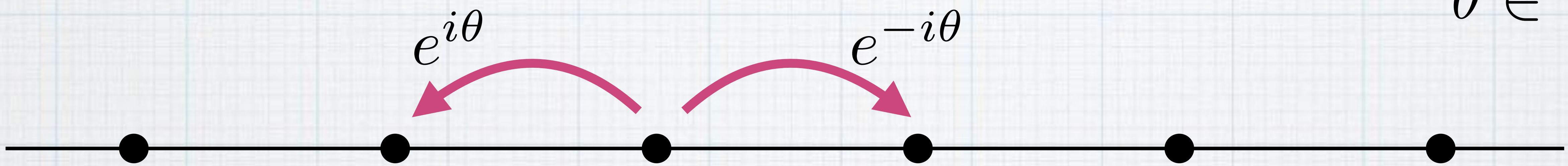
model and initial state

N **non-interacting fermions on the chain** $\{1,\ldots,L\}$
L **large prime,** N **large positive integer, density** $\rho = N/L$

Hamiltonian $\hat{H} = \sum_{x=1}^{L}\{e^{i\theta}\hat{c}_x^{\dagger}\hat{c}_{x+1} + e^{-i\theta}\hat{c}_{x+1}^{\dagger}\hat{c}_x\}$ $\theta \in [0, 2\pi)$



Lemma: all the energy eigenvalues of $\hat{H}$ are non-degenerate for most θ

we choose such θ, e.g, $\theta = (4N)^{-(L-1)/2}$

initial state

pick a normalized state $|\Phi(0)\rangle$ at random (with uniform probability) from the Hilbert space where all particles are in the left half-chain $\{1,\ldots,\frac{L-1}{2}\}$

equilibrium at $T=\infty$ confined in the half-chain

time-evolution and thermalization

time-evolved state $|\Phi(t)\rangle = e^{-i\hat{H}t}|\Phi(0)\rangle$

$\hat{N}_{\rm left}$ the number of particles in the left half-chain $\{1,\ldots,\frac{L-1}{2}\}$

$$\frac{\hat{N}_{\rm left}}{N}|\Phi(0)\rangle = |\Phi(0)\rangle$$

for the choice of $|\Phi(0)\rangle$

Theorem: the following is true with prob. $\geq 1 - e^{-(\rho/3)N}$
there exist sufficiently large $T > 0$ and a set $G \in [0,T]$ with $|G|/T \geq 1 - e^{-(\rho/4)N}$
for any $t \in G$, the measurement result of $\hat{N}_{\rm left}$ satisfies

$$\left|\frac{N_{\rm left}}{N} - \frac{1}{2}\right| \leq \epsilon_0(\rho) \text{ with prob. } \geq 1 - e^{-(\rho/4)N}$$

with $\epsilon_0(\rho) = \sqrt{3\rho/2}$

quantum mechanical probability

time-evolution and thermalization

time-evolved state $|\Phi(t)\rangle = e^{-i\hat{H}t}|\Phi(0)\rangle$

$\hat{N}_{\mathrm{left}}$ the number of particles in the left half-chain $\{1,\ldots,\frac{L-1}{2}\}$

$$\frac{\hat{N}_{\mathrm{left}}}{N}|\Phi(0)\rangle = |\Phi(0)\rangle$$

Theorem: it almost certainly happens that, for sufficiently large and typical time t, the measurement result of $\hat{N}_{\mathrm{left}}$ almost certainly satisfies $\frac{N_{\mathrm{left}}}{N} \simeq \frac{1}{2}$

since $\frac{N_{\mathrm{left}}}{N} = 1$ at $t = 0$, we see thermalization!!

but the precision is $\epsilon_0(\rho) = \sqrt{3\rho/2}$

the result is meaningful only for low enough density ρ

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does thermalization take place only in the special free fermion chain with a prime L ?

of course, the physics should not change when L is not a prime, but this is (so far) the only example where we can prove thermalization without relying on any unproved assumptions

we indeed prove a general thermalization theorem under two assumptions

Assumption 1: energy eigenvalues are non-degenerate

Assumption 2: any energy eigenstate $|\Psi_j\rangle$ satisfies

$$\langle\Psi_j|\hat{P}_{\rm left}|\Psi_j\rangle \le 2^{-N}$$

assumption 1 is very plausible in a generic quantum many-body systems

we have examples of interacting model where assumption 2 is verified assuming assumption 1

why isolated systems? there can't be a completely isolated system!

realistic setting

quantum system of interest

weak interaction with the surrounding environment (bigger system)

our setting

quantum system of interest

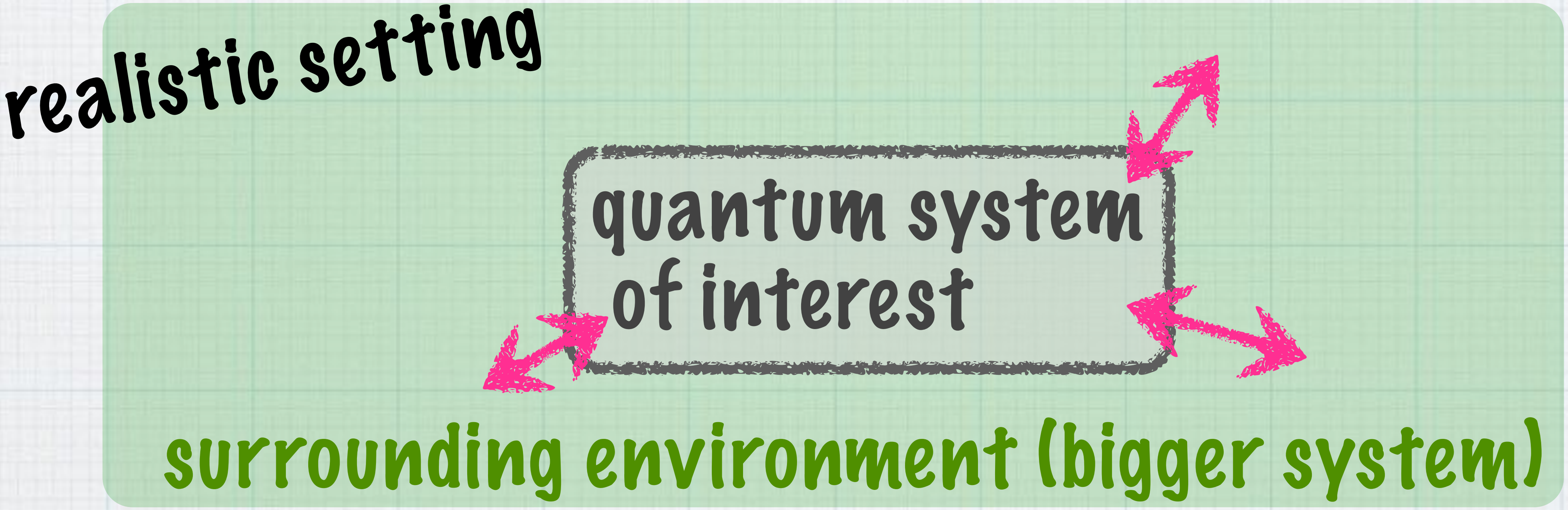
perfectly isolated from the outside world

why isolated systems? there can't be a completely isolated system!

§2. Statistical independence Landau and Lifshitz, "Statistical Mechanics" p.6

The subsystems discussed in §1 are not themselves closed systems; on the contrary, they are subject to the continuous interaction of the remaining parts of the system. But since these parts, which are small in comparison with the whole of the large system, are themselves macroscopic bodies also, we can still suppose that over not too long intervals of time they behave approximately as closed systems. For the particles which mainly take part in the interaction of a subsystem with the surrounding parts are those near the surface of the subsystem; the relative number of such particles, compared with the total number of particles in the subsystem, decreases rapidly when the size of the subsystem increases, and when the latter is sufficiently large the energy of its interaction with the surrounding parts will be small in comparison with its internal energy. Thus we may say that the subsystems are *quasi-closed*. It should be emphasised once more that this property holds only over not too long intervals of time. Over a sufficiently long interval of time, the effect of interaction of subsystems, however weak, will ultimately appear. Moreover, it is just this relatively weak interaction which leads finally to the establishment of statistical equilibrium.

why isolated systems? there can't be a completely isolated system!



fashionable answer

modern experiments in cold atoms!

unfashionable answer

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

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basic concepts and strategies

two main concepts

ETH (energy eigenstate thermalization hypothesis)

all energy eigenstates $|\Psi_j\rangle$ with $E_j \simeq E$ are similar

von Neumann 1929, Deutsch 1991, Srednicki 1994

effective dimension $D_{\rm eff} = \left(\sum_j \left|\langle\Psi_j|\Phi(0)\rangle\right|^4\right)^{-1}$

$D_{\rm eff}$ the effective number of energy eigenstates that constitute the initial state $|\Phi(0)\rangle$

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

essential conditions that guarantee the presence of thermalization

1) a strong version of ETH — von Neumann 1929; Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi 2010

2) a version of ETH and large $D_{\rm eff}$ — Tasaki 1998, Reimann 2008; Linden, Popescu, Short, Winter 2009

3) very large $D_{\rm eff}$ — Goldstein, Hara, Tasaki 2014, Tasaki 2016

basi … ies

believed to be valid in most sufficiently complex quantum many-body systems

two ma…

ETH (energy eigenstate thermalization hypothesis)

all energy eigenstates $|\Psi_j\rangle$ with $E_j \simeq E$ are similar

von Neumann 1929, Deutsch 1991, Srednicki 1994

effective dimension $D_{\rm eff} = \left(\sum_j |\langle \Psi_j | \Phi(0)\rangle|^4\right)^{-1}$

$D_{\rm eff}$ the effective number of energy eigenstates that constitute the initial state $|\Phi(0)\rangle$

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

believed to be very large for realistic nonequilibrium states in sufficiently complex quantum many-body systems

essenti… therma…

1) a strong version of ETH — von Neumann 192… Goldstein, Lebowit… …0

we use this strategy in the present work

2) a version of ETH and large $D_{\rm eff}$ — Tasak… Lind…, Popescu, Short, Winter 2009

3) very large $D_{\rm eff}$ — Goldstein, Hara, Tasaki 2014, Tasaki 2016

why does large D_{eff} lead to thermalization

initial state $|\Phi(0)\rangle = \sum_j \alpha_j |\Psi_j\rangle$

time-evolved state $|\Phi(t)\rangle = e^{-i\hat{H}t}|\Phi(0)\rangle = \sum_j \alpha_j \, e^{-iE_j t}|\Psi_j\rangle$

expectation value of an observable

$$\langle\Phi(t)|\hat{\mathcal{O}}|\Phi(t)\rangle = \sum_{j,k} \alpha_j^* \alpha_k \, e^{-i(E_j - E_k)t}\langle\Psi_j|\hat{\mathcal{O}}|\Psi_k\rangle$$

long-time average

non-degeneracy ($E_j \neq E_k$ if $j \neq k$)

$$\lim_{T\uparrow\infty} \frac{1}{T}\int_0^T dt\langle\Phi(t)|\hat{\mathcal{O}}|\Phi(t)\rangle = \sum_j |\alpha_j|^2\langle\Psi_j|\hat{\mathcal{O}}|\Psi_j\rangle$$

if $D_{\text{eff}} = (\sum_j |\alpha_j|^4)^{-1} \sim D_{\text{tot}}$ **then** $|\alpha_j|^2 \sim D_{\text{tot}}^{-1}$

dimension of the whole Hilbert space

and $\lim_{T\uparrow\infty} \frac{1}{T}\int_0^T dt\langle\Phi(t)|\hat{\mathcal{O}}|\Phi(t)\rangle \sim D_{\text{tot}}^{-1}\sum_j\langle\Psi_j|\hat{\mathcal{O}}|\Psi_j\rangle$

$$= \langle\hat{\mathcal{O}}\rangle_{T=\infty}^{\text{canonical}}$$

(there also is a version for finite T)

structure of the proof

$\mathscr{H}_{\text{left}}$: Hilbert space in which all particles are in the half-chain $\{1, \ldots, \frac{L-1}{2}\}$

$\hat{P}_{\text{left}}$: projection onto $\mathscr{H}_{\text{left}}$

general theory

we prove that a low-density lattice gas exhibits thermalization under the two (plausible) assumptions

Assumption 1: energy eigenvalues are non-degenerate

Assumption 2: any energy eigenstate $|\Psi_j\rangle$ satisfies

$$\langle \Psi_j | \hat{P}_{\text{left}} | \Psi_j \rangle \leq 2^{-N}$$

analysis of the free fermion chain

Assumption 2 can be proved from the exact solution

Assumption 1 can be proved by using results from the number theory general theory

proof that D_{eff} is large

Assumption 2: any energy eigenstate $|\Psi_j\rangle$ satisfies

$$\langle\Psi_j|\hat{P}_{\mathrm{left}}|\Psi_j\rangle \le 2^{-N}$$

D_{left} : dimension of $\mathscr{H}_{\mathrm{left}}$

$|\Phi(0)\rangle$: a random normalized state from $\mathscr{H}_{\mathrm{left}}$

average

standard formula for a random state

$$\overline{|\langle\Phi(0)|\Psi_j\rangle|^4} = \overline{|\langle\Phi(0)|\hat{P}_{\mathrm{left}}|\Psi_j\rangle|^4} = \frac{2}{D_{\mathrm{left}}(D_{\mathrm{left}}+1)}\|\hat{P}_{\mathrm{left}}|\Psi_j\rangle\|^4$$

$$= \frac{2}{D_{\mathrm{left}}(D_{\mathrm{left}}+1)}\langle\Psi_j|\hat{P}_j|\Psi_j\rangle^2$$

$\mathrm{Tr}[\hat{P}_{\mathrm{left}}] = D_{\mathrm{left}}$

$$\overline{D_{\mathrm{eff}}^{-1}} = \sum_j \overline{|\langle\Phi(0)|\Psi_j\rangle|^4} \le \frac{2\times 2^{-N}}{D_{\mathrm{left}}(D_{\mathrm{left}}+1)}\sum_j\langle\Psi_j|\hat{P}_{\mathrm{left}}|\Psi_j\rangle$$

$$= \frac{2\times 2^{-N}}{D_{\mathrm{left}}+1} \le D_{\mathrm{tot}}^{-1}\, e^{(2/3)\rho N}$$

close to D_{tot}^{-1} if ρ is small

analysis of the free fermion chain

proof of the absence of degeneracy

Hamiltonian

must be studied in the number theory!

$\zeta = e^{i\frac{2\pi}{L}}$

energy eigenvalues

$$E_{\boldsymbol{n}} = \sum_{j=0}^{L-1} n_j \cos(\tfrac{2\pi}{L}j + \theta) = \Re[e^{i\theta} \sum_{j=0}^{L-1} n_j\, \zeta^j]$$

occupation numbers $n_j = 0, 1, \quad \sum_{j=1}^{L} n_j = N$

number-theoretic facts

assume L **is an odd prime,** $N \le (L-1)/4$**,** $m_1, \ldots, m_{L-1} \in \mathbb{Z}$

Lemma: if $m_j \neq 0$ **for some** j**, then** $\sum_{j=1}^{L-1} m_j \zeta^j \neq 0$

→ **no degeneracy for most** θ

Lemma: we have $|\sum_{j=1}^{L-1} m_j \zeta^j| \ge (\sum_{j=1}^{L-1} |m_j|)^{-(L-3)/2}$

→ **no degeneracy if** $\theta \neq 0$ **and** $|\theta| \le (4N)^{-(L-1)/2}$

analysis of the free fermion chain

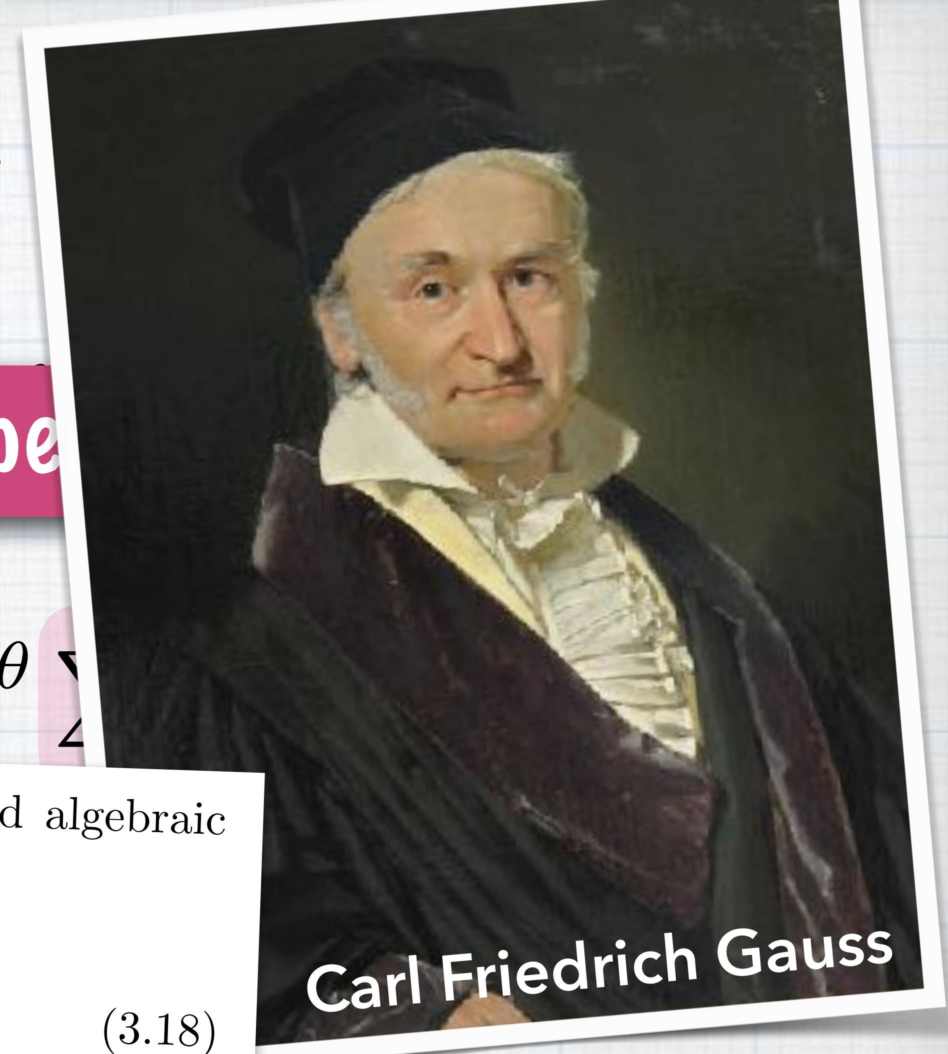
proof of the absence of

Hamiltonian $\hat{H}$

must be studied in the numbe

energy eigenvalues

$$E_n = \sum_{j=0}^{L-1} n_j \cos(\tfrac{2\pi}{L} j + \theta) = \Re[e^{i\theta} \sum$$



Proof: The lemma is proved by using standard facts about the field norm and algebraic integers. See, e.g., [49]. Let $\alpha = \sum_{\mu=1}^{L-1} m_\mu \, \zeta^\mu \in \mathbb{Z}[\zeta] \subset \mathbb{Q}[\zeta]$ and

$$\sigma_j(\alpha) = \sum_{\mu=1}^{L-1} m_\mu \, e^{i2\pi j \mu/L}, \tag{3.18}$$

be its conjugate, where $j = 1, \ldots, L-1$. Note that $\sigma_1(\alpha) = \alpha$, $\sigma_j(\alpha) = \{\sigma_{L-j}(\alpha)\}^*$, and $|\sigma_j(\alpha)| \le M$. Let $N : \mathbb{Q}[\zeta] \to \mathbb{Q}$ denote the field norm of $\mathbb{Q}[\zeta]$. By definition, we have

$$N(\alpha) = \prod_{j=1}^{L-1} \sigma_j(\alpha) = \prod_{j=1}^{(L-1)/2} |\sigma_j(\alpha)|^2. \tag{3.19}$$

Since Lemma 3.3 guarantees $\sigma_j(\alpha) \neq 0$ for all j, we see that $N(\alpha) > 0$. Note that α is an algebraic integer, and hence so are its conjugates $\sigma_j(\alpha)$ and the norm $N(\alpha)$. It is known that an algebraic integer that is rational must be an integer. Since $N(\alpha) \in \mathbb{Q}$, we see $N(\alpha) \in \mathbb{Z}$ and hence $N(\alpha) \ge 1$. This bound, with (3.19), implies

$$|\alpha|^2 \ge \left(\prod_{j=2}^{(L-1)/2} |\sigma_j(\alpha)|^2 \right)^{-1} \ge \frac{1}{M^{L-3}}. \quad ∎ \tag{3.20}$$

$, m_{L-1} \in \mathbb{Z}$

$\neq 0$

$(L-3)/2$

→ no degeneracy if $\theta \neq 0$ and $|\theta| \le (4N)^{-(L-1)/2}$

summary

- ☑ we focused on the problem of thermalization (approach to thermal equilibrium) in isolated macroscopic quantum systems
- ☑ without relying on any unproved assumptions, we proved that a free fermion chain exhibits thermalization (in some weak sense)
- ☑ the key observations were that a random nonequilibrium initial state has a large D_{eff} and that the absence of degeneracy can be proved by using some number-theoretic results
- ☑ it is desirable to have examples of non-integrable systems in which our (plausible) assumptions for the general theory of thermalization can be justified