On the Increase of Boltzmann Entropy of Macroscopic Quantum Systems

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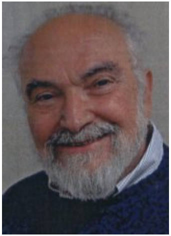
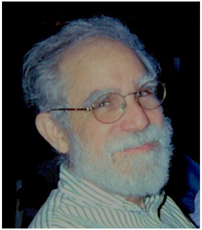


Joel Lebowitz



Shelly Goldstein

Nino Zanghì

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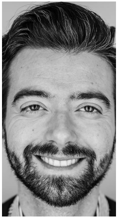


Christian Mastrodonato

Cornelia Vogel

Cedric Igelspacher

Barbara Roos

Motivation

1st law of thermodynamics

"The energy of the universe is constant." (Clausius 1865)

2nd law of thermodynamics

"The entropy of the universe tends toward a maximum." (Clausius 1865)

0th law of thermodynamics

"If two thermodynamic systems are both in thermal equilibrium with a third system, then they are in thermal equilibrium with each other." (Fowler 1939)

"Minus first" law of thermodynamics

"Every macroscopic system sooner or later reaches thermal equilibrium." (Marsland-Brown-Valente 2015)

The theme of my talk is to derive the 2nd and -1st from quantum mechanics.

- Different authors have proposed rather different statements of the 2nd law:
    - I'm interested here in statements about the evolution from certain (low-entropy) states to certain other (high-entropy) states.
- There are different concepts of entropy:
    - I'm interested here in thermal entropy (in and out of thermal equilibrium) following Boltzmann, roughly $S = \log \#$ micro states ($k_{\mathrm{B}} = 1$).
- There are different concepts of thermal equilibrium:
    - "Thermal state" usually means a canonical density matrix $\rho_{\mathrm{can}} = \frac{1}{Z} e^{-\beta H}$ (highly mixed).
    - I'm interested here in thermodynamic behavior of a quantum system in a pure state ψ.
- Our definition of thermalization:
    - Consider a closed system.
    - It is said to thermalize if it is in thermal equilibrium for most $t > 0$.

So we consider

- a macroscopic quantum system (say, $N > 10^{20}$ particles)
- in a bounded volume $\Lambda \subset \mathbb{R}^3$
- isolated, evolves unitarily $i\frac{\partial\psi}{\partial t} = H\psi$ in Hilbert space $\mathscr{H}$
- $H = \sum_\alpha E_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$
- $\mathbb{S}(\mathscr{H}) := \{\psi \in \mathscr{H} : \|\psi\| = 1\}$ unit sphere

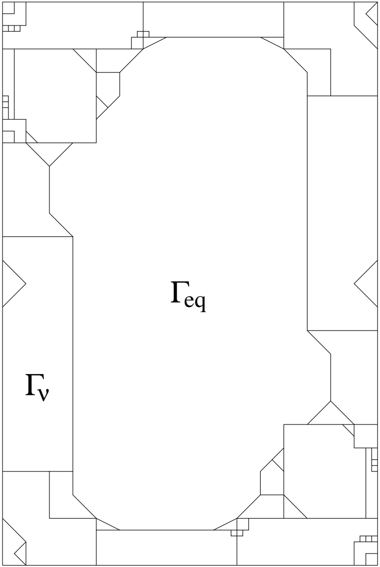
And even in closed quantum systems in pure states, two kinds of thermal equilibrium are relevant:

- **Microscopic thermal equilibrium (MITE):** All local observables have the same Born distribution in ψ as in a thermodynamic ensemble.

  This occurs for most ψ in the ensemble by a theorem known as canonical typicality [Gemmer-Mahler-Michel 2004, Popescu-Short-Winter quant-ph/0511225, Goldstein-Lebowitz-T-Zanghì cond-mat/0511091, for canonical ensemble (GAP measure) Teufel-T-Vogel 2307.15624].
- **Macroscopic thermal equilibrium (MATE):** All macroscopic observables have the same nearly-deterministic value in ψ as in a thermodynamic ensemble.

Setting the stage

Classical mechanics: partition of phase space



- $\Gamma = \cup_\nu \Gamma_\nu$ "macro sets"
- Γ_ν = set of phase points that look like macro state ν
- <u>Ex:</u> $\nu =$ "Between 60 and 61% of the particles are in the left half of the volume."
- Set $\nu(X) = \nu$ with $X \in \Gamma_\nu$, define Boltzmann entropy

$$S_{\mathrm{B}}(X) = \log \mathrm{vol}\, \Gamma_{\nu(X)} = S_{\mathrm{B}}(\nu(X))$$

- Usually, in every energy shell $\Gamma_{\mathrm{mc}} = \{x : E - \Delta E < H(x) \leq E\}$ there is one macro state $\Gamma_\nu = \Gamma_{\mathrm{eq}}$ corresponding to thermal equilibrium and taking up > 99.99% of volume.

$$\max_\nu S_{\mathrm{B}}(\nu) = S_{\mathrm{B}}(\mathrm{eq}) \approx \log \mathrm{vol}\, \Gamma_{\mathrm{mc}}$$

Quantum mechanics: Macro spaces

[von Neumann 1929, van Kampen 1992, Lebowitz 1993]

- $\mathscr{H} = \bigoplus_{\nu \in \mathcal{N}} \mathscr{H}_\nu$. Different macro states ν correspond to mutually orthogonal subspaces $\mathscr{H}_\nu$ ("macro spaces").
- There is some arbitrariness in the choice of $\mathscr{H}_\nu$, but it is expected to not matter much as $N \to \infty$. We regard the $\mathscr{H}_\nu$'s as given.
- $d_\nu := \dim \mathscr{H}_\nu \ggg 1$, of order $10^{10^{10}}$. Notation $P_\nu :=$ proj to $\mathscr{H}_\nu$
- In the micro-canonical "energy shell"

$$\mathscr{H}_{\mathrm{mc}} = \mathrm{span}\Big\{\phi_\alpha : E - \Delta E < E_\alpha \leq E\Big\}$$

($\Delta E =$ resolution of macroscopic energy measurements), usually one of the $\mathscr{H}_\nu$ has most dimensions, "$\nu = \mathrm{eq}$":

$$\frac{\dim \mathscr{H}_{\mathrm{eq}}}{\dim \mathscr{H}_{\mathrm{mc}}} = 1 - \varepsilon\,, \quad \varepsilon \ll 1 \;\; (\text{in practice } \varepsilon \lesssim 10^{-10^5})$$

- quantum Boltzmann entropy $S_{\mathrm{qB}}(\nu) := \log d_\nu$

[Einstein 1914, Lebowitz 1993, Griffiths 1994, GLTZ 1903.11870]

Macroscopic observables

- von Neumann 1929: Macro observables commute exactly. If they don't, adjust them a little ("rounding") so they do.
- Some authors [De Roeck-Maes-Netočný math-ph/0601027, Tasaki 1507.06479] argued that rounding is not essential; but since rounding makes the discussion easier, I will stick with it.
- von Neumann 1929: For macro observables M, the eigenvalue spacing should be the resolution of macroscopic measurements ($\Rightarrow$ M highly degenerate). $\mathscr{H}_\nu$ are just the joint eigenspaces of all macro observables.
- Thus, if $\psi \in \mathscr{H}_{\mathrm{eq}}$, every macro observable M assumes its equilibrium value $m_{\mathrm{eq}} \approx \mathrm{tr}(M\rho_{\mathrm{mc}})$.
- Def: MATE$_\delta$ $:\Leftrightarrow$ $\|P_{\mathrm{eq}}\psi\|^2 \geq 1-\delta$, $\varepsilon \ll \delta \ll 1$.

Fact: Most ψ lie in MATE.

$u_{\mathrm{mc}}(\mathrm{MATE}_\delta) \geq 1 - \varepsilon/\delta \approx 1$ with u_{mc} unif. norm'd measure on $\mathbb{S}(\mathscr{H}_{\mathrm{mc}})$.

(By the way, most $\psi \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ also lie in MITE [GHLT 1506.07494].)

Thermalization, or the -1st Law

Eigenstate thermalization hypothesis (ETH)

Every eigenvector ϕ_α of H is in thermal equilibrium.

MATE-ETH

$\forall\alpha: \quad \phi_\alpha \in \mathsf{MATE}_\delta$

Proposition: MATE-ization [GLMTZ 0911.1724, this version RSTTV 2408.15832]

Suppose H satisfies MATE-ETH. Then for every $\psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ and $(1-\varepsilon)$-most $t > 0$, $\psi_t \in \mathsf{MATE}_{\delta/\varepsilon}$.

MITE-ETH [Srednicki cond-mat/9403051]

For every small spatial region s (and s^c = complement),

- $\forall\alpha: \quad \mathrm{tr}_{s^c}|\phi_\alpha\rangle\langle\phi_\alpha| \approx \mathrm{tr}_{s^c}\,\rho_{\mathrm{mc}}$
- $\forall E_\alpha \neq E_\beta: \quad \mathrm{tr}_{s^c}|\phi_\alpha\rangle\langle\phi_\beta| \approx 0$

Proposition: MITE-ization [Srednicki chao-dyn/9511001, this version ITV 2601.03253]

Suppose H satisfies MITE-ETH, and the maximal degeneracy of eigenvalue gaps is not too large. Then for every $\psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ and most $t > 0$, $\psi_t \in \mathsf{MITE}$.

A nice thing about ETH

It is a clear mathematical condition on H that suffices for thermalization of every ψ_0.

Some alternative approaches cover *most* ψ_0.

[Reimann 0810.3092, Linden-Popescu-Short-Winter 0812.2385, Tasaki-Shirasishi 2310.18880]

Theorem: Most H satisfy MATE-ETH [GLMTZ 0911.1724]

Given any subspace $\mathscr{H}_{\mathrm{eq}}$ with high dimension and $\dim \mathscr{H}_{\mathrm{eq}} / \dim \mathscr{H} > 1 - \varepsilon$, and any non-degenerate values E_α. Choose the eigenbasis $\{\phi_\alpha\}$ of H purely randomly (i.e., uniformly over all ONBs). Then MATE-ETH is satisfied with probability near 1.

- However, such random H are not realistic because they thermalize ultrafast (in $\hbar k_{\mathrm{B}}/T \approx 10^{-13}$ seconds at room temperature).
  [Goldstein-Hara-Tasaki 1307.0572, 1402.3380, Reimann 1603.00669]
- There do exist exceptional Hamiltonians that don't satisfy MATE-ETH (e.g., non-interacting, many-body localization).
- (By the way, most H with uniform eigenbasis also satisfy MITE-ETH [Mori-Ikeda-Kaminishi-Ueda 1712.08790].)

A concrete H that satisfies MATE-ETH

Theorem [Tasaki-Shiraishi 2310.18880, Tasaki 2404.04533, this version RSTTV 2408.15832]

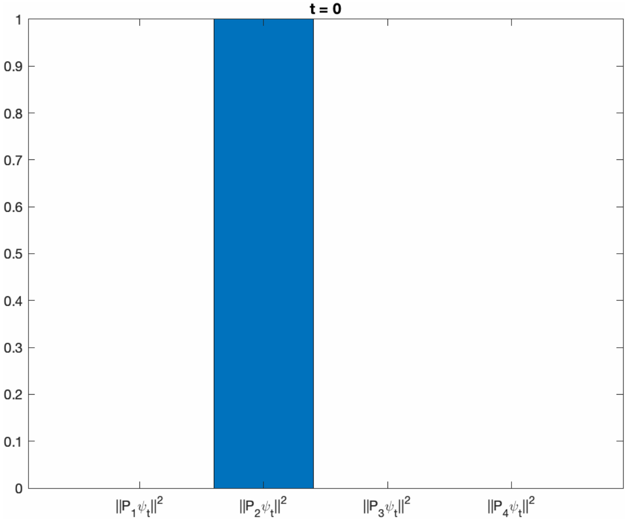
Let $\mathscr{H}$ be the Hilbert space of $N \gg 1$ fermions on a 1d finite periodic lattice, $H = H_0$ the discrete Laplacian ("free Fermi gas"), and $\mathscr{H}_{\mathrm{eq}}$ the subspace with (say) particle number in the left half of the lattice between $\frac{N}{2} - \eta N$ and $\frac{N}{2} + \eta N$ for some $\eta > 0$. Under some technical assumptions, H satisfies MATE-ETH.

Theorem [RSTTV 2408.15832]

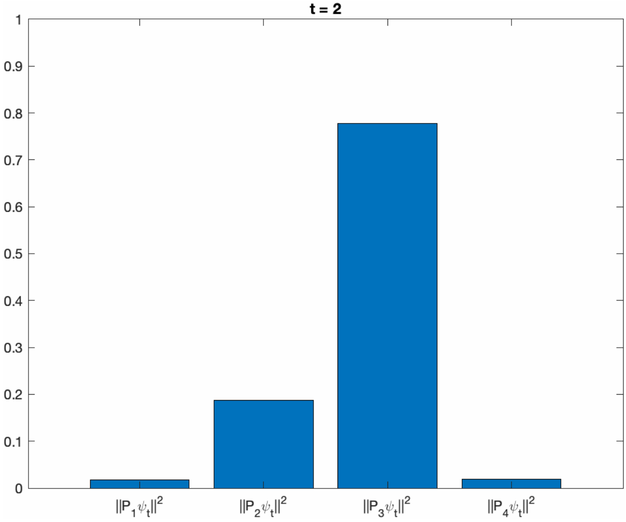
Consider the free Fermi gas H_0 with $N \gg 1$ on a d-dimensional periodic lattice with any $d \geq 1$ and $\mathscr{H}_{\mathrm{eq}}$ as before. Let $H = H_0 + \lambda V$, where V is a generic perturbation. Then for every sufficiently small $\lambda > 0$, H satisfies MATE-ETH.

The macro history $(\nu, t) \mapsto \|P_\nu \psi_t\|^2$

Simulation by Cornelia Vogel:



Simulation by Cornelia Vogel:



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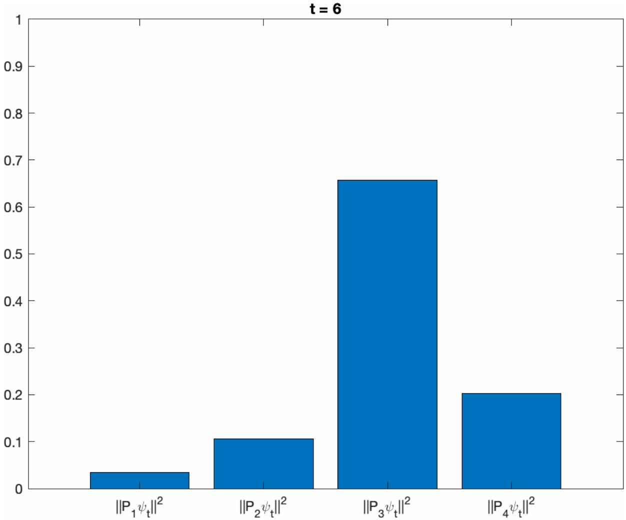

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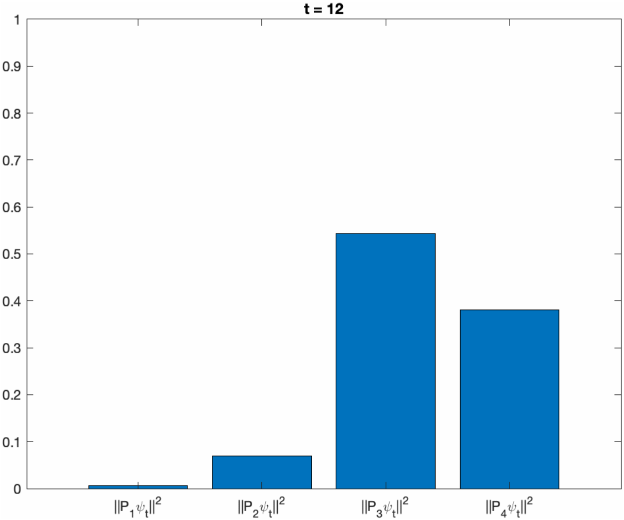

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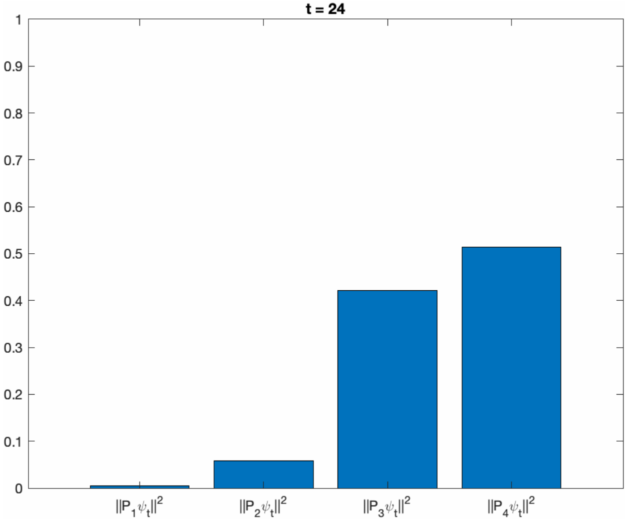

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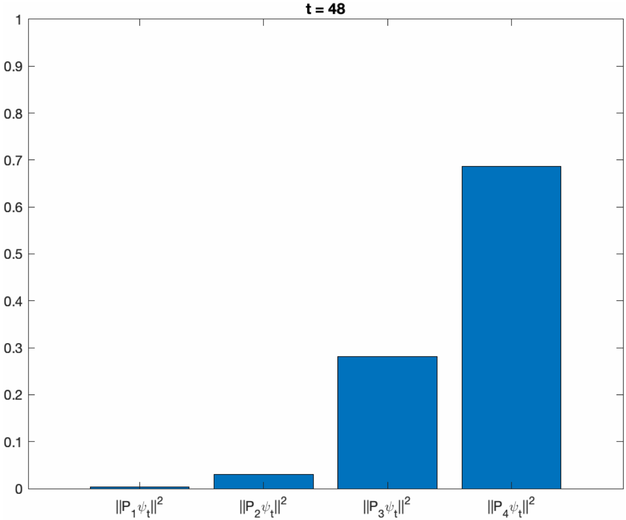
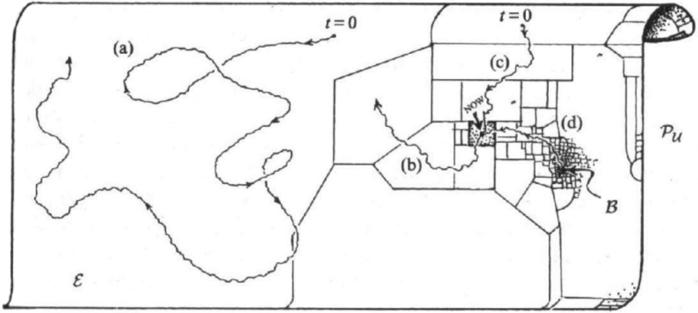


Entropy and the 2nd law

Entropy increase, classically

- Hamiltonian flow Φ_t in phase space, $X_t = \Phi_t(X)$.
- Boltzmann entropy usually increases: Phase point typically moves to larger and larger macro sets Γ_ν.

Drawing: R. Penrose



- Def: quantum Boltzmann entropy $S_{\mathrm{qB}}(\nu) := \log d_\nu$
- Indeed, the d_ν are vastly different.
- $S_{\mathrm{qB}}(\mathrm{eq}) \approx \log \dim \mathscr{H}_{\mathrm{mc}}$
- S_{qB} is additive: For a composite system $s = a \cup b$, if $\mathscr{H}_s = \mathscr{H}_a \otimes \mathscr{H}_b$, $\nu = (\nu_a, \nu_b)$, $\mathscr{H}_\nu = \mathscr{H}_{\nu_a} \otimes \mathscr{H}_{\nu_b}$, then $S_{\mathrm{qB}}(\nu) = S_{\mathrm{qB}}(\nu_a) + S_{\mathrm{qB}}(\nu_b)$.
- Since a general ψ is a superposition of different ν's, it is also a superposition of different entropy values.
- If macro states ν follow an autonomous, deterministic evolution law $\nu \mapsto \nu_t$, then S_{qB} increases, i.e.,

$$\text{if } e^{-i\hat{H}t}\mathscr{H}_\nu \subseteq \mathscr{H}_{\nu'}, \text{ then } S_{\mathrm{qB}}(\nu) \leq S_{\mathrm{qB}}(\nu').$$

- But in general, it is not obvious what it means to say that entropy increases.
- I will present some options.

- It is natural to define the entropy operator

$$\hat{S} = \sum_{\nu \in \mathcal{N}} S_{\mathrm{qB}}(\nu)\, P_\nu$$

with P_ν the projection to $\mathscr{H}_\nu$.

- Here, the foundations of statistical mechanics touch the foundations of quantum mechanics. The Copenhagen interpretation is too vage.
    - Many-worlds or
    - spontaneous collapse (such as GRW) or
    - hidden variables (such as Bohmian mechanics)

  provide principled answers.

- In Bohmian mechanics, an actual macro state cannot always be defined, but in practical cases it can. Then the net amount of probability transported $\nu' \to \nu$ per time plausibly agrees with the discrete probability current of QM,

$$J_{\nu\nu'} = 2\,\mathrm{Im}\langle\psi|P_\nu H P_{\nu'}|\psi\rangle\,.$$

Goal: "Strong 2nd law"

For reasonable H and macro spaces $\mathscr{H}_\nu$, any ν_0, and most $\psi_0 \in \mathbb{S}(\mathscr{H}_{\nu_0})$, the discrete current

$$J_{\nu\nu'} = 2\,\mathrm{Im}\langle\psi_t|P_\nu H P_{\nu'}|\psi_t\rangle$$

points overwhelmingly from smaller $\mathscr{H}_{\nu'}$ to larger $\mathscr{H}_\nu$ for $t \in [0, T]$, where T is the time scale of reaching MATE.

"Weak 2nd law"

For reasonable H and macro spaces $\mathscr{H}_\nu$, any ν_0, and most $\psi_0 \in \mathbb{S}(\mathscr{H}_{\nu_0})$, the histogram $(\nu, t) \mapsto \|P_\nu\psi_t\|^2$ is approximately right-moving for $t \in [0, T]$, where T is the time scale of reaching MATE, and we order ν by size: $\nu < \nu'$ $:\Leftrightarrow d_\nu < d_{\nu'} \Leftrightarrow S_{\mathrm{qB}}(\nu) < S_{\mathrm{qB}}(\nu')$.

It would be nice

to have a mathematical condition (like ETH) on H and the P_ν's that is sufficient for the weak or the strong 2nd law and holds in realistic examples of macroscopic systems.

Approaches to deriving this version of the 2nd law

van Kampen's hypothesis [1992]

$p_\nu(t) := \|P_\nu \psi_t\|^2$ evolves approximately like the distribution of a Markov process on the set $\mathscr{N}$ of macro states with jump rates $\sigma_{\nu\nu'}$.

Strasberg-Winter-Gemmer-Wang [2209.07977] gave arguments in support of it and the following

Hypothesis of local detailed balance

$$\frac{\sigma_{\nu\nu'}}{\sigma_{\nu'\nu}} \approx \frac{d_\nu}{d_{\nu'}} \tag{1}$$

Together, these two hypotheses imply the weak 2nd law.

Results for special types of H (1)

Def: A Wigner matrix is a random Hermitian $d \times d$ matrix H, where

- $\{\mathrm{Re}\, h_{ij}, \mathrm{Im}\, h_{ij} : 1 \leq i < j \leq d\} \cup \{\sqrt{2}\, h_{ii} : 1 \leq i \leq d\}$ are i.i.d.
- $\mathbb{E} h_{ij} = 0$ and $\mathbb{E}|h_{ij}|^2 = 1/d$ for all i, j

Ex: GUE is a special case.

Theorem [Igelspacher 2026, using Cipolloni-Erdős-Schröder 2102.09975]

Suppose all $d_\nu \gg 1$ and $d_{\nu_0} \gg \sum_{\nu<\nu_0} d_\nu$. Then a typical Wigner matrix H satisfies the strong 2nd law within a tolerance of 2.5%, i.e., the total time-integrated current to the left is $\leq 2.5\%$ of the total current to the right.

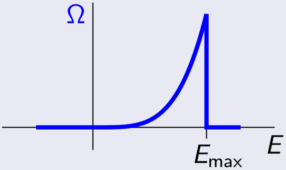
Results for special types of H (2)

Added September 14, 2026: I am retracting the claims that I made on this slide. They were based on a mistake.

Theorem [T 2026]

Suppose

- all $d_\nu \gg 1$ and $d_{\nu_0} \gg \sum_{\nu<\nu_0} d_\nu$
- H has uniformly distributed eigenbasis
- the eigenvalues are distributed according to a curve $\Omega(E)$ (density of states)
- $\Omega(E) = 0$ for $E \leq 0$ and $E > E_{\max}$ ("microcanonical")
- the function $\Omega(\cdot)$ is smooth, increasing and convex on $[0, E_{\max}]$.



Then the strong 2nd law holds.

Still, that is a case with ultrafast (unrealistic) thermalization.

Results for special types of H (3)

A random block-band matrix: still a toy model, but more realistic

Let $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2 \oplus \mathscr{H}_3$ with $d_1 \ll d_2 \ll d_3 = d_{\mathrm{eq}}$.
Take H to be a Wigner-type Hermitian random matrix, i.e., h_{ij} are independent for $i \leq j$, $\mathbb{E}h_{ij} = 0$, and $\mathbb{E}|h_{ij}|^2 = s_{ij}$ with

$$S = (s_{ij}) = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & S_{23} \\ 0 & S_{32} & S_{33} \end{pmatrix},$$

where each block $S_{\nu\nu'}$ has all entries equal.

Theorem [Erdős-Henheik-Vogel 2506.17177]

For $d_2/d_1 = d_3/d_2$, a suitable choice of the entries of $S_{\nu\nu'}$ (that allows explicit calculations), and any $\psi_0 \in \mathscr{H}_{\nu_0}$, it has probability near 1 that for times t that are large ($> \mathcal{O}(d_2/d_1)$) but not too large (¡ recurrence times $\mathcal{O}(e^d)$), the $\|P_\nu \psi_t\|^2$ evolve monotonically (up to small errors) towards d_ν/d. In particular, if $d_2/d_1 \gg 1$, then the weak 2nd law holds (right-moving distribution), but thermalization is not ultrafast.

For discussion see also [Igelspacher 2026].

Thank you for your attention