Time evolution of closed macroscopic quantum systems towards thermal equilibrium

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14 May 2024

Main reference: arXiv 2210.10018

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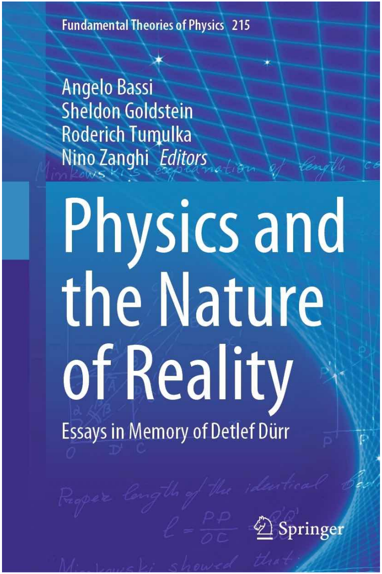
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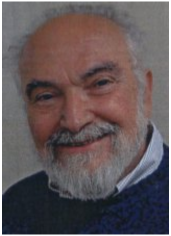
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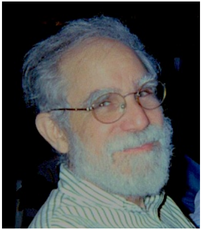
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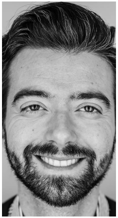
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Motivation

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 the talk is to derive the 2nd and -1st from quantum mechanics.

- Different authors have proposed rather different statements of the 2nd law:
  - some concern only thermal equilibrium states,
  - some the impossibility of certain (perpetual motion) machines,
  - some the knowledge of observers.
  - 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:
  - Shannon entropy $S_{\mathrm{S}} = -\sum_i p_i \log p_i$ measures the width of a probability distribution $(p_i)_i$.
  - Entanglement entropy quantifies the amount of entanglement between 2 systems.
  - 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 thermalization:
  - Some authors consider a system coupled to an infinite reservoir or to random perturbations.
  - But thermalization is not limited to open systems or stochastic evolution: Consider the isolated system consisting of a hot brick touching a cold one. The temperatures will even out.
  - I'm interested here in the thermalization of a closed system.
- There are different concepts of thermal equilibrium:
  - "Thermal state" usually means a canonical density matrix $\rho = \frac{1}{Z} e^{-\beta H}$ (highly mixed).
  - I'm interested here in thermodynamic behavior of a quantum system in a pure state ψ ("thermalization in the strong sense").
  - Such behavior has been studied in particular in connection with the *eigenstate thermalization hypothesis* [Deutsch 1991, Srednicki cond-mat/9403051], but also [von Neumann 1929, Schrödinger 1952, Lebowitz 1993, Tasaki cond-mat/9707253, Popescu-Short-Winter quant-ph/0511225, Reimann 0710.4214, Gemmer-Mahler-Michel 2004]

So we consider

- a macroscopic quantum system (say, $N > 10^{20}$ particles)
- in a bounded volume $\Lambda \subset \mathbb{R}^3$
- isolated, evolves unitarily $i\dfrac{\partial\psi}{\partial t} = H\psi$ 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 occur:

- **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.
  I will focus on this kind.

Setting the stage

Macro spaces

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

- $\mathscr{H} = \bigoplus_{\nu \in \mathscr{N}} \mathscr{H}_\nu$. Different macro states ν correspond to mutually orthogonal subspaces $\mathscr{H}_\nu$ ("macro spaces"). Vectors in the same $\mathscr{H}_\nu$ should "look macroscopically the same."
- Ex: $\nu =$ "Between 60 and 61% of the particles are in the left half of the volume."
- 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.
- Classical analog: partition of phase space into "macro sets."
- $d_\nu := \dim \mathscr{H}_\nu \ggg 1$, 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, "$\nu = \mathrm{eq}$":

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

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 $\mathbb{S}(\mathscr{H}_{\mathrm{mc}})$.

Proof: $\mathbb{E}_\psi \langle\psi|P_{\mathrm{eq}}|\psi\rangle = \mathrm{tr}(P_{\mathrm{eq}}\rho_{\mathrm{mc}}) = \dim \mathscr{H}_{\mathrm{eq}} / \dim \mathscr{H}_{\mathrm{mc}} = 1-\varepsilon$, but the average of $f(\psi) = \langle\psi|P_{\mathrm{eq}}|\psi\rangle$ could not be that high if less than $1-\varepsilon/\delta$ of all ψ's had $f(\psi) \geq 1-\delta$ (Markov ineq). □

Thermalization, or the -1st Law

Eigenstate thermalization hypothesis (ETH)

Every eigenvector ϕ_α of H is in thermal equilibrium.

Different concepts of thermal equilibrium lead to different versions of ETH; a strong one has been proven for Wigner-type random matrices [Riabov-Erdős 2404.17512]. We only need

MATE-ETH

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

Let $\dim \mathscr{H} < \infty$, $\mathscr{H}_{\mathrm{eq}} \subset \mathscr{H}$ any subspace, P_{eq} projection to $\mathscr{H}_{\mathrm{eq}}$.

Proposition: Approach to MATE [GLMTZ 0911.1724]

Let $\eta, \varepsilon > 0$, $\delta = \eta\varepsilon$. If H is non-degenerate and MATE-ETH holds, then any $\psi_0 \in \mathbb{S}(\mathscr{H})$ will spend $(1-\varepsilon)$-most of the time in MATE_η, i.e.,

$$\liminf_{T\to\infty} \frac{1}{T}\left|\left\{0 < t < T : \langle \psi_t | P_{\mathrm{eq}} | \psi_t \rangle > 1 - \eta\right\}\right| > 1 - \varepsilon \,.$$

$|M|$ = Lebesgue measure of M

Proof

time average $\overline{f(t)} = \lim_{T\to\infty} \frac{1}{T}\int_0^T f(t)\,dt$

$\overline{\langle\psi_t|P_{\mathrm{eq}}|\psi_t\rangle} = ?$

$$\psi_0 = \sum_{\alpha=1}^{\dim\mathscr{H}} c_\alpha|\phi_\alpha\rangle\,, \qquad \psi_t = \sum_{\alpha=1}^{\dim\mathscr{H}} e^{-iE_\alpha t} c_\alpha|\phi_\alpha\rangle$$

$$\begin{aligned}\overline{\langle\psi_t|P_{\mathrm{eq}}|\psi_t\rangle} &= \sum_{\alpha,\beta} \underbrace{\overline{e^{i(E_\alpha - E_\beta)t}}}_{\delta_{\alpha\beta}} c_\alpha^* c_\beta \langle\phi_\alpha|P_{\mathrm{eq}}|\phi_\beta\rangle \\ &= \sum_\alpha |c_\alpha|^2 \underbrace{\langle\phi_\alpha|P_{\mathrm{eq}}|\phi_\alpha\rangle}_{>1-\eta\varepsilon} \\ &> 1 - \eta\varepsilon\end{aligned}$$

If $\mathrm{error}(t) > \eta$ for more than ε of the time then $\overline{\mathrm{error}(t)} > \eta\varepsilon$.

Thus, $\langle\psi_t|P_{\mathrm{eq}}|\psi_t\rangle > 1 - \eta$ for $(1-\varepsilon)$-most of the time. □

Theorem: Most H satisfy ETH [GLMTZ 0911.1724]

Let $\varepsilon, \delta > 0$, E_α pairwise distinct real values, $\{\phi_\alpha\}$ a random ONB of $\mathscr{H}$ with uniform distribution, $H = \sum_\alpha E_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$.
If $\dim \mathscr{H} > D_0(\varepsilon, \delta)$ and

$$\frac{\dim \mathscr{H}_{\mathrm{eq}}}{\dim \mathscr{H}} > 1 - \varepsilon\,,$$

then $\mathrm{MATE}_{2\varepsilon}$-ETH is $(1-\delta)$-typically satisfied, i.e.,

$$\mathrm{Prob}\Big\{ \langle\phi_\alpha|P_{\mathrm{eq}}|\phi_\alpha\rangle > 1 - 2\varepsilon \quad \forall \alpha = 1, \ldots, \dim \mathscr{H} \Big\} > 1 - \delta\,.$$

- There do exist exceptional Hamiltonians that don't satisfy MATE-ETH (e.g., non-interacting, Anderson localization).

A concrete H that satisfies MATE-ETH

Theorem [after Tasaki-Shiraishi 2310.18880, Tasaki 2404.04533]

Let $\eta > 0$, $\mathscr{H}$ the Hilbert space of N fermions on a 1d periodic lattice with L sites, H the discrete Laplacian with nonzero magnetic field through the ring (no interaction between the fermions), 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 N and L/N sufficiently large and under some technical assumptions, H satisfies MATE-ETH.

Ultrafast thermalization

[Goldstein-Hara-Tasaki 1307.0572,1402.3380, Reimann 1603.00669]

Theorem

If the eigenbasis $(\phi_\alpha)_\alpha$ of H is random with uniform distribution and $\nu_0 \neq \mathrm{eq}$, then with probability near 1, most $\psi \in \mathbb{S}(\mathscr{H}_{\nu_0})$ reach MATE in a time of the order of the Boltzmann time $\hbar/k_{\mathrm{B}}T$ ($T =$ temperature), which is about 10^{-13} seconds at room temperature.

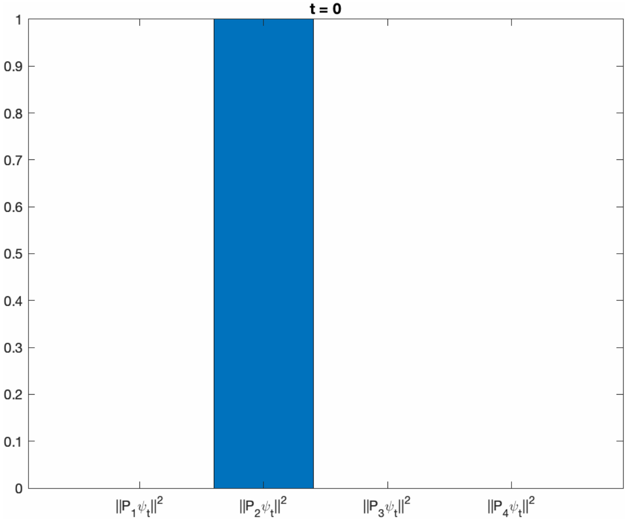
- This doesn't happen in reality, which shows that such random H are not realistic.
- This class of random matrices includes GUE. Also H satisfying the strong ETH display ultrafast thermalization [Riabov-Erdős 2404.17512].
- The reason behind the theorem is that H provides transition elements for any ψ to directly go to $\mathscr{H}_{\mathrm{eq}}$.
- The reason this doesn't happen in reality is local conservation laws.

Does this fact invalidate typicality reasoning?

No. It shows that $(\phi_\alpha)_\alpha$ and the joint eigenbasis of P_ν are not unrelated.

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

Simulation by Cornelia Vogel:



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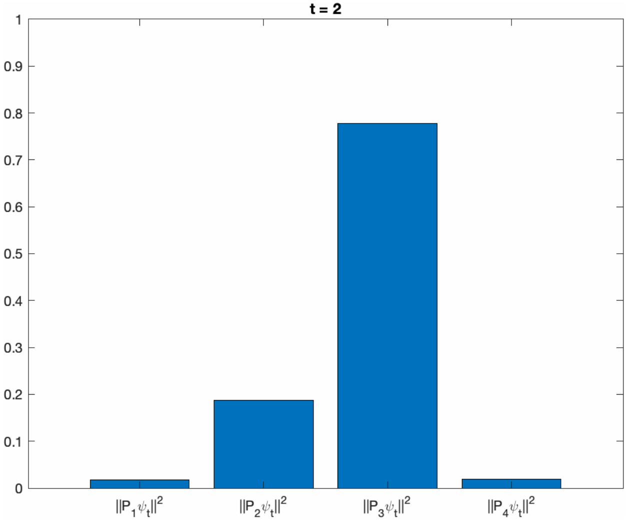

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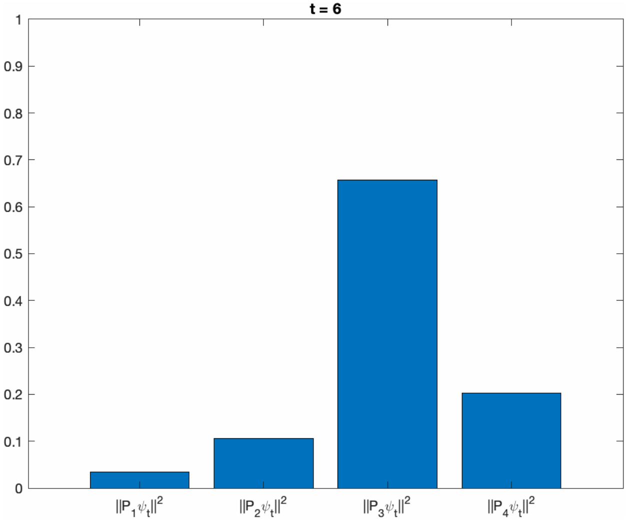

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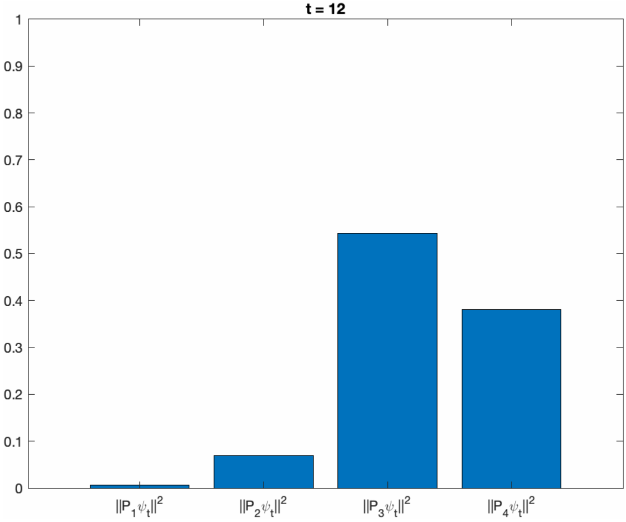

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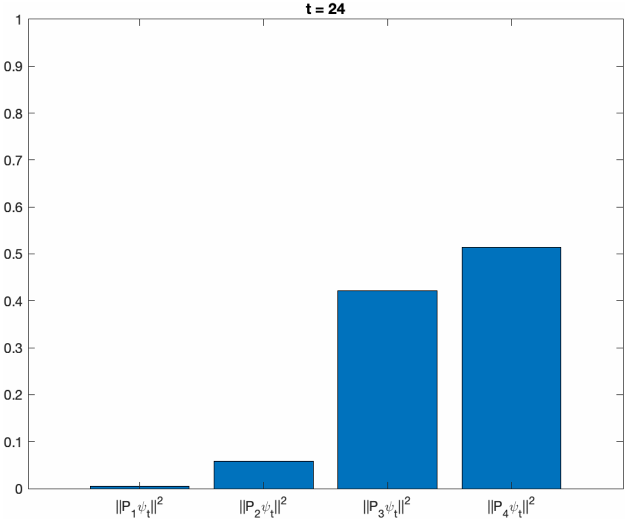

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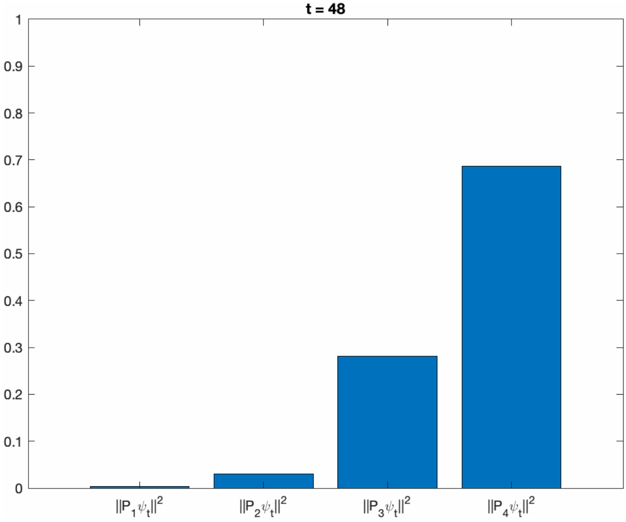


Dynamical typicality

[Bartsch-Gemmer 0902.0927, Reimann 1805.07085, rigorously Müller-Gross-Eisert 1003.4982]

- I present here only a simplified statement: Most $\psi_0 \in \mathbb{S}(\mathscr{H}_{\nu_0})$ have the same macro history $(\nu, t) \mapsto \|P_\nu \psi_t\|^2$ (for a long time).

Theorem [Teufel-T-Vogel 2210.10018]

Let

$$w_{\nu_0\nu}(t) := \frac{1}{d_{\nu_0}} \mathrm{tr}\Big[P_{\nu_0} \exp(iHt) P_\nu \exp(-iHt)\Big] = \mathbb{E}_{\psi_0 \sim u_{\mathbb{S}(\mathscr{H}_{\nu_0})}} \|P_\nu \psi_t\|^2 .$$

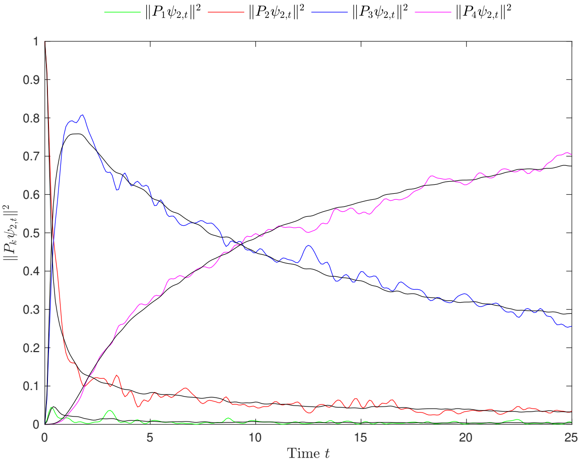
For every $t \in \mathbb{R}$, $T > 0$, $\varepsilon > 0$, and $(1-\varepsilon)$-most $\psi_0 \in \mathbb{S}(\mathscr{H}_{\nu_0})$,

$$\Big| \|P_\nu \psi_t\|^2 - w_{\nu_0\nu}(t) \Big| \leq \frac{1}{\sqrt{\varepsilon d_{\nu_0}}}$$

and

$$\frac{1}{T} \int_0^T dt \, \Big| \|P_\nu \psi_t\|^2 - w_{\nu_0\nu}(t) \Big|^2 \leq \frac{1}{\varepsilon d_{\nu_0}} .$$

Numerical example



For a random Gaussian band matrix, we can show that also the *relative* errors are small, and thus cover the case of small $w_{\nu_0\nu}$ [T-T-V 2303.13242].

Fraction equilibrium = generalized normal equilibrium

- Most $\psi \in \mathbb{S}(\mathscr{H})$ have $\|P_\nu \psi\|^2 = d_\nu / d$ (the "normal histogram").
- Von Neumann proposed to take this as the definition of thermal equilibrium. But it is not really a *thermal* equilibrium, it is a different kind of equilibrium ("normal equilibrium").
- But it tends to occur in the long run:

Theorem on normal typicality [von Neumann 1929, GLMTZ 0907.0108]

Let $\varepsilon > 0$, and let H have arbitrary distinct eigenvalues with nondegenerate gaps and a uniformly distributed eigenbasis. Under some technical conditions, with probability close to 1, every $\psi \in \mathbb{S}(\mathscr{H})$ satisfies for most $t \in [0, \infty)$ that

$$\left| \|P_\nu \psi_t\|^2 - \frac{d_\nu}{d} \right| < \varepsilon \frac{d_\nu}{d} \,.$$

Let's move away from the unrealistic assumption that $(\phi_\alpha)_\alpha$ is uniformly distributed: Every initial macro state ν_0 has a typical long-time histogram, $\|P_\nu \psi_t\|^2 \approx M_{\nu_0 \nu}$.

Theorem on fraction equilibrium [Teufel-T-Vogel 2210.10018]

Let ν_0, ν be any macro states, and let H have eigenvalues $e \in \mathcal{E}$, eigenprojections Π_e, maximal degeneracy D_E and maximal gap degeneracy D_G. Define

$$M_{\nu_0 \nu} := \frac{1}{d_{\nu_0}} \sum_{e \in \mathcal{E}} \mathrm{tr}\left(P_{\nu_0} \Pi_e P_\nu \Pi_e\right) . \tag{1}$$

Then for any $\varepsilon, \delta > 0$, $(1-\varepsilon)$-most $\psi_0 \in \mathbb{S}(\mathscr{H}_{\nu_0})$ are such that for $(1-\delta)$-most $t \in [0, \infty)$

$$\left| \|P_\nu \psi_t\|^2 - M_{\nu_0 \nu} \right| \leq 4 \sqrt{\frac{D_E D_G}{\delta \varepsilon d_{\nu_0}} \min\left\{1, \frac{d_\nu}{d_{\nu_0}}\right\}} .$$

Entropy and the 2nd law

- Def: quantum Boltzmann entropy $S_{\mathrm{B}}(\nu) := \log d_\nu$ [Lebowitz 1993, Griffiths 1994, Goldstein-Lebowitz-T-Zanghì 1903.11870].
- $S_{\mathrm{B}}(\mathrm{eq}) \approx \log \dim \mathscr{H}_{\mathrm{mc}}$
- Since a general ψ is a superposition of different ν's, it is also a superposition of different entropy values.
- Thus, it is not obvious what it means to say that entropy increases.

- Some authors have considered the *average* entropy $\sum_\nu \|P_\nu \psi_t\|^2 \, S(\nu)$. But we don't just want the average, we want the entropy *in our branch of the wave function*.
- Here, the foundations of statistical mechanics touch the foundations of quantum mechanics. Orthodox QM is too vage. Many-worlds or spontaneous collapse (such as GRW) or hidden variables (such as Bohmian mechanics) provide justified 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: the "strong 2nd law"

For reasonable H and macro spaces $\mathscr{H}_\nu$, any ν_0, and most $\psi \in \mathbb{S}(\mathscr{H}_{\nu_0})$, 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.

Slightly weaker version

For reasonable H and macro spaces $\mathscr{H}_\nu$, any ν_0, and most $\psi \in \mathbb{S}(\mathscr{H}_{\nu_0})$, 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.

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,

$$\frac{dp_\nu}{dt} = \sum_{\nu' \neq \nu} \big(\sigma_{\nu\nu'}\, p_{\nu'}(t) - \sigma_{\nu'\nu}\, p_\nu(t)\big) \tag{2}$$

with jump rates $\sigma_{\nu\nu'}$ given for $\nu \neq \nu'$ by

$$\sigma_{\nu\nu'} = \frac{1}{\tau d_{\nu'}} \mathrm{tr}\big(e^{iH\tau} P_\nu e^{-iH\tau} P_{\nu'}\big) = \frac{1}{\tau} \mathbb{E}_{\psi_0 \sim u_{\mathbb{S}(\mathscr{H}_{\nu'})}} \|P_\nu \psi_\tau\|^2 \tag{3}$$

for $\tau > 0$ that is small (so the expression doesn't depend much on τ) but not too small (or else $\sigma_{\nu\nu'} = 0$).

Van Kampen gave some heuristic reasons for his hypothesis, Strasberg-Winter-Gemmer-Wang [2209.07977] further arguments in support of it and the following

Hypothesis of local detailed balance

$$\frac{\sigma_{\nu\nu'}}{\sigma_{\nu'\nu}} \approx \frac{d_\nu}{d_{\nu'}} \tag{4}$$

Whether (2), (3), (4) are satisfied in practice remains an open problem.

Together, (2), (3), (4) almost imply the strong 2nd law.

They do imply that the histogram of S_{qB} is approximately right-moving. If $J_{\nu\nu'} \approx \sigma_{\nu\nu'} p_{\nu'} - \sigma_{\nu'\nu} p_\nu$, which at least seems plausible, then also the strong 2nd law is fulfilled.

Thank you for your attention