Of MITE and MATE
or
Macroscopic and Microscopic Thermal Equilibrium

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Overview

Macroscopic thermal equilibrium (MATE)

A quantum system in state $\psi \in \mathscr{H}$ is in MATE when all macro observables assume rather sharp values in ψ that agree with their thermodynamic equilibrium values.
(As we will discuss, most ψ in a given micro-canonical energy shell are in MATE.)

For generic macroscopic systems most ψ have a stronger property:

Microscopic thermal equilibrium (MITE)

A quantum system in state $\psi \in \mathscr{H}$ is in MITE when all micro observables (i.e., those referring only to a small subsystem S) have a probability distribution in ψ that coincides with their thermal probability distribution.
(This property is a sign of a high degree of entanglement in ψ between S and its complement.)

"Ordinary" systems (satisfying eigenstate thermalization hypothesis = ETH) approach MATE and MITE.
Systems with many-body Anderson localization (MBL) do not necessarily.

ρ versus X

- One often says that

> "a system with Hamiltonian H is in a thermal state if $\rho = Z^{-1}e^{-\beta H}$ for some $\beta \in \mathbb{R}$" (classically or quantum)

- But one often wants to consider an individual closed, macroscopic system in thermal equilibrium. Is *this particular* thermos bottle of coffee in thermal equilibrium?
- A classical system always has a phase point X, not a probability distribution ρ over phase space Γ.
- So a system should be in thermal equilibrium whenever X belongs to a certain set Γ_{eq}. This set does not necessarily have a precise definition, just as it is not precisely defined which 0-1 sequences of length N "look random."
- Just like a randomly chosen 0-1 sequence looks random with high probability, a phase point chosen with distribution $\rho = Z^{-1}e^{-\beta H}$ lies in Γ_{eq} with high probability.

Thermal equilibrium in classical mechanics

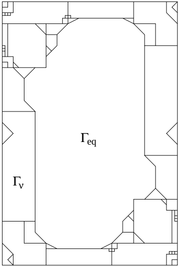
- State: point $X = (\mathbf{q}_1, \ldots, \mathbf{q}_N, \mathbf{p}_1, \ldots, \mathbf{p}_N)$ in phase space
- energy shell $\Gamma_{\mathrm{mc}} = \{X : E - \Delta E \leq H(X) \leq E\}$
- depending on a choice of macro-variables, partition Γ_{mc} into macro-states Γ_ν corresponding to different (small ranges of) values of the macro-variables,

$$\Gamma_{\mathrm{mc}} = \bigcup_\nu \Gamma_\nu$$

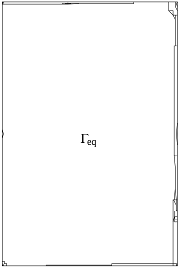
- one cell Γ_{eq} has the overwhelming majority of volume,

$$\frac{\mathrm{vol}\,\Gamma_{\mathrm{eq}}}{\mathrm{vol}\,\Gamma_{\mathrm{mc}}} \approx 1.$$

- <u>Def:</u> A system is in equilibrium $\Leftrightarrow$ its phase point lies in the set Γ_{eq}.



or rather:



ρ versus ψ

- Like a classical pure state $X \in \Gamma$, a quantum pure state $\psi \in \mathscr{H}$ can be in thermal equilibrium.
- Example: Put a hot brick on top of a cold one. What happens? Thermal behavior: Energy gets transported from the hot to the cold one.
- This occurs also, of course, for a pure state ψ during unitary evolution (say, if the system of two bricks is closed). Interaction with an environment is not needed.

Notation and terminology

- $H = \sum_\alpha E_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$
- micro-canonical energy shell $\mathscr{H}_{\mathrm{mc}}$ spanned by eigenvectors ϕ_α of H with $E - \Delta E \leq E_\alpha \leq E$
- The width ΔE represents the macroscopic resolution of energy.
- Typically, $d_{\mathrm{mc}} := \dim \mathscr{H}_{\mathrm{mc}} \approx 10^{10^{10}}$.
- P_{mc} = projection to $\mathscr{H}_{\mathrm{mc}}$
- $\rho_{\mathrm{mc}} = d_{\mathrm{mc}}^{-1} P_{\mathrm{mc}}$ micro-canonical density matrix
- $\mathbb{S}(\mathscr{H}_{\mathrm{mc}}) = \Big\{\psi \in \mathscr{H}_{\mathrm{mc}} : \|\psi\| = 1\Big\}$ = unit sphere
- u_{mc} = uniform probability measure on $\mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ (normalized area)

Macro states in quantum mechanics

- macro states correspond to subspaces $\mathscr{H}_\nu$, mutually orthogonal,

$$\mathscr{H}_{\mathrm{mc}} = \bigoplus_\nu \mathscr{H}_\nu$$

- thermal equilibrium subspace $\mathscr{H}_{\mathrm{eq}} \subset \mathscr{H}_{\mathrm{mc}}$ with

$$\frac{\dim \mathscr{H}_{\mathrm{eq}}}{\dim \mathscr{H}_{\mathrm{mc}}} = 1 - \varepsilon$$

In practice, usually $\varepsilon \leq \exp(-10^{-15} N)$ for N degrees of freedom, so $\varepsilon < 10^{-10^5}$ for $N > 10^{20}$.

Def: A system is in MATE $\Leftrightarrow$ ψ is close to $\mathscr{H}_{\mathrm{eq}}$ $\Leftrightarrow$

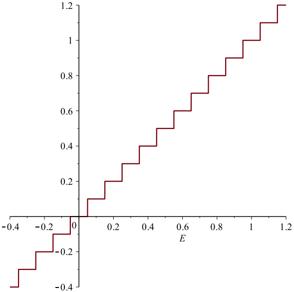
$$\langle \psi | P_{\mathrm{eq}} | \psi \rangle \geq 1 - \delta$$

say with $\delta = 10^{-200}$, so $0 < \varepsilon \ll \delta$.

Macro observables

John von Neumann 1929

- $M_1, \ldots, M_K$ macro observables (e.g., net spin in a macro 3-region)
- The M_j commute approximately.
- Change the M_j a little so as to make them commute exactly.
- Coarse grain the M_j to macro resolution.
- The joint eigenspaces of the M_j provide an orthogonal decomposition $\mathscr{H} = \oplus_\nu \mathscr{H}_\nu$ into macro spaces $\mathscr{H}_\nu$.



Are almost commuting operators near commuting ones?

Theorem (Huaxin Lin 1995): Yes for 2 operators

If $\|[A,B]\| \ll 1$ then there are $\tilde{A}$ and $\tilde{B}$ near A, B with $[\tilde{A},\tilde{B}] = 0$.

Theorem (M.D.Choi 1988): No in general

There are self-adjoint $d \times d$ matrices A_1, A_2, A_3 with $\|[A_i, A_j]\| \leq 3/d$, so that for any commuting $\tilde{A}_1, \tilde{A}_2, \tilde{A}_3$,

$$\|A_1 - \tilde{A}_1\| + \|A_2 - \tilde{A}_2\| + \|A_3 - \tilde{A}_3\| \geq \sqrt{1 - 8/d}\,.$$

Theorem (Yoshiko Ogata 2013): Yes for averages

Let $\mathscr{H} = (\mathbb{C}^d)^N$, let L_{jk} be $L_j : \mathbb{C}^n \to \mathbb{C}^n$ acting on the k-th factor space, and let

$$A_{jN} = \frac{1}{N}\sum_{k=1}^{N} L_{jk}\,.$$

Then there are commuting operators M_{jN} with $\lim_{N\to\infty} \|M_{jN} - A_{jN}\| = 0$.

Fact: Most ψ lie in MATE.

$u_{\mathrm{mc}}(MATE) > 1 - \varepsilon/\delta \approx 1$.

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 no more than $1 - \varepsilon/\delta$ of all ψ's had $f(\psi) > 1 - \delta$. $\square$

Most $\psi \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ lie not only in MATE but have a stronger property based on canonical typicality: Microscopic thermal equilibrium = MITE

Canonical typicality

- Let S be a small subsystem and $\rho_S^\psi = \mathrm{tr}_{S^c} |\psi\rangle\langle\psi|$ the reduced density operator.
- For most $\psi \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ is ρ_S^ψ "canonical,"

$$\rho_S^\psi \approx \rho_S^{\mathrm{can}}$$

with $\rho_S^{\mathrm{can}} = \mathrm{tr}_{S^c}\, \rho^{\mathrm{can}}$. If the interaction between S and S^c is weak, then $\rho_S^{\mathrm{can}} = (1/Z_S)\, e^{-\beta H_S}$.

Def: $\psi \in \mathit{MITE} \Leftrightarrow \left\|\rho_S^\psi - \rho_S^{\mathrm{can}}\right\| < \varepsilon$ for every spatial subsystem S with diameter $\leq \ell_0$,
where ℓ_0 is such that $\rho_S^{\mathrm{mc}} \approx \rho_S^{\mathrm{can}}$ for subsystems with diameter $\leq \ell_0$.

In classical mechanics there is no analog of MITE for pure states

because every subsystem is then also in a pure state and not close to a thermal ρ.

Theorem about canonical typicality (Popescu-Short-Winter 2005)

Let $\varepsilon > 0$, $\mathscr{H}_S, \mathscr{H}_{S^c}$ of finite dimension d_S, d_{S^c}, and $\mathscr{H}_{\mathrm{mc}} \subset \mathscr{H}_S \otimes \mathscr{H}_{S^c}$ an arbitrary subspace of dimension d_{mc}. If $d_S < \frac{1}{2}\varepsilon\sqrt{d_{\mathrm{mc}}}$, then

$$u_{\mathrm{mc}}\Big\{\psi \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}}) : \big\|\rho_S^\psi - \rho_S^{\mathrm{mc}}\big\| < \varepsilon\Big\} \geq 1 - 4\exp\Big(-\frac{d_{\mathrm{mc}}\varepsilon^2}{72\pi^3}\Big),$$

where $\|A\| = \mathrm{tr}\sqrt{A^*A}$ (trace norm).

This means for a system of N spins that, for any subsystem S of up to $N/2$ spins, $\rho_S^\psi \approx \rho_S^{\mathrm{mc}}$. For small S (e.g., 10^{-3} of full diameter), $\rho_S^{\mathrm{mc}} \approx \rho_S^{\mathrm{can}}$ (equivalence of ensembles) $\Rightarrow$ canonical typicality.

Rule of thumb: For subsystems of $< \frac{1}{2}$ the volume, typically $\rho_S^\psi \approx \rho_S^{\mathrm{mc}}$.

One can show that that is not so for subsystems of $> \frac{1}{2}$ the volume.

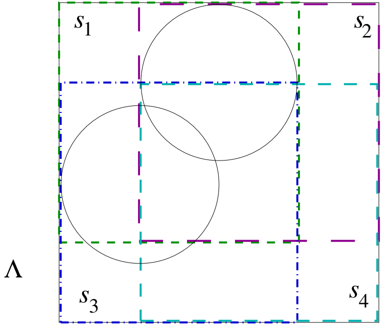
Entanglement-driven

Canonical typicality reflects the high degree of entanglement between S and S^c.

Most ψ are in MITE

Subsubsystem property

If $\rho_S^\psi \approx \rho_S^{\mathrm{mc}}$ for some subsystem S, then the same is true for every smaller $S' \subset S$. (Take the partial trace on both sides.)



In a cube of side length 1, there are 8 smaller cubes s_i of side length $0.79 < 2^{1/3}$ and thus volume $< \frac{1}{2}$ so that every set of diameter < 0.29 is contained in one s_i.

Corollary

Most $\psi \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ lie in MITE.

General framework of MATE and MITE

Def: Let $\mathscr{A}$ be a set of observables. A system (in ψ or ρ) is in $\mathscr{A}$-TE iff for every $A \in \mathscr{A}$, the probability distribution over the spectrum of A is approximately equal to the thermal distribution defined by ρ^{mc}.

- $\mathscr{A}_{\mathsf{MATE}} = \{M_1, \ldots, M_K\}$ = macro observables
- $\mathscr{A}_{\mathsf{MITE}} = \bigcup_S \mathscr{A}_S$ over all regions S of diameter $\leq \ell_0$ and $\mathscr{A}_S$ = all observables in S.

MATE = TE relative to all macro observables
MITE = TE relative to all "local" observables

Since every macro observable has a dominant eigenvalue (whose eigenspace has > 99% of dimensions), the thermal distribution is essentially concentrated on that one value; thus, $\mathscr{A}_{\mathsf{MATE}}$-TE $= \{P_{\mathrm{eq}}\}$-TE. Different for local observables: non-trivial distribution.

MITE implies MATE for macro systems

because macro observables M_j are sums of local observables referring to spatial cells of size L. Since realistically $L \leq \ell_0$ for macro systems, $\psi \in$ MITE displays thermal behavior for local observ.s and thus for M_j.

Example of $\psi \in$ MATE, $\psi \notin$ MITE

$N \gg 1$ spins-$\frac{1}{2}$, $\mathscr{H} = (\mathbb{C}^2)^{\otimes N}$, $H = 0$, $\mathscr{H}_{\mathrm{mc}} = \mathscr{H}$. Choose

$$\psi = \otimes_i \psi_i \qquad \text{at random.}$$

MATE: $M_j =$ total spin in j-th macro cell, thermal value $= 0 \Rightarrow$ YES
MITE: $\rho_S^{\psi} = |\psi_i\rangle\langle\psi_i| \neq \frac{1}{2} I = \rho_S^{\mathrm{mc}} \quad \Rightarrow$ NO

Dynamical approach to thermal equilibrium

ETH = eigenstate thermalization hypothesis (Srednicki 1994)

The energy eigenstates ϕ_α are in thermal equilibrium.
MATE-ETH: all $\phi_\alpha \in \mathrm{MATE}_{\delta^2}$

That's a condition on H.

Theorem: approach to MATE

If $\dim \mathscr{H}_{\mathrm{mc}} < \infty$, H is non-degenerate, and MATE-ETH holds, then every $\psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ sooner or later reaches MATE_δ and spends there most of the time in the long run, i.e.,

$$\liminf_{T\to\infty} \frac{1}{T}\left|\left\{0 < t < T : \psi_t \in \mathrm{MATE}_\delta\right\}\right| > 1-\delta\,.$$

Proof: approach to MATE

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

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

$$\psi_0 = \sum_{\alpha=1}^{d_{\rm mc}} c_\alpha|\phi_\alpha\rangle\,, \qquad \psi_t = \sum_{\alpha=1}^{d_{\rm mc}} e^{-iE_\alpha t} c_\alpha|\phi_\alpha\rangle$$

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

If error$(t) > \delta$ for more than the fraction δ of time then $\overline{\text{error}(t)} > \delta^2$.

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

When is ETH satisfied?

Examples that violate ETH

- non-interacting H
- MBL $=$ many-body localization

Yet, *every* macro system satisfies almost MATE-ETH: most $\phi_\alpha \in$ MATE

Proof: $d_{\mathrm{mc}}^{-1} \sum_{\alpha=1}^{d_{mc}} \langle \phi_\alpha | P_{\mathrm{eq}} | \phi_\alpha \rangle = d_{\mathrm{mc}}^{-1} \operatorname{tr}(P_{\mathrm{eq}}) = 1 - \varepsilon$, and since $0 \leq \langle \phi_\alpha | P_{\mathrm{eq}} | \phi_\alpha \rangle \leq 1$, most of these terms must be close to 1. □

Theorem (GLMTZ 2010): random H satisfies ETH

If d_{mc} is sufficiently large and $d_{\mathrm{eq}}/d_{\mathrm{mc}}$ sufficiently close to 1, then most ONBs of $\mathscr{H}_{\mathrm{mc}}$ have all basis vectors in MATE_{δ^2}.

Numerical evidence (Kim-Ikeda-Huse 2014)

points to the existence of systems with realistic interactions for which all energy eigenstates are in MITE and thus also in MATE.

Approach to MITE

Assumptions:

1. $d_{\mathrm{mc}} < \infty$
2. H is non-degenerate
3. MITE_{δ^2}-ETH
4. non-degenerate energy gaps, i.e.,

$$E_\alpha - E_\beta \neq E_{\alpha'} - E_{\beta'} \text{ unless } \begin{cases} \text{either } \alpha = \alpha' \text{ and } \beta = \beta' \\ \text{or } \alpha = \beta \text{ and } \alpha' = \beta' \,, \end{cases}$$

Theorem (Reimann 2008, Linden-Popescu-Short-Winter 2009)

Assuming 1–4, most $\psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ spend most of the time in MITE_δ.

Theorem (Rigol-Dunjko-Olshanii 2008)

Assume 1–4 and the following off-diagonal extension of ETH:

$$\Big|\langle\phi_\alpha|A|\phi_\beta\rangle\Big| < \delta^2 \qquad \forall\alpha \neq \beta,\ \forall A \in \mathscr{A}_{\mathrm{MITE}}\,.$$

Then all $\psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{mc}})$ spend $(1-\delta)$-most of the time in MITE_δ.

MBL = many-body localization

- generalization of Anderson localization
- no general definition
- Some eigenstates ϕ_α of H are in some sense "localized."
- Most ϕ_α have a short range of entanglement.
- In fact, typically $(|\phi_\alpha\rangle\langle\phi_\alpha|)_S$ for small spatial region S has substantially lower von Neumann entropy than ρ_S^{can}.
- As a consequence, most ϕ_α fail to be in MITE.
- This remains true under local perturbations.
- As a consequence, many ψ may fail to thermalize.
- We know that *every* H must have most ϕ_α in MATE.
- In some MBL systems, $\forall\alpha$ either $\phi_\alpha \in \mathscr{H}_{\mathrm{eq}}$ or $\phi_\alpha \perp \mathscr{H}_\alpha$ (approximately).
- In that case, MATE-ETH is violated as strongly as possible, and contributions $\perp \mathscr{H}_{\mathrm{mc}}$ never thermalize in either MATE or MITE.

Thank you for your attention