Of MITE and MATE
or
Macroscopic and Microscopic Thermal Equilibrium

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<table>
<thead>
<tr>
<th>Macroscopic thermal equilibrium (MATE)</th>
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<td>A quantum system in state $\psi \in \mathcal{H}$ is in MATE when all macro observables assume rather sharp values in $\psi$ that agree with their thermodynamic equilibrium values. (As we will discuss, most $\psi$ in a given micro-canonical energy shell are in MATE.)</td>
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For generic macroscopic systems most $\psi$ have a stronger property:

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<td>A quantum system in state $\psi \in \mathcal{H}$ is in MITE when all micro observables (i.e., those referring only to a small subsystem $S$) have a probability distribution in $\psi$ that coincides with their thermal probability distribution. (This property is a sign of a high degree of entanglement in $\psi$ between $S$ and its complement.)</td>
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“Ordinary” systems (satisfying eigenstate thermalization hypothesis = ETH) approach MATE and MITE.

Systems with many-body Anderson localization (MBL) do not necessarily.
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 $\rho$ over phase space $\Gamma$.

So a system should be in thermal equilibrium whenever $X$ belongs to a certain set $\Gamma_{\text{eq}}$. 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 $\Gamma_{\text{eq}}$ with high probability.
Thermal equilibrium in classical mechanics

- **State**: point $X = (q_1, \ldots, q_N, p_1, \ldots, p_N)$ in phase space

- **Energy shell**
  $\Gamma_{mc} = \{X : E - \Delta E \leq H(X) \leq E\}$

- Depending on a choice of macro-variables, partition $\Gamma_{mc}$ into macro-states $\Gamma_\nu$ corresponding to different (small ranges of) values of the macro-variables,

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

- One cell $\Gamma_{eq}$ has the overwhelming majority of volume,

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

- **Def**: A system is in equilibrium $\iff$ its phase point lies in the set $\Gamma_{eq}$. 

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Macroscopic and Microscopic Thermal Equilibrium
Like a classical pure state $X \in \Gamma$, a quantum pure state $\psi \in \mathcal{H}$ 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 $\psi$ 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 \( \mathcal{H}_{mc} \) spanned by eigenvectors \( \phi_\alpha \) of \( H \) with \( E - \Delta E \leq E_\alpha \leq E \)
- The width \( \Delta E \) represents the macroscopic resolution of energy.
- Typically, \( d_{mc} := \text{dim} \mathcal{H}_{mc} \approx 10^{10^{10}} \).
- \( P_{mc} \) = projection to \( \mathcal{H}_{mc} \)
- \( \rho_{mc} = d_{mc}^{-1} P_{mc} \) micro-canonical density matrix
- \( S(\mathcal{H}_{mc}) = \{ \psi \in \mathcal{H}_{mc} : \|\psi\| = 1 \} = \text{unit sphere} \)
- \( u_{mc} = \text{uniform probability measure on } S(\mathcal{H}_{mc}) \) (normalized area)
Macro states in quantum mechanics

- Macro states correspond to subspaces $\mathcal{H}_\nu$, mutually orthogonal,

$$\mathcal{H}_{mc} = \bigoplus \mathcal{H}_\nu$$

- Thermal equilibrium subspace $\mathcal{H}_{eq} \subset \mathcal{H}_{mc}$ with

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

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 $\iff \psi$ is close to $\mathcal{H}_{eq}$ $\iff$

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

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 $\mathcal{H} = \bigoplus \nu \mathcal{H}_\nu$ into macro spaces $\mathcal{H}_\nu$. 
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 $\mathcal{H} = (\mathbb{C}^d)^N$, 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 $\lim_{N \to \infty} \|M_{jN} - A_{jN}\| = 0$. 

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Macroscopic and Microscopic Thermal Equilibrium
Fact: Most $\psi$ lie in MATE.

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

Proof: $\mathbb{E}_\psi \langle \psi | P_{eq} | \psi \rangle = \text{tr}(P_{eq} \rho_{mc}) = \dim \mathcal{H}_{eq} / \dim \mathcal{H}_{mc} = 1 - \varepsilon$, but the average of $f(\psi) = \langle \psi | P_{eq} | \psi \rangle$ could not be that high if no more than $1 - \varepsilon/\delta$ of all $\psi$’s had $f(\psi) > 1 - \delta$. \hfill \Box

Most $\psi \in \mathcal{S}(\mathcal{H}_{mc})$ lie not only in MATE but have a stronger property based on canonical typicality: Microscopic thermal equilibrium $= \text{MITE}$
Let $S$ be a small subsystem and $\rho_S^\psi = \text{tr}_{S^c} |\psi\rangle\langle\psi|$ the reduced density operator.

For most $\psi \in S(H_{mc})$ is $\rho_S^\psi$ “canonical,”

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

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

**Def:** $\psi \in MITE \iff \|\rho_S^\psi - \rho_S^{\text{can}}\| < \varepsilon$ for every spatial subsystem $S$ with diameter $\leq \ell_0$,

where $\ell_0$ is such that $\rho_S^{mc} \approx \rho_S^{\text{can}}$ 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 $\rho$. 
Theorem about canonical typicality (Popescu-Short-Winter 2005)

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

$$u_{mc} \left\{ \psi \in \mathcal{S}(\mathcal{H}_{mc}) : \| \rho^\psi_S - \rho^{mc}_S \| < \varepsilon \right\} \geq 1 - 4 \exp \left( - \frac{d_{mc} \varepsilon^2}{72 \pi^3} \right),$$

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

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

Rule of thumb: For subsystems of $< \frac{1}{2}$ the volume, typically $\rho^\psi_S \approx \rho^{mc}_S$.

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 $S^c$. 
Subsystem property

If $\rho^\psi_S \approx \rho^\text{mc}_S$ 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 $\psi \in S(\mathcal{H}_\text{mc})$ lie in MITE.
**Def:** Let $\mathcal{A}$ be a set of observables. A system (in $\psi$ or $\rho$) is in $\mathcal{A}$-TE iff for every $A \in \mathcal{A}$, the probability distribution over the spectrum of $A$ is approximately equal to the thermal distribution defined by $\rho^{mc}$.

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

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, $\mathcal{A}_{\text{MATE}}$-TE = $\{P_{eq}\}$-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, $\psi \in \text{MITE}$ displays thermal behavior for local observables and thus for $M_j$.

**Example of $\psi \in \text{MATE}, \psi \notin \text{MITE}$**

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

$$\psi = \otimes_i \psi_i$$

at random.

**MATE**: $M_j =$ total spin in $j$-th macro cell, thermal value $= 0 \Rightarrow \text{YES}$

**MITE**: $\rho_S^\psi = |\psi_i\rangle \langle \psi_i| \neq \frac{1}{2} I = \rho_S^{\text{mc}} \Rightarrow \text{NO}$
Dynamical approach to thermal equilibrium

ETH = eigenstate thermalization hypothesis (Srednicki 1994)

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

That’s a condition on $H$.

Theorem: approach to MATE

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

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

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

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

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

$\langle \psi_t | P_{eq} | \psi_t \rangle = \sum_{\alpha, \beta} \left( \frac{e^{i(E_{\alpha} - E_{\beta}) t}}{\delta_{\alpha \beta}} \right) c^*_{\alpha} c_{\beta} \langle \phi_{\alpha} | P_{eq} | \phi_{\beta} \rangle$

$= \sum_{\alpha} |c_{\alpha}|^2 \langle \phi_{\alpha} | P_{eq} | \phi_{\alpha} \rangle$

$> 1 - \delta^2$

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

Thus, $\langle \psi_t | P_{eq} | \psi_t \rangle > 1 - \delta$ for $(1 - \delta)$-most of the time. $\square$
When is ETH satisfied?

Examples that violate ETH

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

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

Proof: 
\[
  d_{mc}^{-1} \sum_{\alpha=1}^{d_{mc}} \langle \phi_\alpha | P_{eq} | \phi_\alpha \rangle = d_{mc}^{-1} \text{tr}(P_{eq}) = 1 - \varepsilon,
\]

and since
\[
  0 \leq \langle \phi_\alpha | P_{eq} | \phi_\alpha \rangle \leq 1,
\]
most of these terms must be close to 1.

Theorem (GLMTZ 2010): random $H$ satisfies ETH

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

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

$$E_\alpha - E_\beta \neq E_{\alpha'} - E_{\beta'}$$

unless

$$\begin{align*}
\text{either } \alpha &= \alpha' \text{ and } \beta = \beta' \\
\text{or } \alpha &= \beta \text{ and } \alpha' = \beta',
\end{align*}$$

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

Assuming 1–4, most $\psi_0 \in S(H_{mc})$ spend most of the time in $MITE_\delta$.

Theorem (Rigol-Dunjko-Olshanii 2008)

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

$$\langle \phi_\alpha | A | \phi_\beta \rangle < \delta^2 \quad \forall \alpha \neq \beta, \forall A \in \mathcal{A}_{MITE}.$$ 

Then all $\psi_0 \in S(H_{mc})$ spend $(1 - \delta)$-most of the time in $MITE_\delta$. 

generalization of Anderson localization
no general definition
Some eigenstates $\phi_\alpha$ of $H$ are in some sense “localized.”
Most $\phi_\alpha$ 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 $\rho_S^{\text{can}}$.
As a consequence, most $\phi_\alpha$ fail to be in MITE.
This remains true under local perturbations.
As a consequence, many $\psi$ may fail to thermalize.
We know that every $H$ must have most $\phi_\alpha$ in MATE.
In some MBL systems, $\forall \alpha$ either $\phi_\alpha \in \mathcal{H}_{\text{eq}}$ or $\phi_\alpha \perp \mathcal{H}_\alpha$ (approximately).
In that case, MATE-ETH is violated as strongly as possible, and contributions $\perp \mathcal{H}_{\text{mc}}$ never thermalize in either MATE or MITE.
Thank you for your attention