Statistical ensembles without typicality

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"Gibbs' trick": Assign canonical ensemble.

$$\{\rho : \mathrm{Tr}(\rho H) = e\} =: \; (e, H) \longrightarrow \gamma_e(H) \; := \frac{e^{-\beta(e)H}}{\mathrm{Tr}(e^{-\beta(e)H})} \in (e, H)$$

"macrostate" "microstate"

Why does this work?

- Complete Passivity:

  CEs is only family of microstates from which no work can be extracted.

- Jaynes' Principle (Max-Ent):

  Out of microstates compatible with information should assign the one with maximal entropy.

- (Canonical) Typicality: [Popescu et al., Goldstein et al., '06]

  Vast majority of microstates compatible with coarse-grained information behaves like can. ensemble wrt property of interest.

$$\frac{V_{\mu_{\mathrm{Haar}}}[\{|\psi\rangle \in \mathcal{H}_{mc} \mid \mathcal{D}(Tr_{\bar{S}}(|\psi\rangle\langle\psi|), \gamma_S) \geq \epsilon\}]}{V_{\mu_{\mathrm{Haar}}}[\{|\psi\rangle \in \mathcal{H}_{mc}\}]} \leq \epsilon'$$

Provide a novel way to motivate Gibbs' trick that is independent of any measure or Jaynes-like reasoning:

The states that can be reached thermodynamically from a macrostate are exactly those that can be reached if the initial state was the corresponding canonical ensemble.

Thermodynamically, any macrostate is *operationally equivalent* to its corresponding canonical ensemble.

1. Two models of thermodynamic transitions

$$\rho \longrightarrow O_{\mathrm{mic.}} \longrightarrow \rho_f \qquad\qquad (e, H) \longrightarrow O_{\mathrm{mac.}} \longrightarrow \rho_f$$

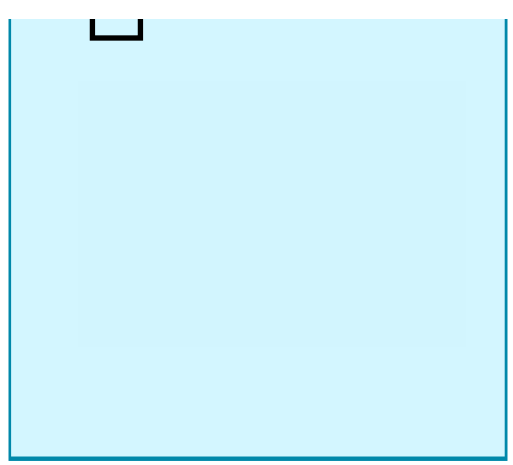
"theoretical setting" "lab setting"

2. Compare via reachable state sets

$$\rho \xrightarrow{\mathrm{mic.}} \rho_f \overset{?}{\Leftrightarrow} (e, H) \xrightarrow{\mathrm{mac.}} \rho_f$$

3. Find "operational equivalence"

$$\gamma_e(H) \xrightarrow{\mathrm{mic.}} \rho_f \Leftrightarrow (e, H) \xrightarrow{\mathrm{mac.}} \rho_f$$



1. Bath states:

$$\gamma_\beta(E^i) = \frac{e^{-\beta H_{E^i}}}{tr(e^{-\beta H_{E^i}})}$$

2. Evolution:

S and E evolve unitarily, such that total average energy and entropy preserved

Microstate Operations

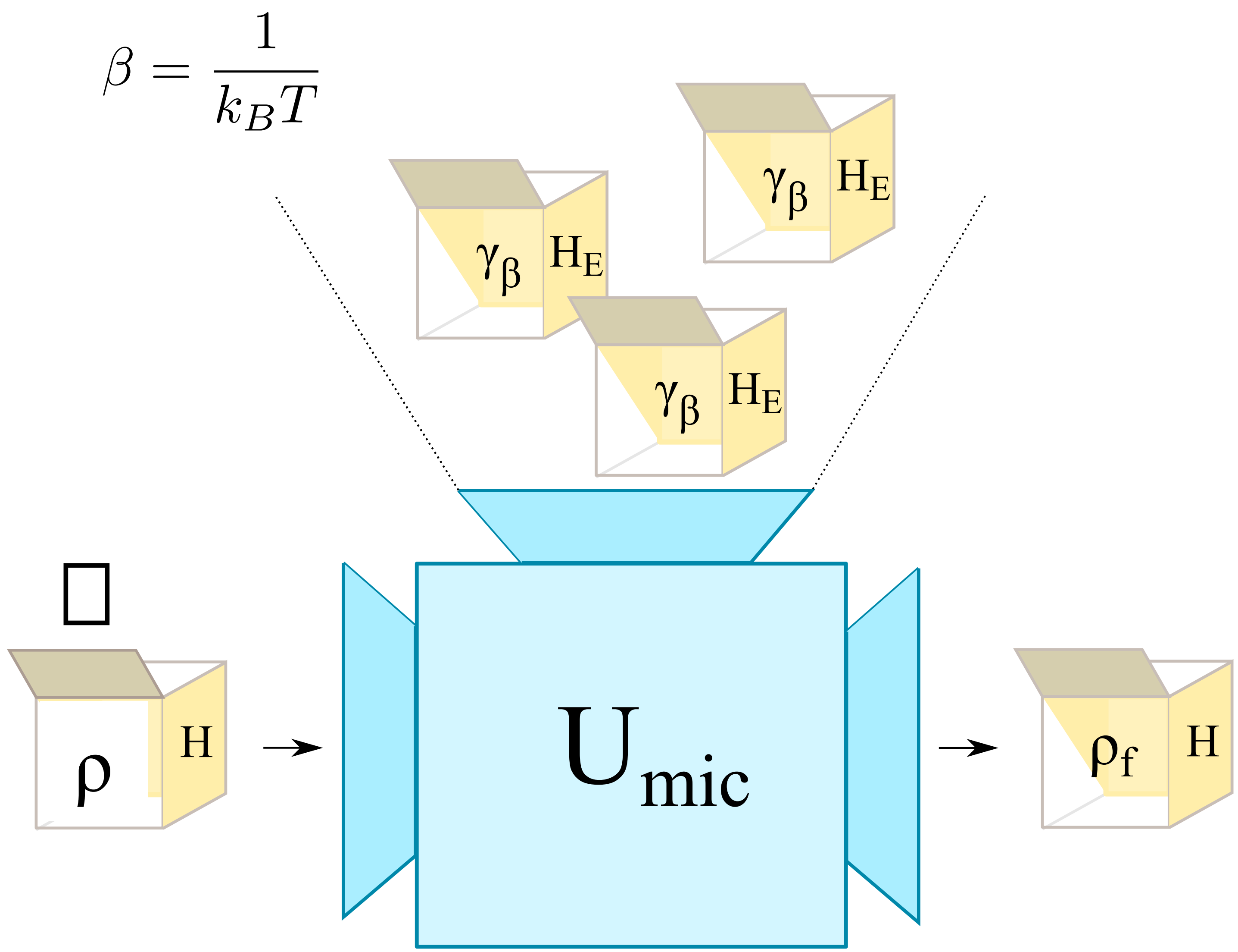
$$\rho \xrightarrow{\beta-\text{mic.}} \rho_f$$

if $\quad \forall\, \epsilon, \epsilon' > 0,\ \exists\ \{H_{E^1}, \ldots, H_{E^N}\}, U$ s.t.

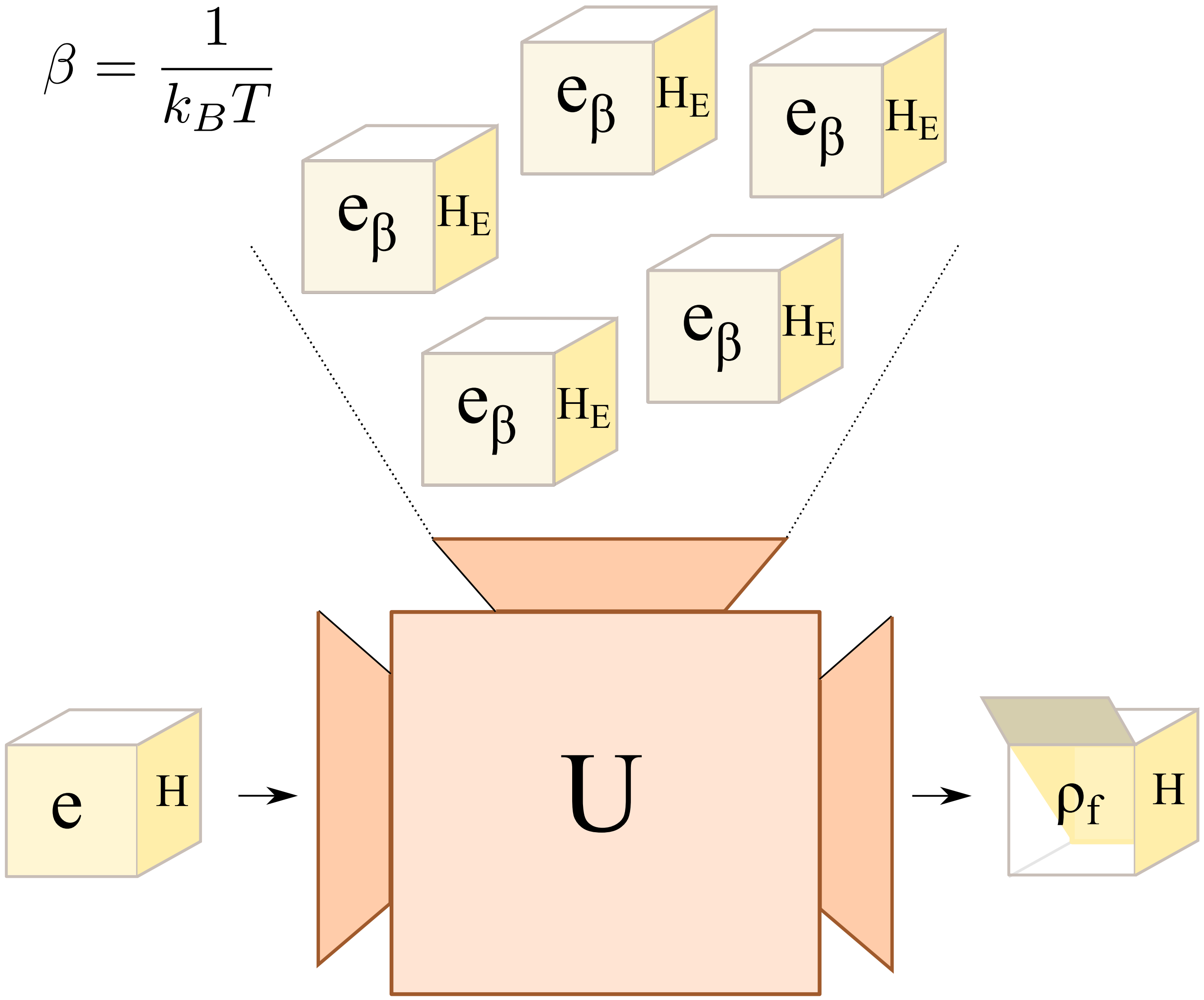
$$\rho_f \approx_\epsilon tr_E \left(U\, \rho \bigotimes_{i=1}^{N} \gamma_\beta(H_{E^i})\, U^\dagger \right)$$

and

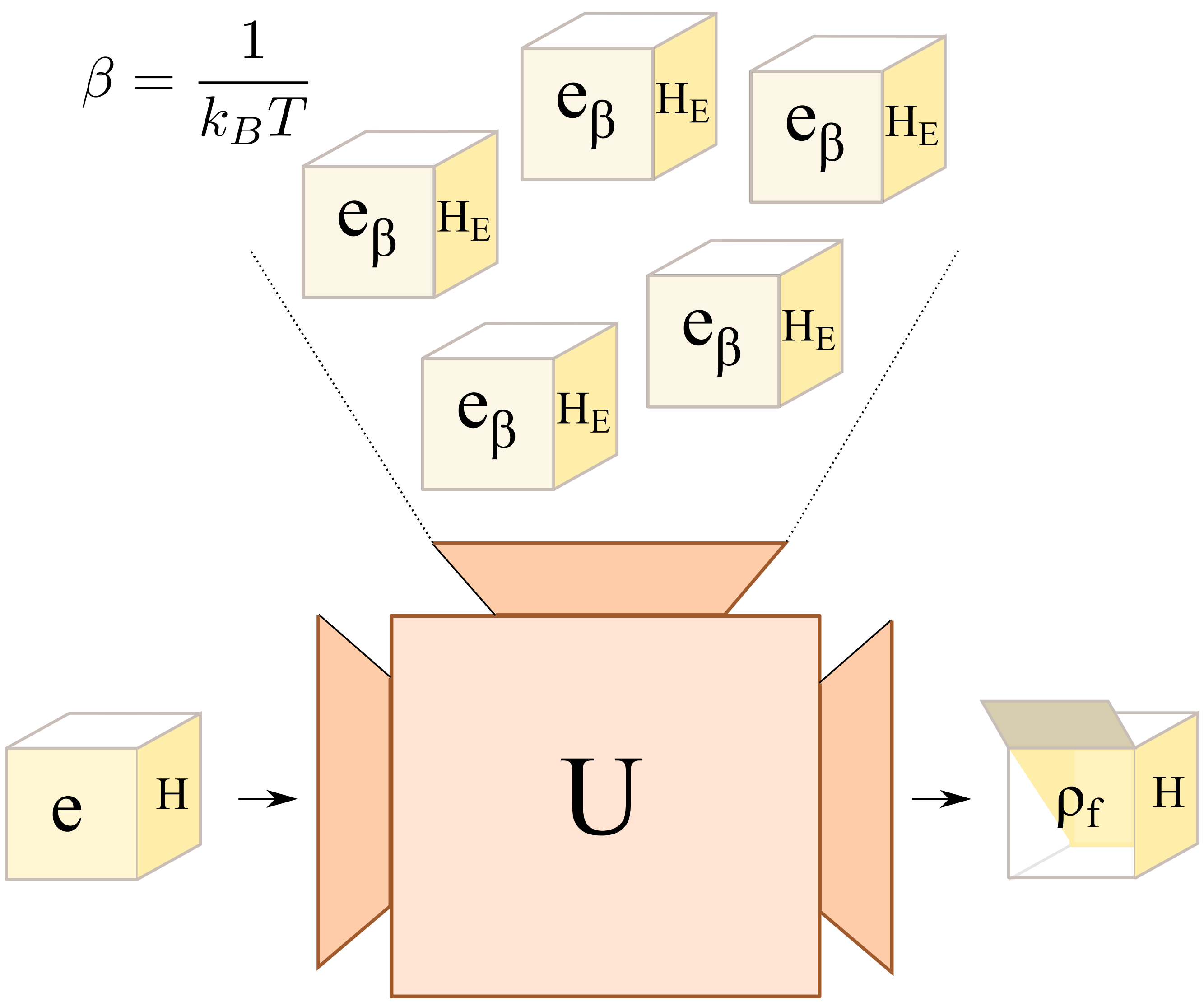
$$\mathcal{E} \left(U\, \rho \bigotimes_{i=1}^{N} \gamma_\beta(H_{E^i})\, U^\dagger \right) \approx_{\epsilon'} \mathcal{E} \left(\rho \bigotimes_{i=1}^{N} \gamma_\beta(H_{E^i}) \right)$$


$\beta = \frac{1}{k_B T}$
γ_β
H_E
γ_β
H_E
γ_β
H_E
ρ
H
U_{mic}
ρ_f
H

$$\beta = \frac{1}{k_B T}$$



Macrostate Operations



1. Bath states:

$$(e_\beta(H_{E^i}), H_{E^i}),$$
$$e_\beta(H_{E^i}) := \mathcal{E}(\gamma_\beta(H_{E^i}))$$

2. Evolution:

S and E evolve unitarily,
such that total
average energy and entropy
preserved

Macrostate Operations

$$\boxed{(e, H) \xrightarrow{\beta-\text{mac.}} \rho_f}$$

if $\forall\, \epsilon, \epsilon' > 0,\ \exists\ \{H_{E^1}, \ldots, H_{E^N}\}, U$ s.t.

$$\forall \rho \in (e, H), \sigma^{(i)} \in (e_\beta, H_{E^i})$$

$$\rho_f \approx_\epsilon tr_E \left(U\, \rho \bigotimes_{i=1}^{N} \sigma^{(i)}\, U^\dagger \right)$$

and

$$\mathcal{E}\left(U\, \rho \bigotimes_{i=1}^{N} \sigma^{(i)}\, U^\dagger \right) \approx_{\epsilon'} \mathcal{E}\left(\rho \bigotimes_{i=1}^{N} \sigma^{(i)} \right)$$

Macrostate Operations

(e, H)

$$\rho = |E\rangle\langle E|$$

$$\rho = \gamma_e(H)$$

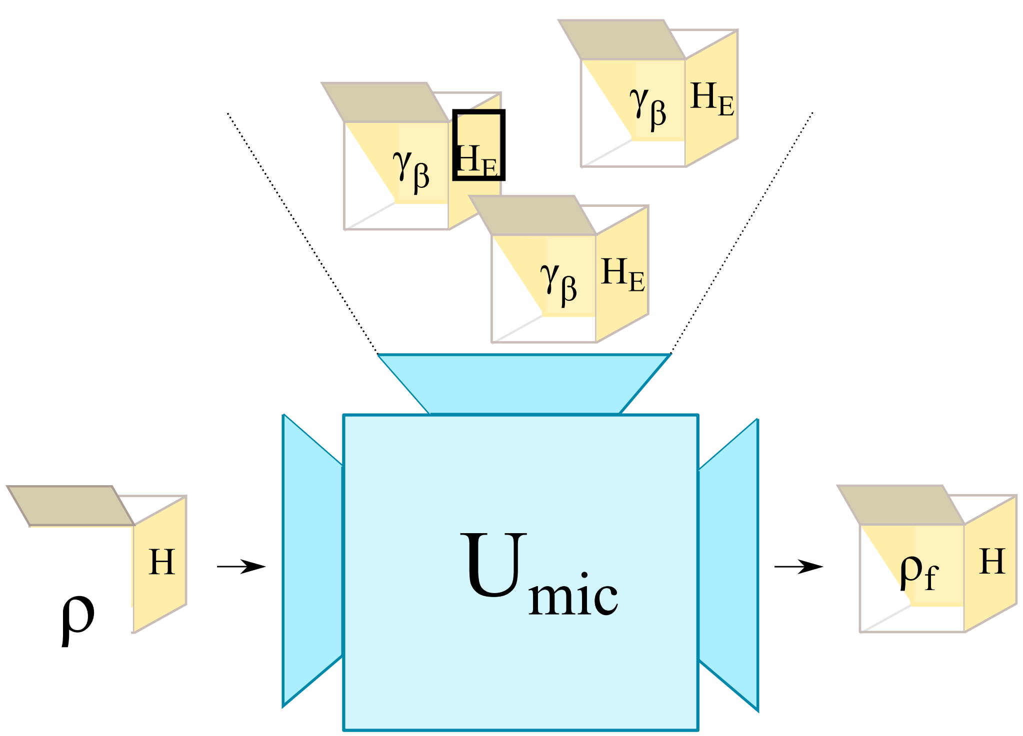
Same:

- Fixed bath temperature
- Unitary Evolution
- Average energy preservation
- No initial correlations
- Final state is Microstate

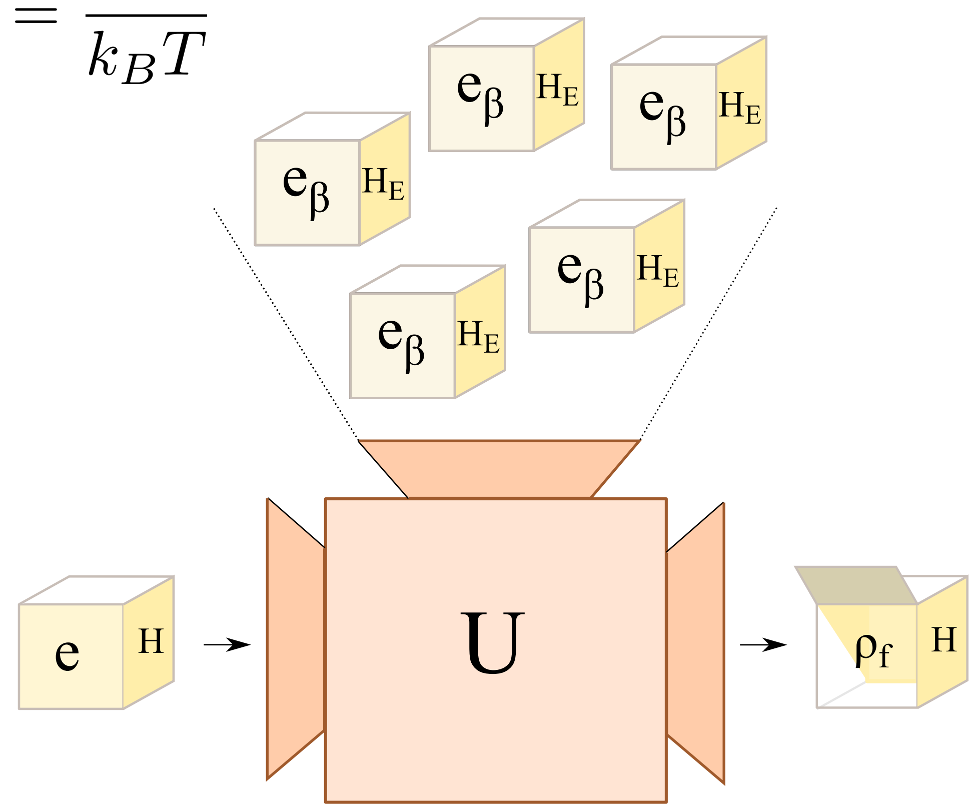
Different:

- Initial states
- Constraint on Unitary

$$\beta = \frac{1}{k_B T}$$



$$\beta = \frac{1}{k_B T}$$



$$(e, H) \sim_\beta \rho$$

$$:=$$

$$(e, H) \xrightarrow{\beta-\text{mac.}} \rho_f \Leftrightarrow \rho \xrightarrow{\beta-\text{mic.}} \rho_f$$

<u>Theorem</u>

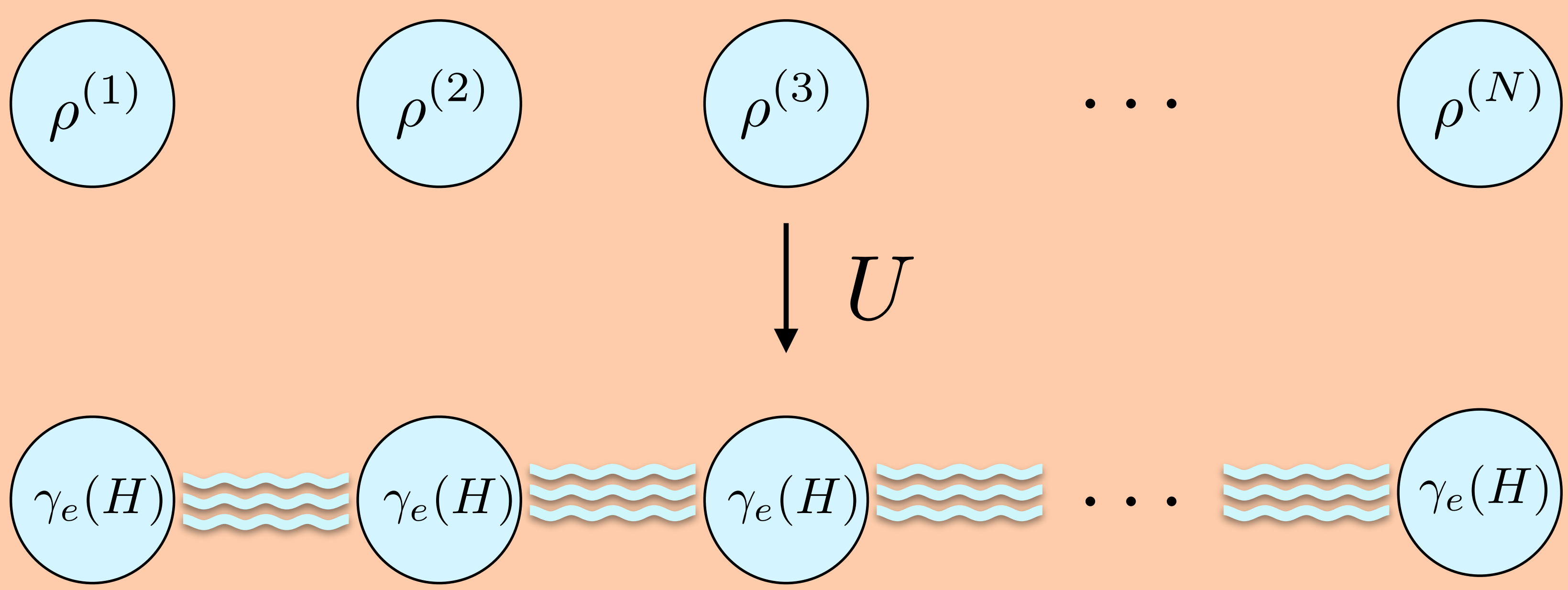
$$(e, H) \sim_\beta \gamma_e(H), \quad \forall\, e, H, \beta > 0$$

"The canonical ensemble is the one and only microstate that encodes the possible thermodynamic state transitions of a system whenever one only has partial information about system, bath and evolution."

Proof Sketch

Key Lemma

$$\exists \rho_f : \bigotimes_{l=1}^{N} (e, H) \overset{\beta\text{-mac}}{\rightarrow} \rho_f \ \text{ s.t. } \ tr_{\bar{l}}(\rho_f) \overset{N \to \infty}{\longrightarrow} \gamma_e(H).$$



Re-deriving phenomenological TD

$$(e, H) \stackrel{\beta\text{-mac}}{\to} \gamma_e(H)$$

Work extraction

$$\Delta W \leq \Delta \mathcal{F}_S, \quad \mathcal{F}_S := \Delta \mathcal{E}_S - T\Delta \mathcal{S}_S$$

Second Law

$$(e, H) \stackrel{\beta\text{-mac}}{\to} \rho_f \Leftrightarrow \mathcal{F}_S(\gamma_e(H)) \geq \mathcal{F}_S(\rho_f).$$

Clausius Inequality

$$(e, H) \stackrel{\beta\text{-mac}}{\to} (e, H) \Leftrightarrow \Delta Q \leq T\Delta S$$

cf. Skrzypczyk et al., Nat. Comm. 5, 4185 (2016)

Do we cheat by letting bath have thermal energy?

$$(H_E, \beta) \mapsto f(H_E, \beta)$$

Any choice other than $f(H_E, \beta) = \mathcal{E}(\gamma_\beta(H_E))$ would trivialise the operations.

Stronger setting: Unitary commutes

Exact commutation instead of average preservation.

$$[U, H_S + H_E] = 0$$

Operational equivalence breaks down!

$$H \neq 0, \beta < \infty \Rightarrow \exists\, e \text{ s.t. } (e, H) \overset{\text{c}}{\not\sim}_\beta \gamma_e(H)$$

NB: Is recovered locally in thermodynamic limit.

Can generalise all of this to the case of any set of commuting observables (GGEs).

$$(\mathbf{v}, \mathcal{Q}) \sim_{\beta} \gamma_{\mathbf{v}}(\mathcal{Q})$$

$$\gamma_{\mathbf{v}}(\mathcal{Q}) := \frac{e^{-\sum_j \beta_S^j(\mathbf{v}) Q^j}}{\mathrm{tr}(e^{-\sum_j \beta_S^j(\mathbf{v}) Q^j})}$$

cf. Guryanova et al./Yunger-Halpern et al., Nat. Comm. 7, 12049/12051 (2016)

Summary

- Provided novel justification for use of canonical ensembles in (quantum) statistical mechanics by showing operational equivalence wrt possible thermodynamic transitions.
- Re-derive phenomenological TD without assuming can. ensemble.
- Operational equivalence breaks down for exactly commuting case.
- Can be generalised for commuting observables.

Thanks