Freie Universität Berlin

Statistical ensembles without typicality

Paul Boes, Henrik Wilming, Jens Eisert, Rodrigo Gallego

QIP'18

A frequent question in thermodynamics

Given a (quantum) system of which you only know its average energy e wrt some Hamiltonian H, how will it behave thermodynamically?

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Given a (quantum) system of which you only know its average energy e wrt some Hamiltonian H, how will it behave thermodynamically?

Difficult problem, due to lack of information about underlying state of system.

“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?

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E.g.: Canonical Typicality
(Popescu et al., Goldstein et al., '06)

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

This talk

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

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

Idea

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$$(e, H) \to \rho_f \overset{?}{\Leftrightarrow} \rho \to \rho_f$$

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1. Two models of thermodynamic transitions

$$\rho \longrightarrow O_1 \longrightarrow \rho_f \qquad (e, H) \longrightarrow O_2 \longrightarrow \rho_f$$

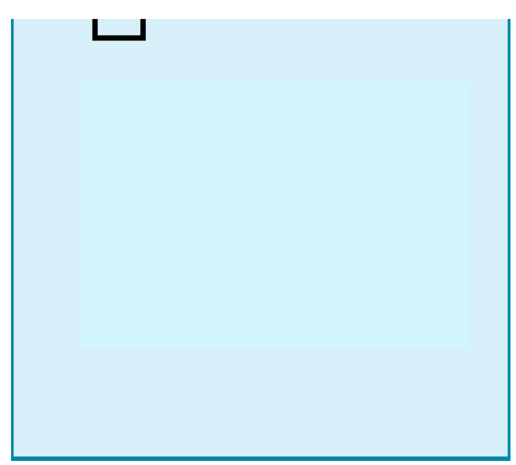
2. Compare via reachable state sets

$$(e, H) \to \rho_f \overset{?}{\Leftrightarrow} \rho \to \rho_f$$

3. Show equivalence between macrostates and canonical ensembles

$$(e, H) \sim \gamma_e(H)$$

Setting



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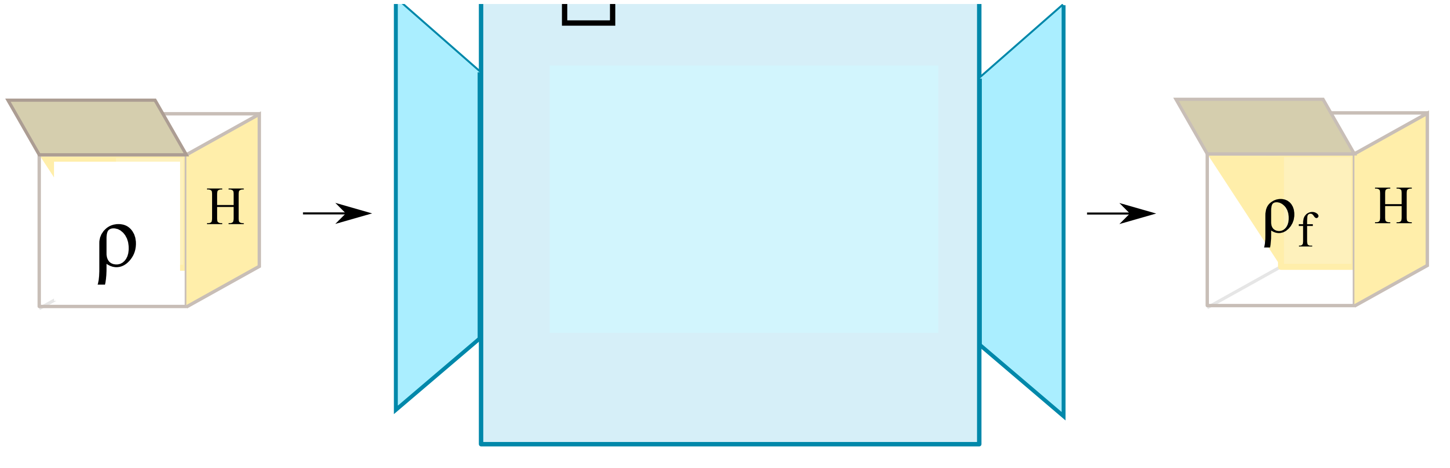
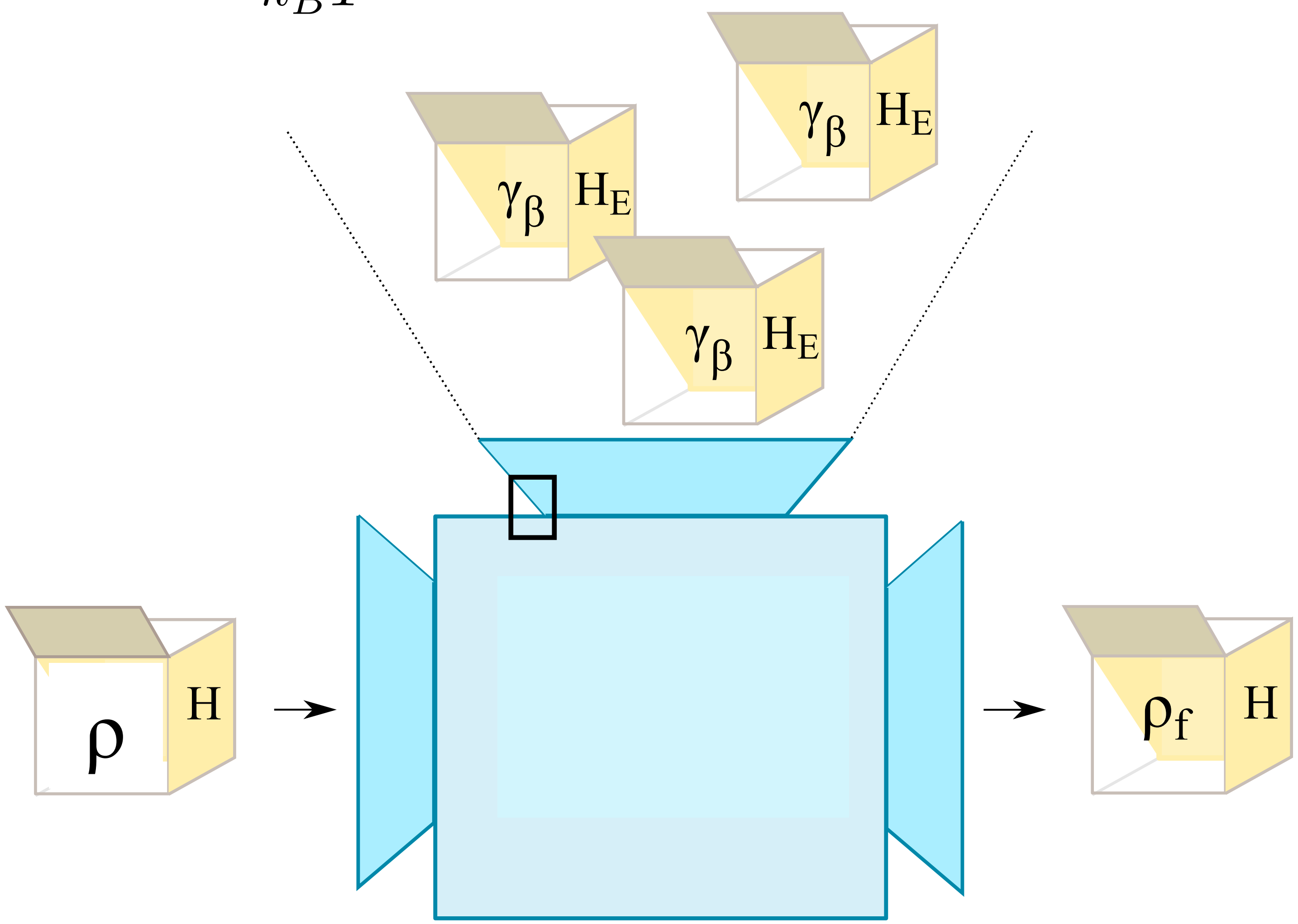


Setting

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



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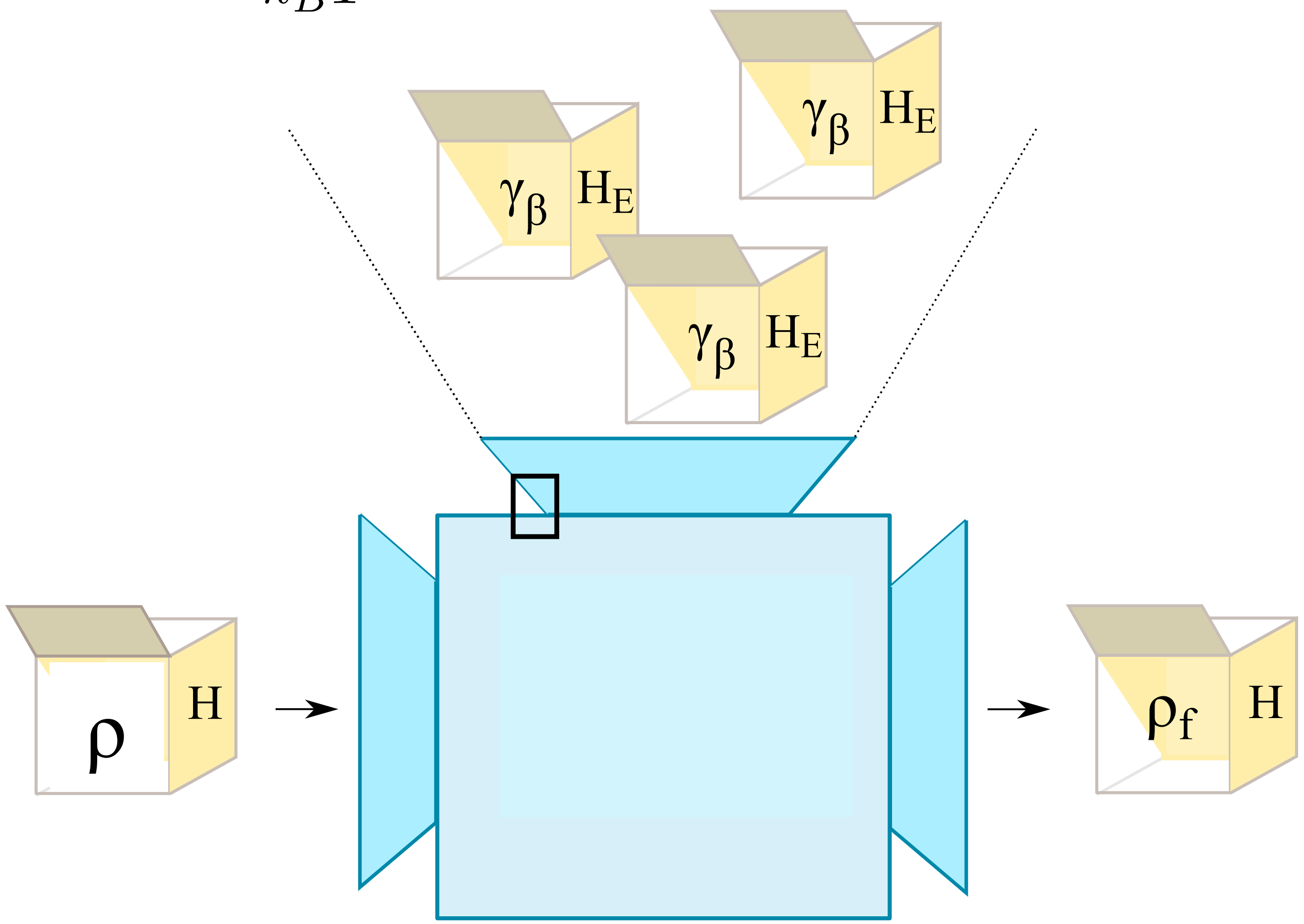

1. Bath states:

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

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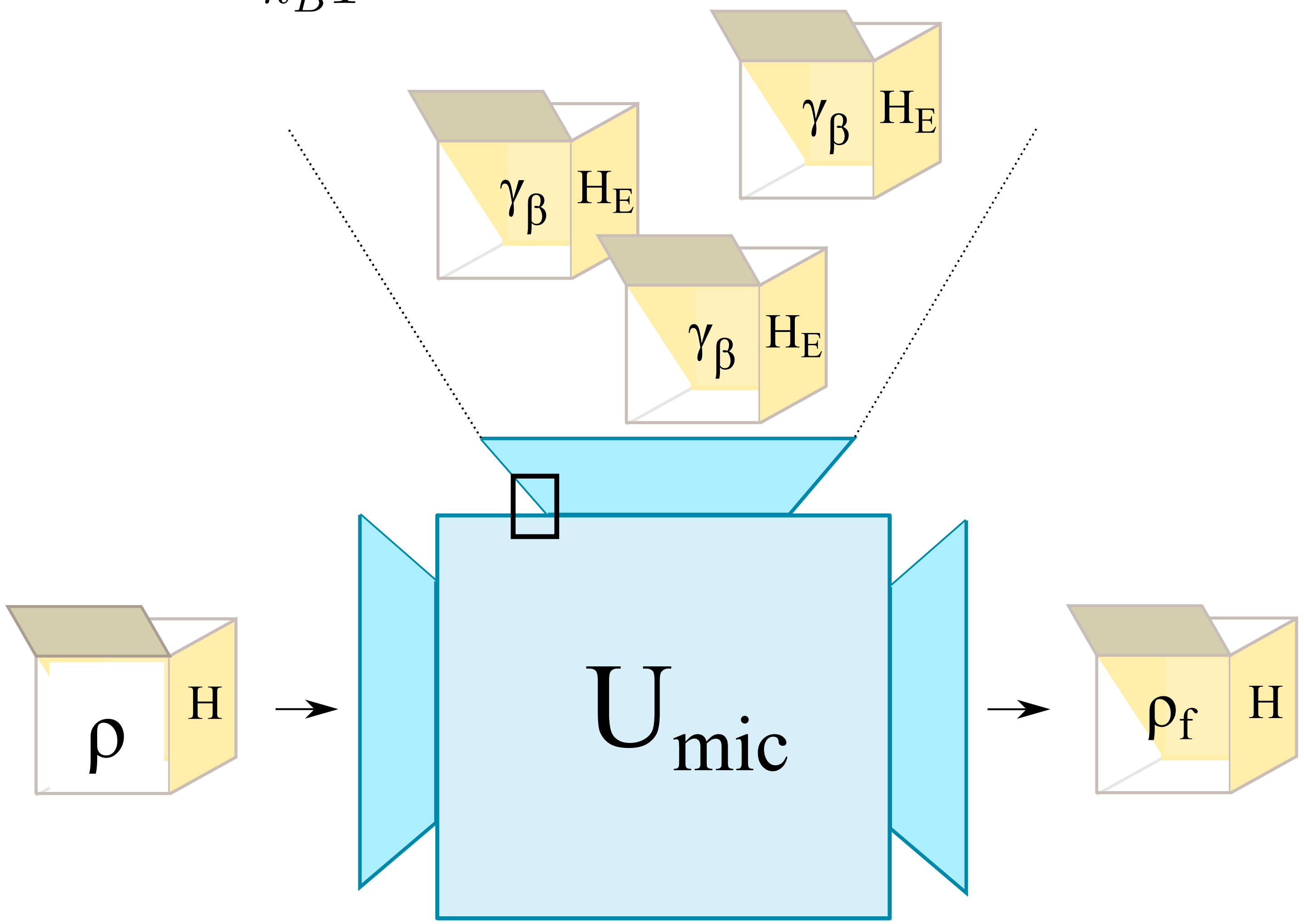

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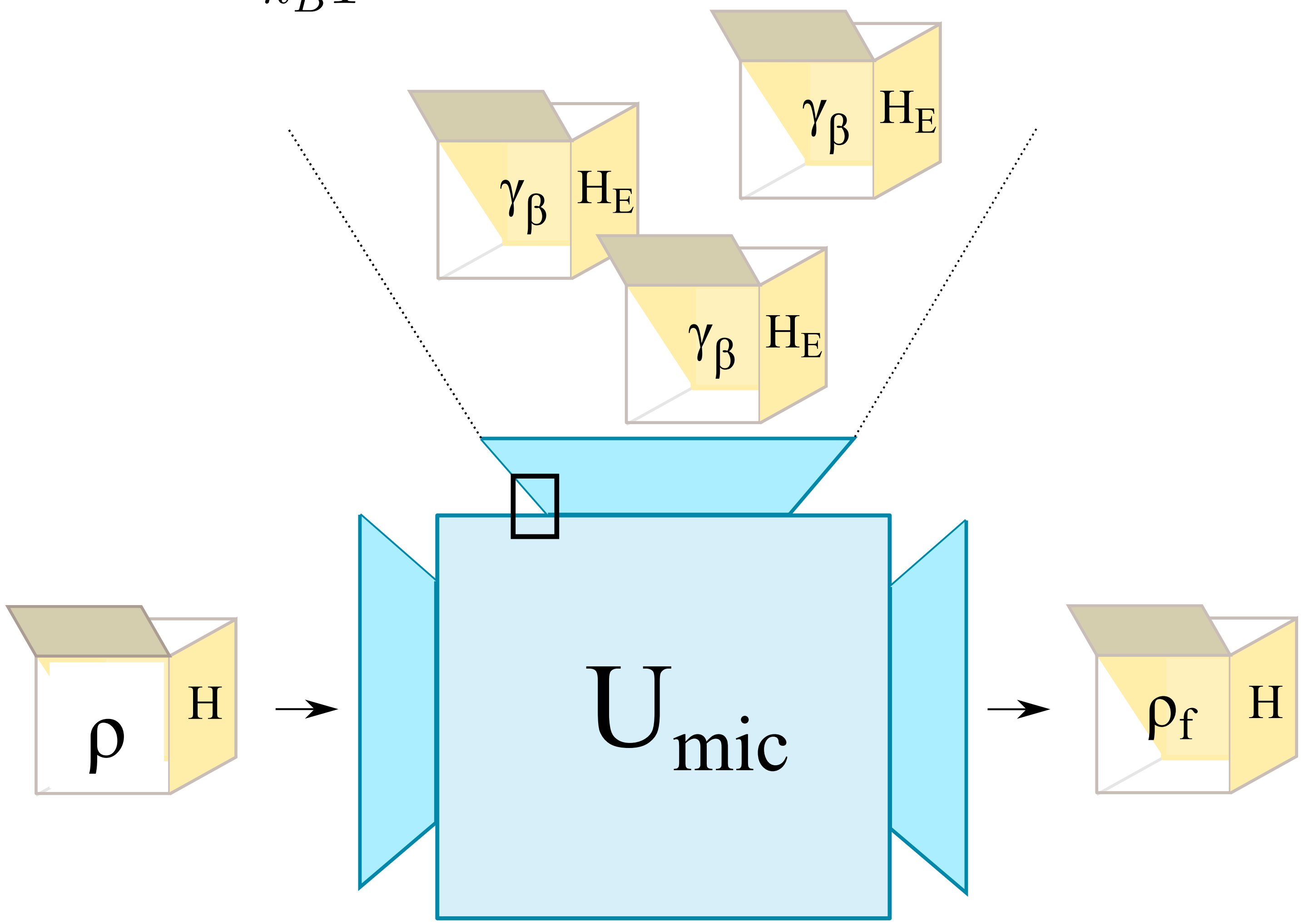

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2. Evolution:

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

Microstate Operations

$$\boxed{\rho \overset{\beta-\text{mic.}}{\longrightarrow} \rho_f}$$

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

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

and

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

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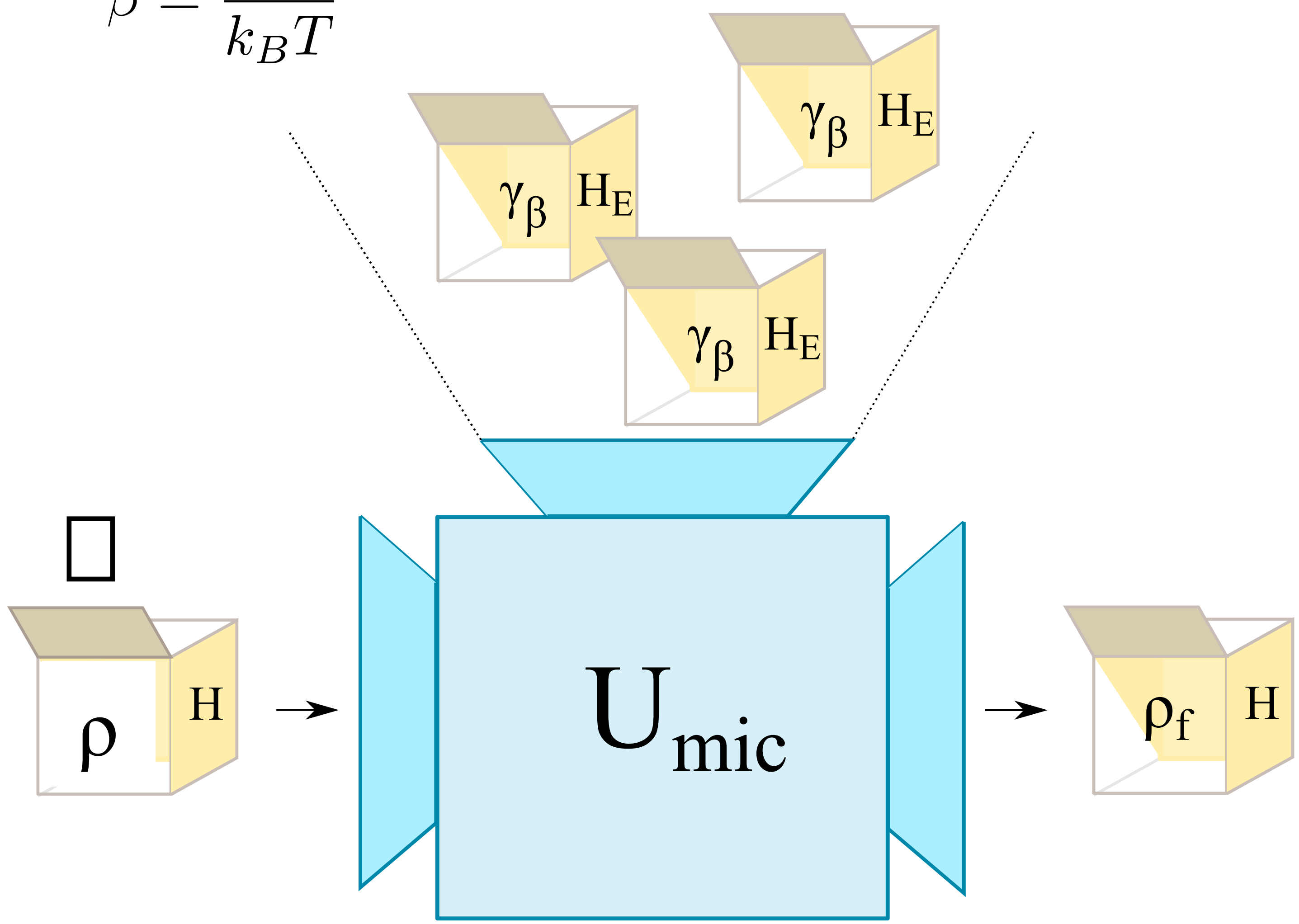

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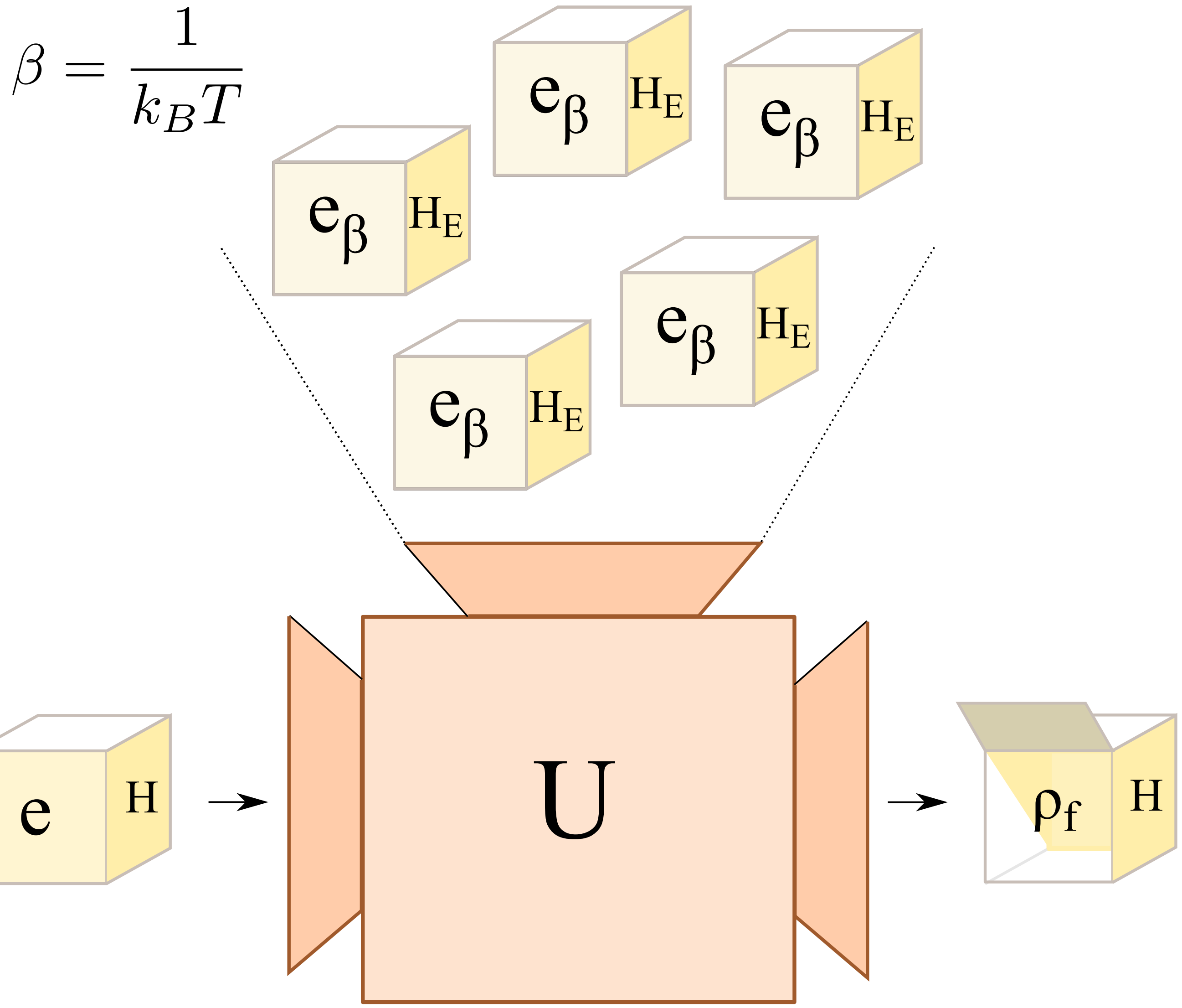

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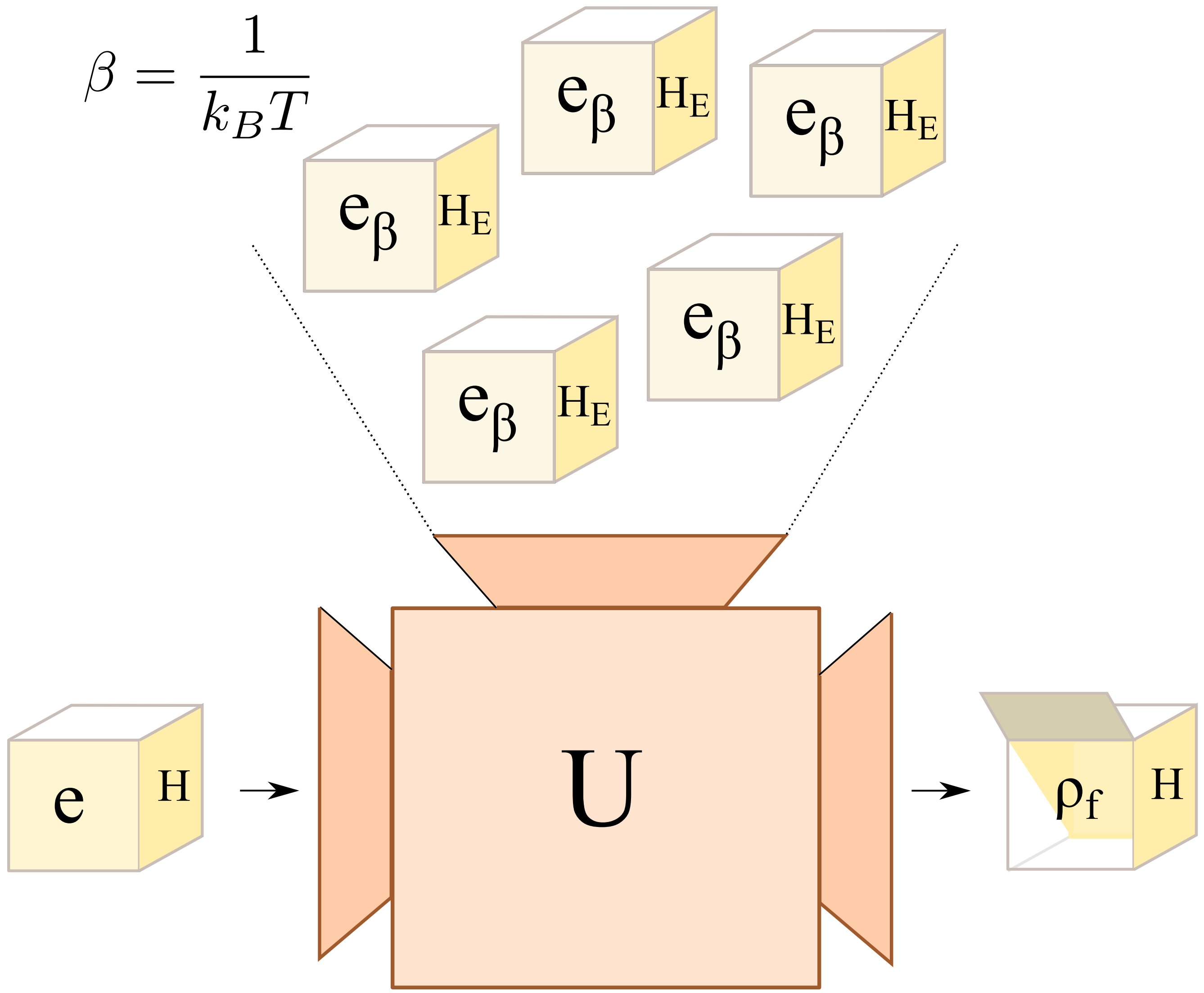

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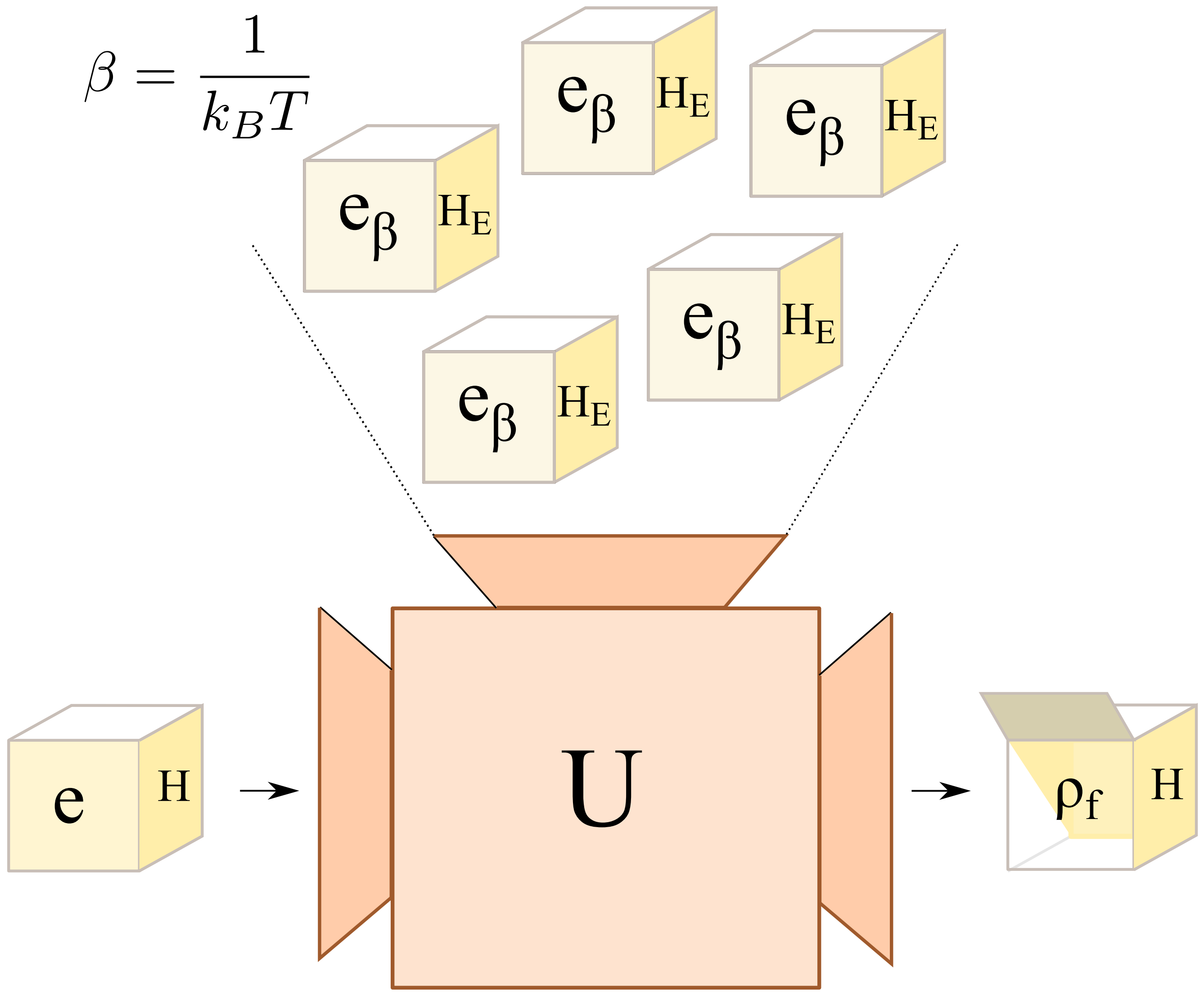
$$\left(e_\beta(H_{E^i}), H_{E^i}\right),$$

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

Setting



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

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

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Setting

Same:

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

Different:

- Initial states
- Constraint on Unitary

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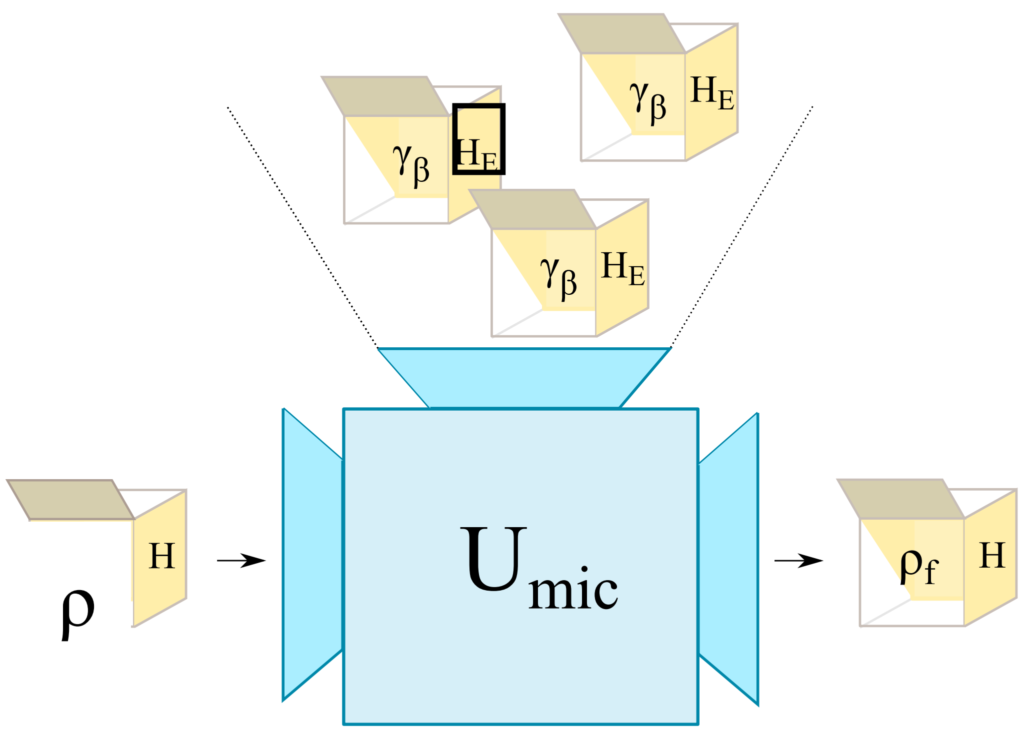

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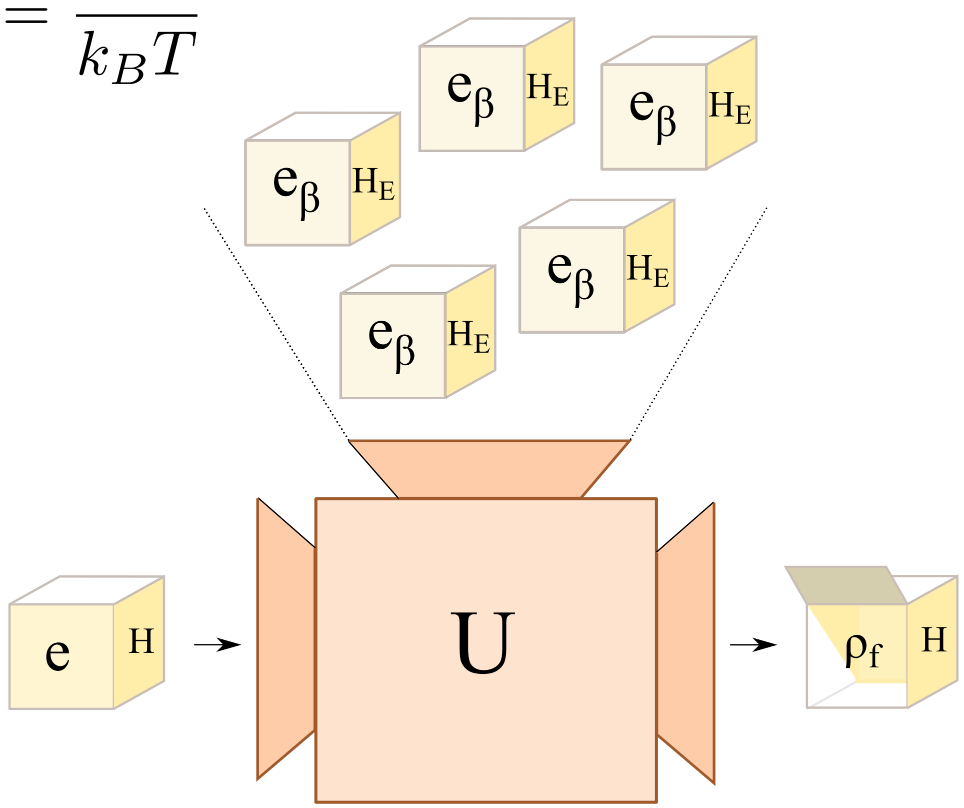

Operational Equivalence

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

$$\equiv$$

$$(e, H) \stackrel{\beta-\mathrm{mac.}}{\longrightarrow} \rho_f \Leftrightarrow \rho \stackrel{\beta-\mathrm{mic.}}{\longrightarrow} \rho_f$$

Main Result

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

Motivating the success of Gibbs' trick

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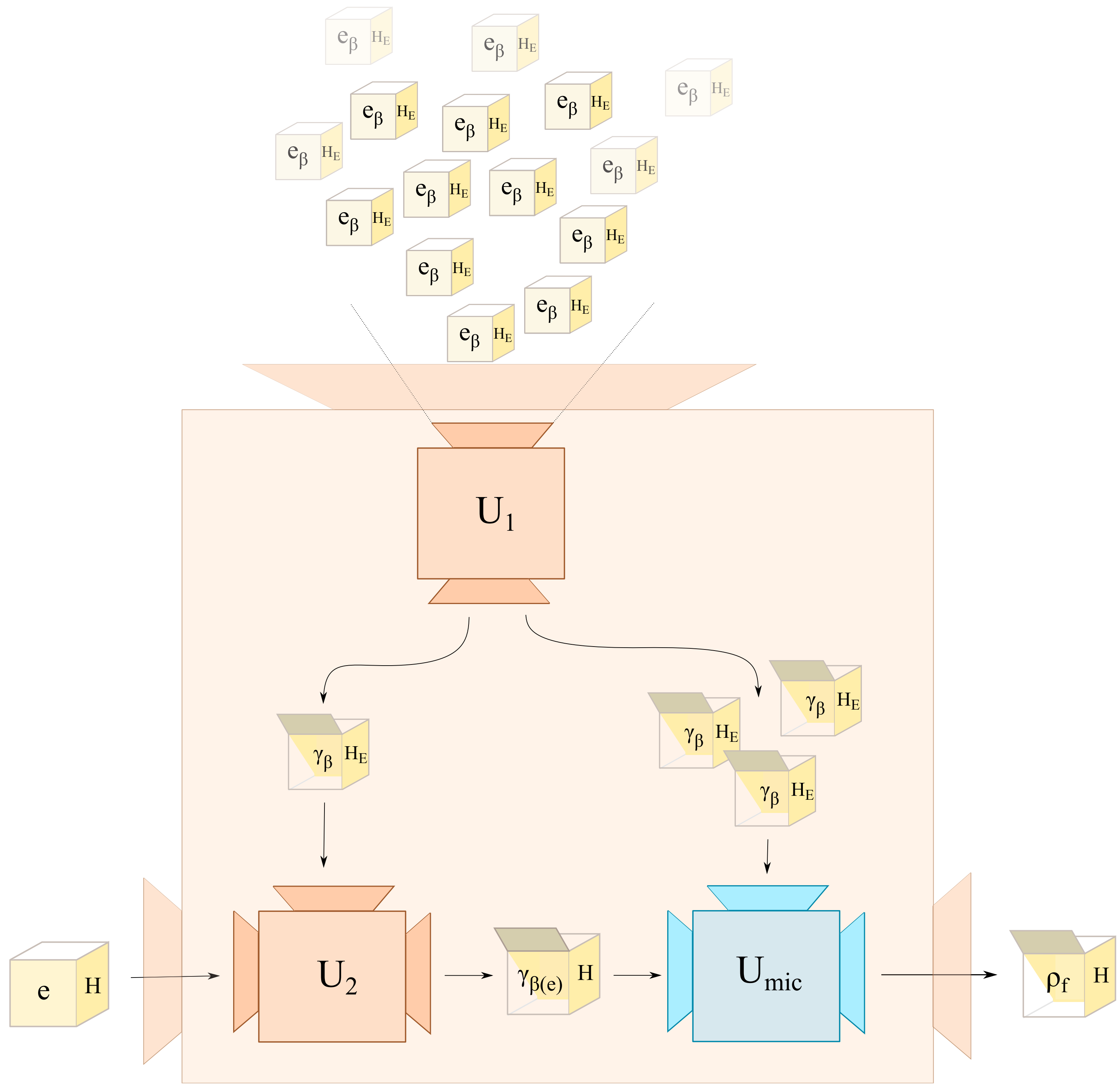
The canonical ensemble is the one and only microstate that encodes the possible thermodynamic state transitions of a system whenever one only has partial information about system, bath and evolution.

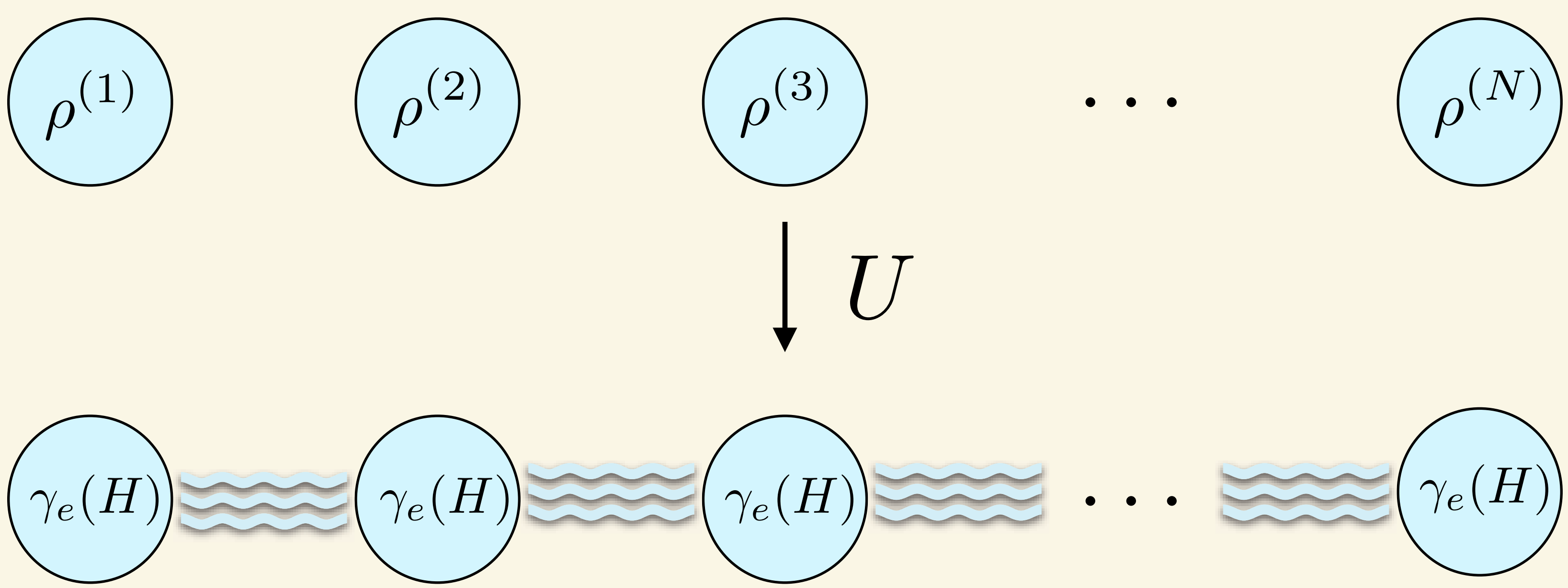
Proof Sketch



Proof Sketch

Key Lemma

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



Re-deriving phenomenological TD

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

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Work extraction

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

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

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Second Law

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

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Clausius Inequality

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

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Stronger setting: Unitary commutes

Exact commutation instead of average preservation.

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

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Can be recovered for special cases,
e.g. locally in thermodynamic limit.

Generalizable to GGE setting

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.

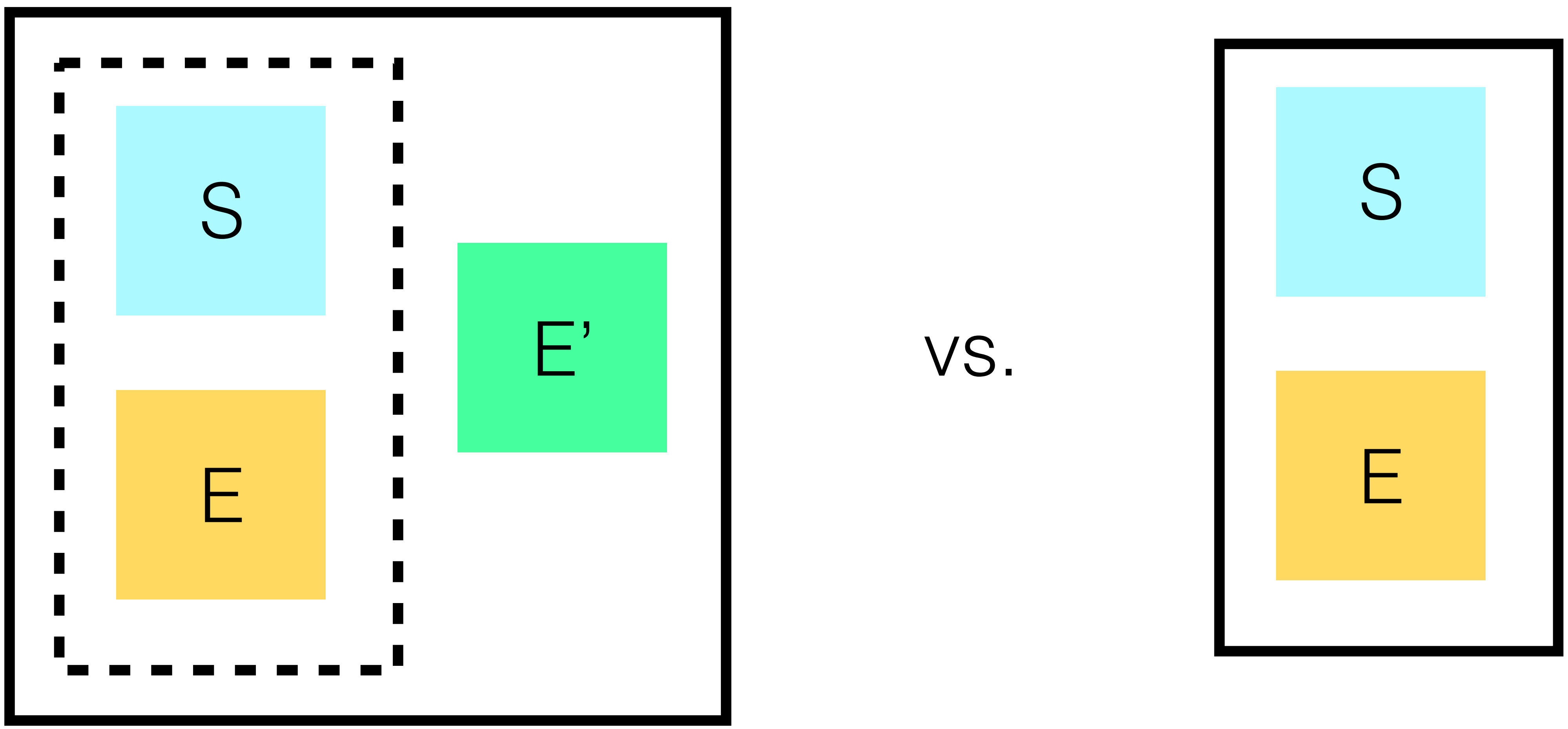
- Re-derive phenomenological TD without assuming can. ensemble.

- Operational equivalence breaks down for exactly commuting case.

- Can be generalised for commuting observables.

Thank you

arxiv: 1707.08218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