[Mark Rothko]

The Kirkwood-Dirac Distribution:

Quantum Thermodynamics and Nonclassicality

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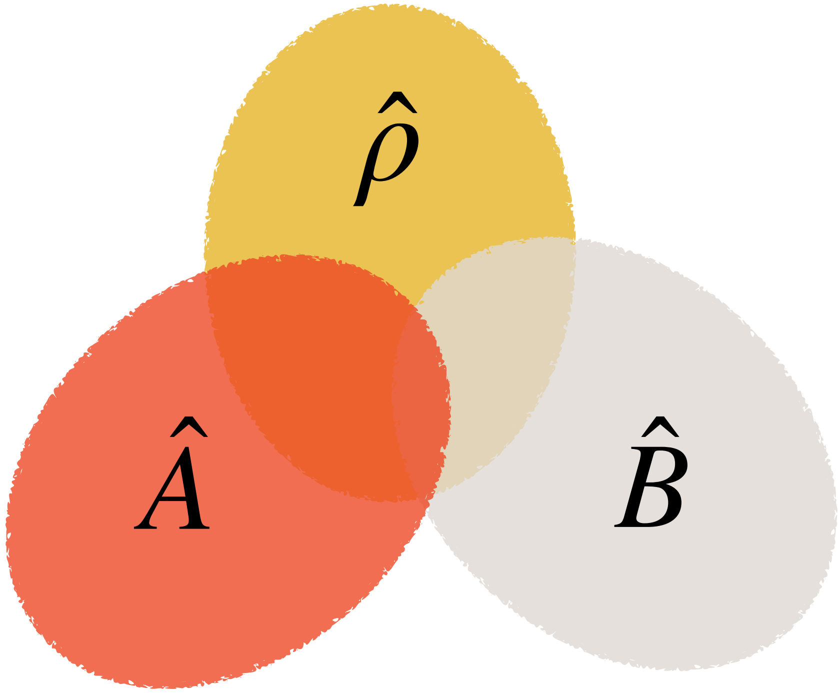

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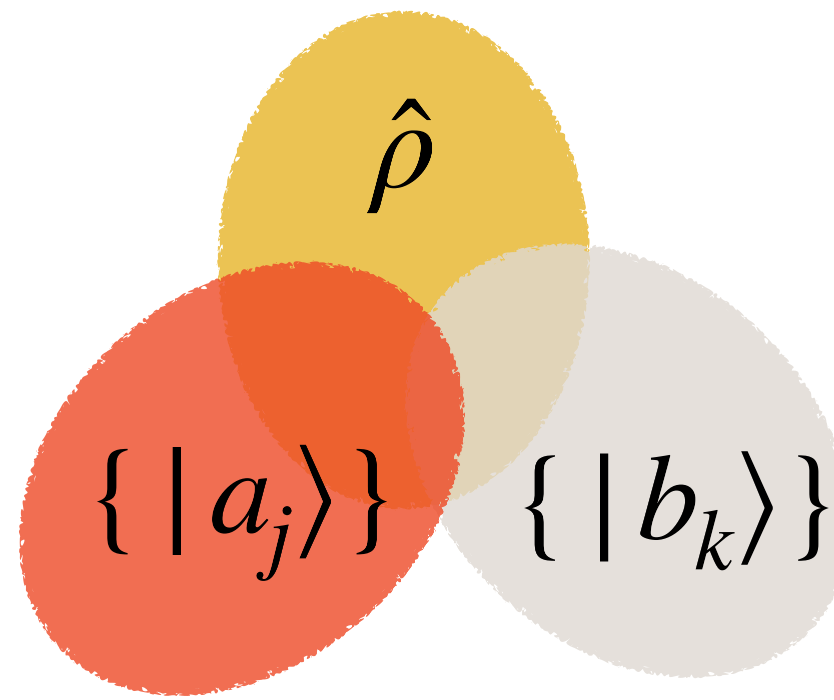

Outline

1. Quantum Thermodynamics

- Classical fluctuation theorems
- Issues with quantizing fluctuation theorems
- Kirkwood-Dirac distributions enable quantization

2. Kirkwood-Dirac Physical Nonclassicality

- Contextuality as rigorous nonclassicality
- Kirkwood-Dirac distribution witness contextuality

Kirkwood-Dirac Distribution

Complex Hilbert space $\mathscr{H}$ of dimension d.

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Kirkwood-Dirac quasiprobability:

$$q^{\rho}(a_j, b_k) := \mathrm{Tr}\big(|b_k\rangle\langle b_k|a_j\rangle\langle a_j|\rho\big) = \langle b_k|a_j\rangle\langle a_j|\rho|b_k\rangle$$

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Expansion coefficients given a particular operator basis:

$$\rho = \sum_{j,k} \frac{|a_j\rangle\langle b_k|}{\langle b_k|a_j\rangle} q^{\rho}(a_j, b_k)$$

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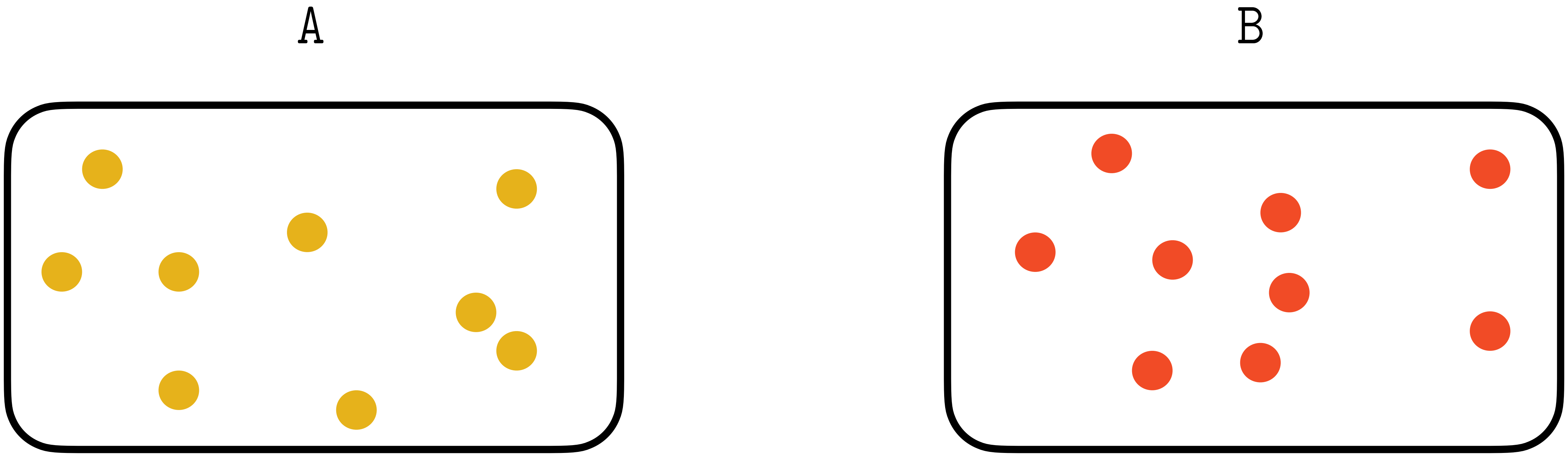
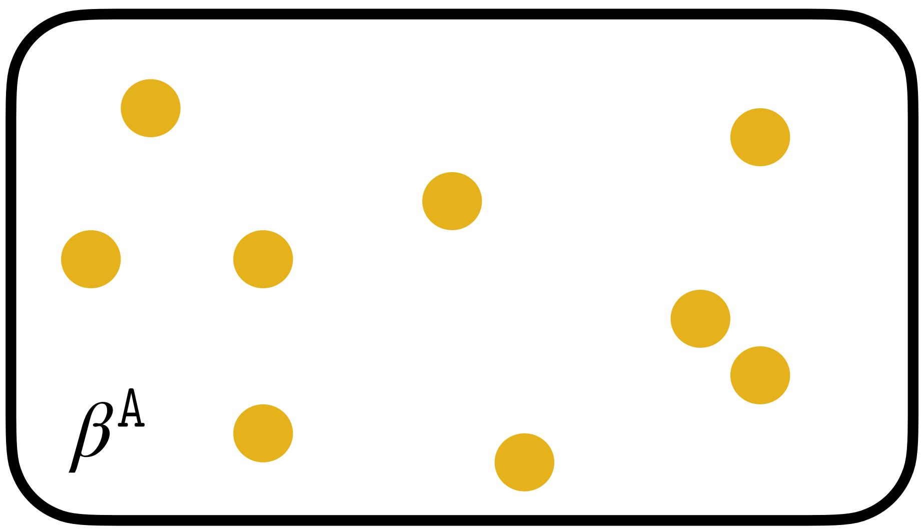
Why $\{ |a_j\rangle \}$ and $\{ |b_k\rangle \}$?

Classical Exchange Fluctuation Theorem



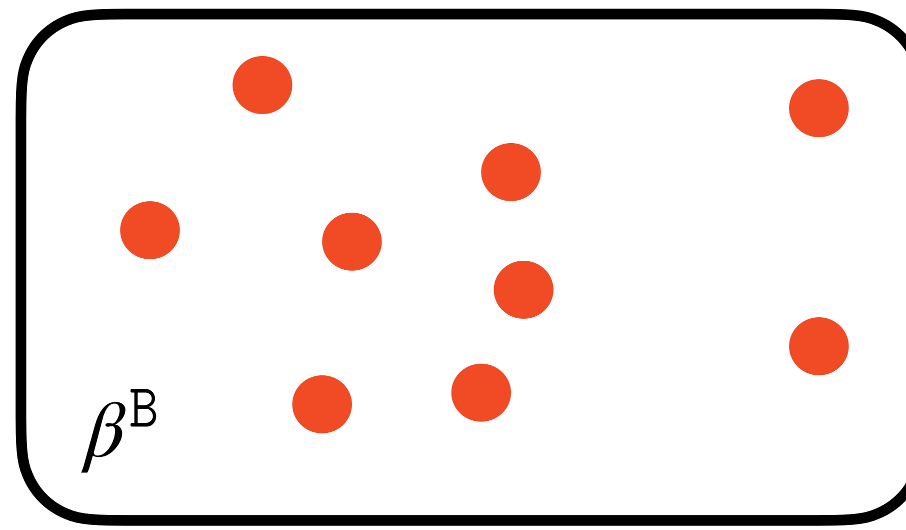
Classical Exchange Fluctuation Theorem

A



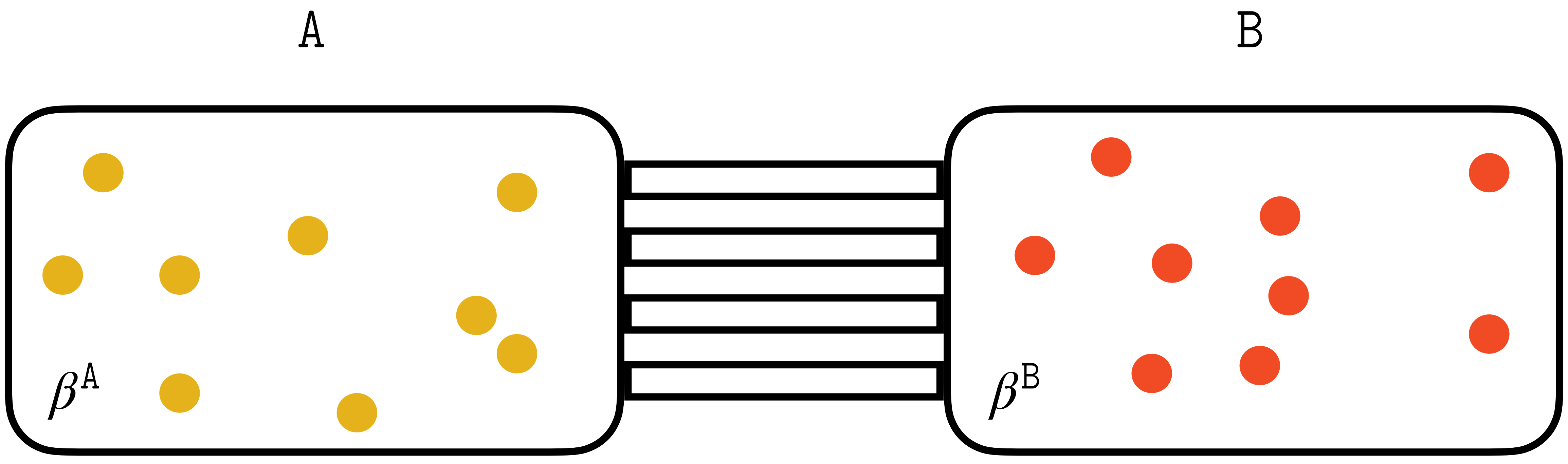
$$p(E^{\mathtt{A}}) = \frac{\exp(-\beta^{\mathtt{A}} E^{\mathtt{A}})}{Z^{\mathtt{A}}}$$

B



$$p(E^{\mathtt{B}}) = \frac{\exp(-\beta^{\mathtt{B}} E^{\mathtt{B}})}{Z^{\mathtt{B}}}$$

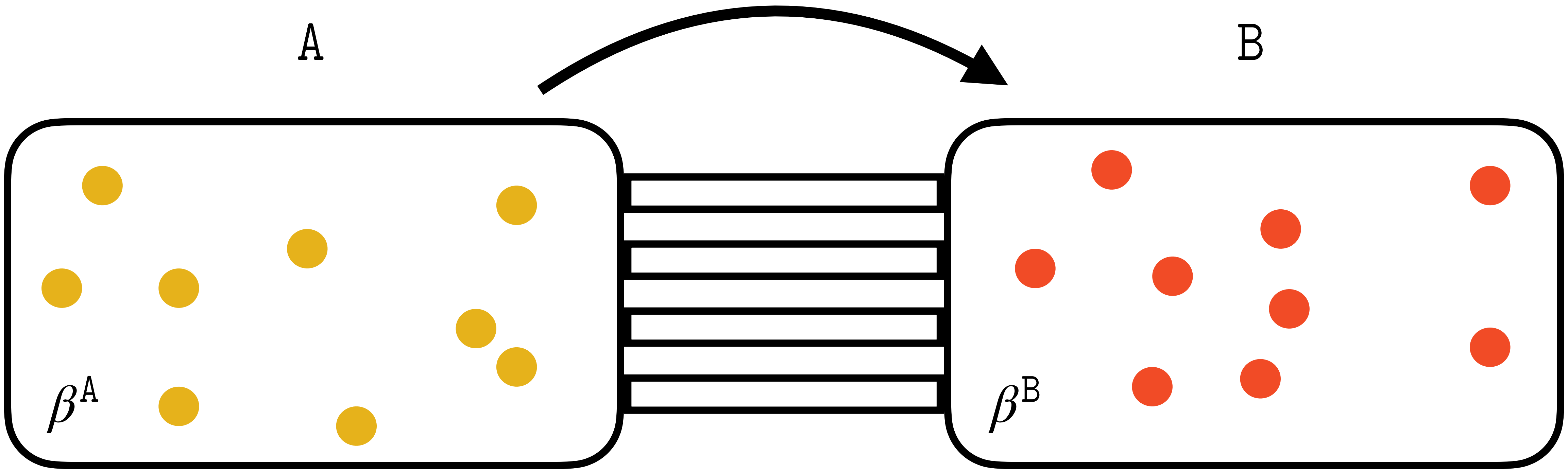
Classical Exchange Fluctuation Theorem



$$p(E^{\mathtt{A}}) = \frac{\exp(-\beta^{\mathtt{A}} E^{\mathtt{A}})}{Z^{\mathtt{A}}} \qquad p(E^{\mathtt{B}}) = \frac{\exp(-\beta^{\mathtt{B}} E^{\mathtt{B}})}{Z^{\mathtt{B}}}$$

Classical Exchange Fluctuation Theorem

$$Q = E_{\mathrm{f}}^{\mathrm{B}} - E_{\mathrm{i}}^{\mathrm{B}} = -\left(E_{\mathrm{f}}^{\mathrm{A}} - E_{\mathrm{i}}^{\mathrm{A}}\right)$$



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$$p(E^{\mathrm{B}}) = \frac{\exp(-\beta^{\mathrm{B}} E^{\mathrm{B}})}{Z^{\mathrm{B}}}$$

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Trajectories $\gamma_{\rm F}(t) : (E_{\rm i}^{\tt A}, E_{\rm i}^{\tt B} \mapsto E_{\rm f}^{\tt A}, E_{\rm f}^{\tt B})$

[Jarzynski and Wójcik, PRL 92, 230602 (2004)]

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$$\frac{p\left(\gamma_{\mathrm{F}}(t)\right)}{p\left(\gamma_{\mathrm{R}}(t)\right)}$$

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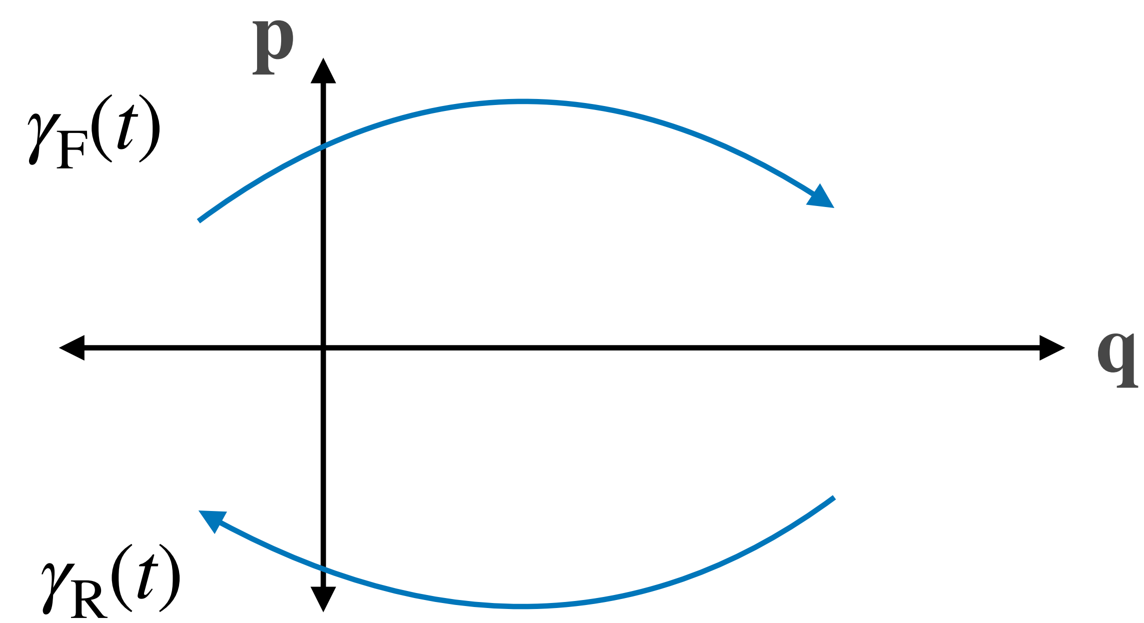

$$\frac{p\big(\gamma_{\mathrm{F}}(t)\big)}{p\big(\gamma_{\mathrm{R}}(t)\big)} = \frac{p\big(\gamma_{\mathrm{F}}(0)\big)}{p\big(\gamma_{\mathrm{R}}(0)\big)}$$

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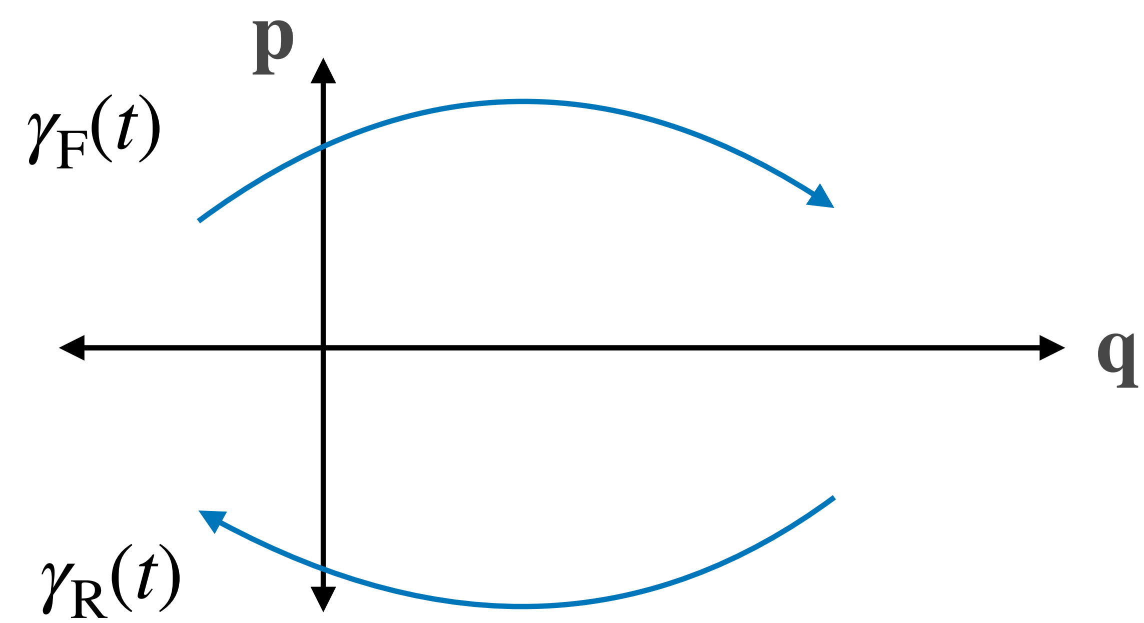

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$$= \frac{\exp(-\beta^{\mathrm{A}} E_{\mathrm{i}}^{\mathrm{A}})}{Z^{\mathrm{A}}} \frac{\exp(-\beta^{\mathrm{B}} E_{\mathrm{i}}^{\mathrm{B}})}{Z^{\mathrm{B}}}$$

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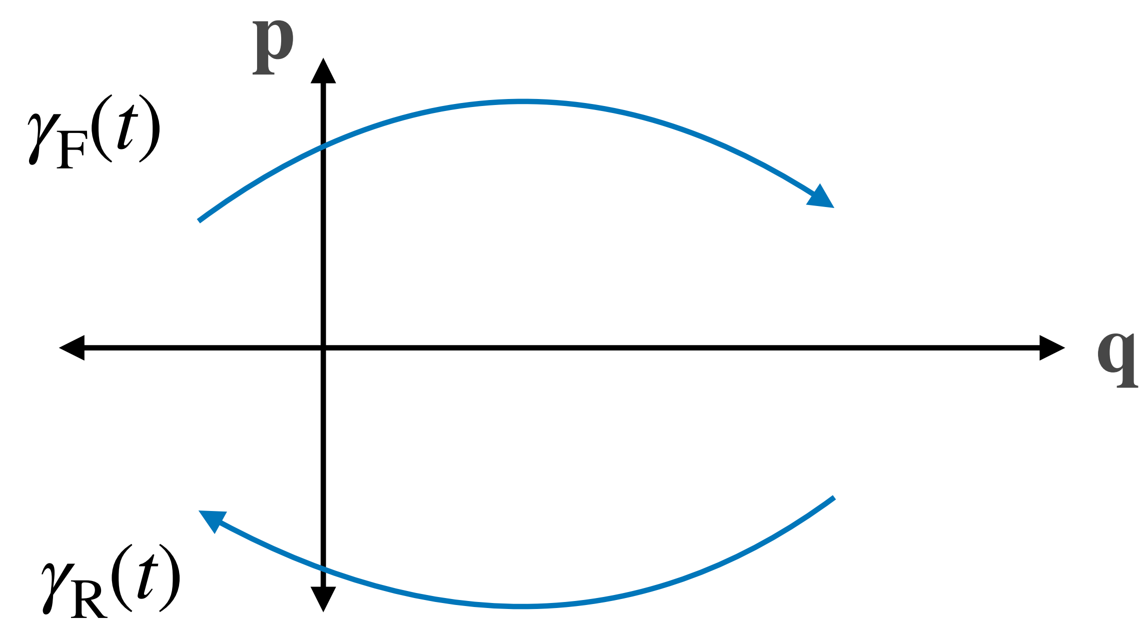

Trajectories $\gamma_{\mathrm{F}}(t) : (E_{\mathrm{i}}^{\mathtt{A}}, E_{\mathrm{i}}^{\mathtt{B}} \mapsto E_{\mathrm{f}}^{\mathtt{A}}, E_{\mathrm{f}}^{\mathtt{B}})$

$\gamma_{\mathrm{R}}(t) : (E_{\mathrm{f}}^{\mathtt{A}}, E_{\mathrm{f}}^{\mathtt{B}} \mapsto E_{\mathrm{i}}^{\mathtt{A}}, E_{\mathrm{i}}^{\mathtt{B}})$

$$\frac{p\big(\gamma_{\mathrm{F}}(t)\big)}{p\big(\gamma_{\mathrm{R}}(t)\big)} = \frac{p\big(\gamma_{\mathrm{F}}(0)\big)}{p\big(\gamma_{\mathrm{R}}(0)\big)}$$

$$= \frac{\exp(-\beta^{\mathtt{A}} E_{\mathrm{i}}^{\mathtt{A}})}{Z^{\mathtt{A}}} \frac{\exp(-\beta^{\mathtt{B}} E_{\mathrm{i}}^{\mathtt{B}})}{Z^{\mathtt{B}}}$$

$$= \frac{\exp(-\beta^{\mathtt{A}} E_{\mathrm{i}}^{\mathtt{A}} - \beta^{\mathtt{B}} E_{\mathrm{i}}^{\mathtt{B}})}{\exp(-\beta^{\mathtt{A}} E_{\mathrm{f}}^{\mathtt{A}} - \beta^{\mathtt{B}} E_{\mathrm{f}}^{\mathtt{B}})}$$

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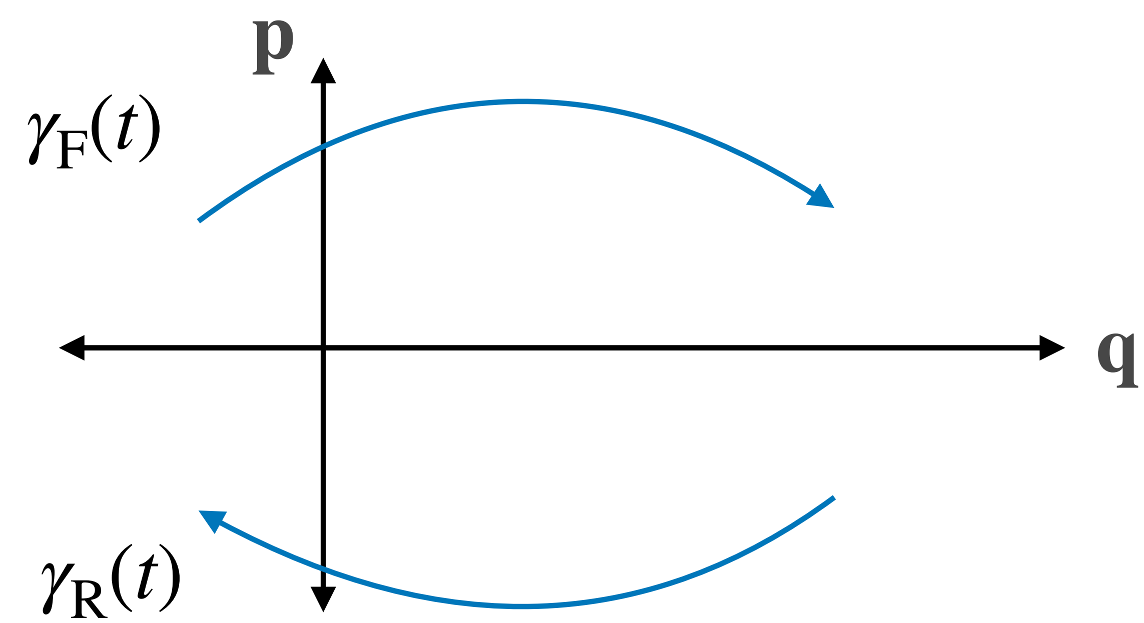
$\gamma_{\rm R}(t) : (E_{\rm f}^{\rm A}, E_{\rm f}^{\rm B} \mapsto E_{\rm i}^{\rm A}, E_{\rm i}^{\rm B})$



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$$= \frac{\exp(-\beta^{\rm A} E_{\rm i}^{\rm A} - \beta^{\rm B} E_{\rm i}^{\rm B})}{\exp(-\beta^{\rm A} E_{\rm f}^{\rm A} - \beta^{\rm B} E_{\rm f}^{\rm B})}$$

$$= \exp[\beta^{\rm A}(E_{\rm f}^{\rm A} - E_{\rm i}^{\rm A}) + \beta^{\rm B}(E_{\rm f}^{\rm B} - E_{\rm i}^{\rm B})]$$

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Classical Exchange Fluctuation Theorem

Trajectories $\gamma_F(t) : (E_i^A, E_i^B \mapsto E_f^A, E_f^B)$

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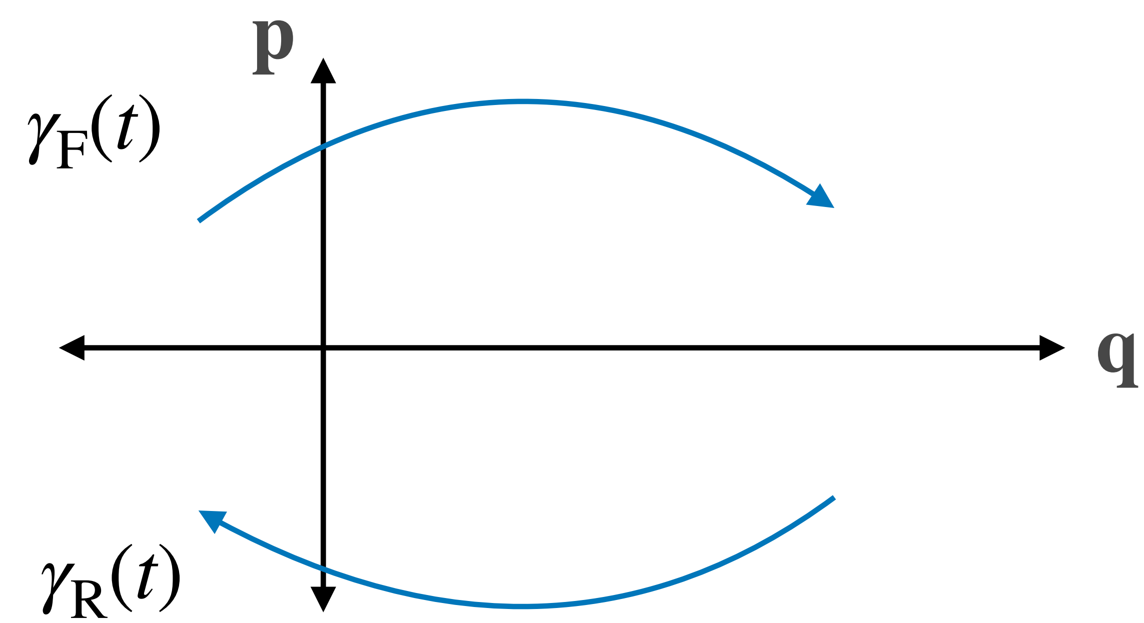

$$\frac{p\big(\gamma_F(t)\big)}{p\big(\gamma_R(t)\big)} = \frac{p\big(\gamma_F(0)\big)}{p\big(\gamma_R(0)\big)}$$

$$= \frac{\exp(-\beta^A E_i^A)}{Z^A} \frac{\exp(-\beta^B E_i^B)}{Z^B}$$

$$= \frac{\exp(-\beta^A E_i^A - \beta^B E_i^B)}{\exp(-\beta^A E_f^A - \beta^B E_f^B)}$$

$$= \exp[\beta^A (E_f^A - E_i^A) + \beta^B (E_f^B - E_i^B)]$$

$$= \exp[-\beta^A Q + \beta^B Q]$$

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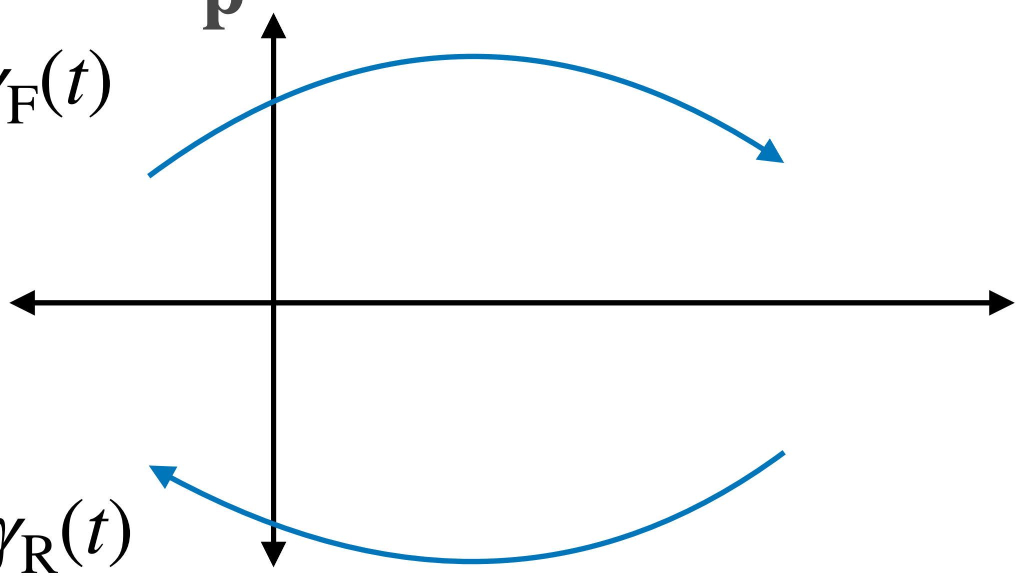

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$$\Delta\beta := \beta^B - \beta^A$$

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$$= \exp(\Delta\beta Q)$$

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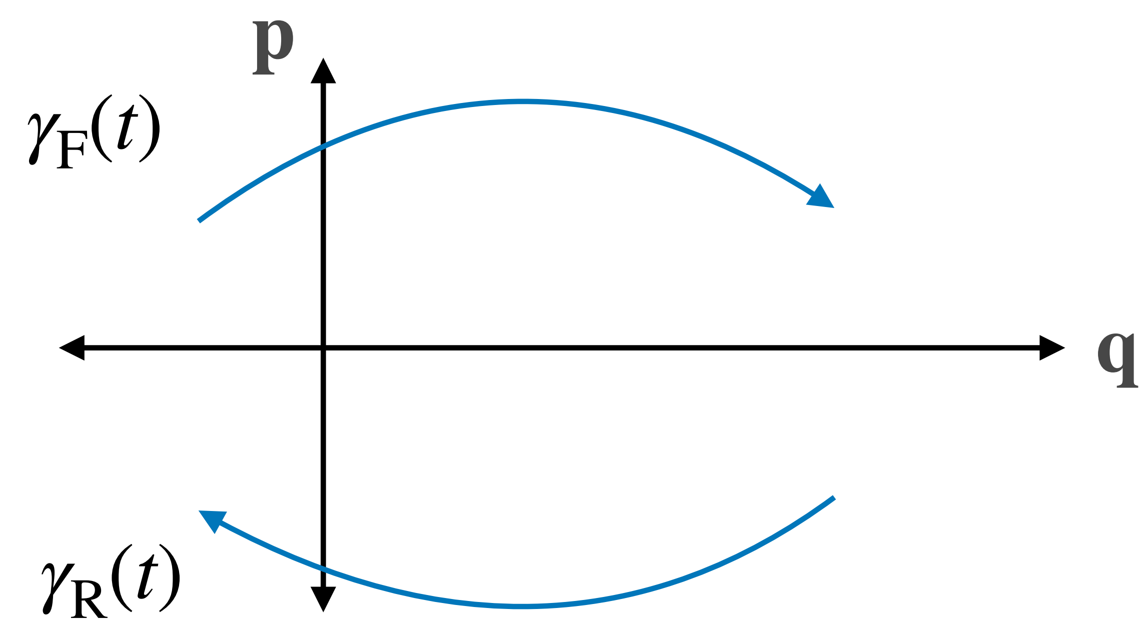

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$$\Delta\beta := \beta^B - \beta^A$$

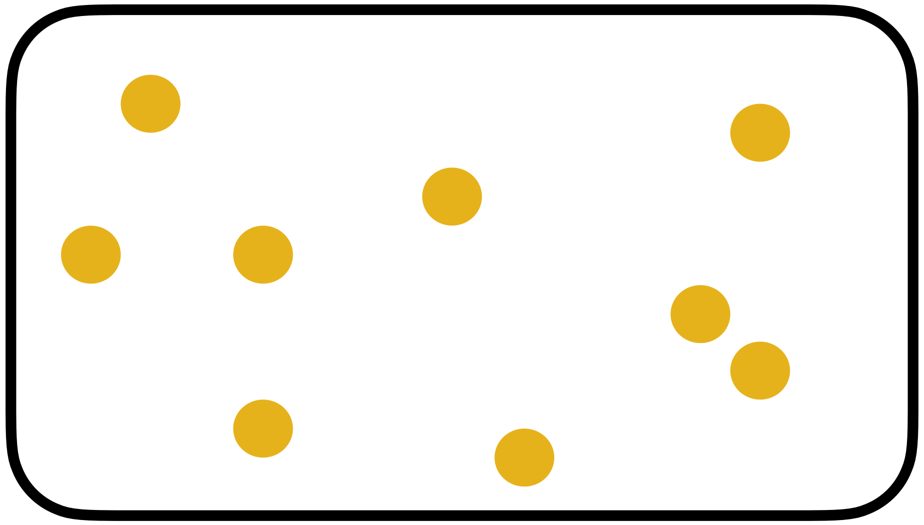
$$= \exp[-\beta^A Q + \beta^B Q]$$

$$= \exp(\Delta\beta Q) \qquad \Longrightarrow \quad (\beta^B - \beta^A)\langle Q\rangle \geq 0$$

[Jarzynski and Wójcik, PRL 92, 230602 (2004)]

Quantization Issues?

A



$$\rho^{\mathtt{A}} = \frac{\exp(-\beta^{\mathtt{A}} H^{\mathtt{A}})}{Z^{\mathtt{A}}}$$

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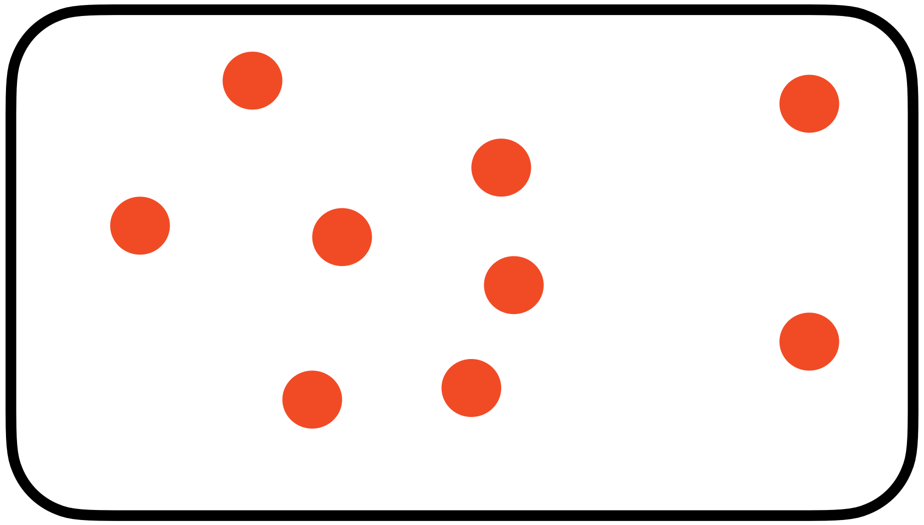

$$\rho^{\mathtt{B}} = \frac{\exp(-\beta^{\mathtt{B}} H^{\mathtt{B}})}{Z^{\mathtt{B}}}$$

Evolve according to energy conserving unitary U: $[U, H^{\mathtt{A}} + H^{\mathtt{B}}] = 0$.

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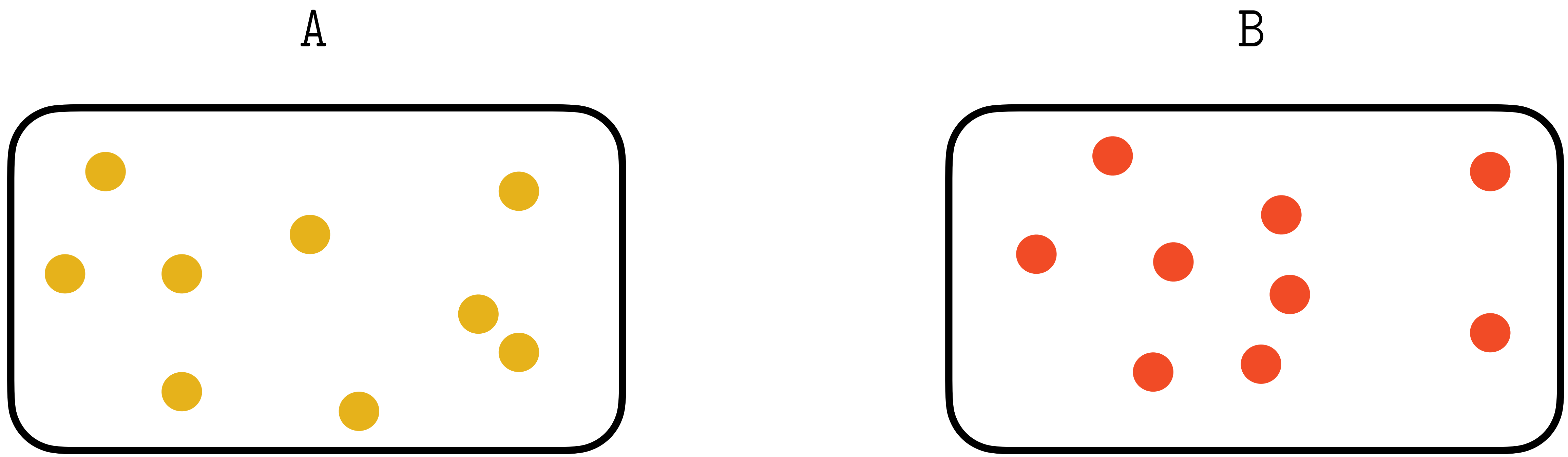

$$\rho^{\mathtt{A}} = \frac{\exp(-\beta^{\mathtt{A}} H^{\mathtt{A}})}{Z^{\mathtt{A}}} \qquad \rho^{\mathtt{B}} = \frac{\exp(-\beta^{\mathtt{B}} H^{\mathtt{B}})}{Z^{\mathtt{B}}}$$

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Access statistics associate with $\rho^{\mathtt{A}} \otimes \rho^{\mathtt{B}} \rightarrow U(\rho^{\mathtt{A}} \otimes \rho^{\mathtt{B}})U^{\dagger}$: measure energies before and after the unitary is implemented.

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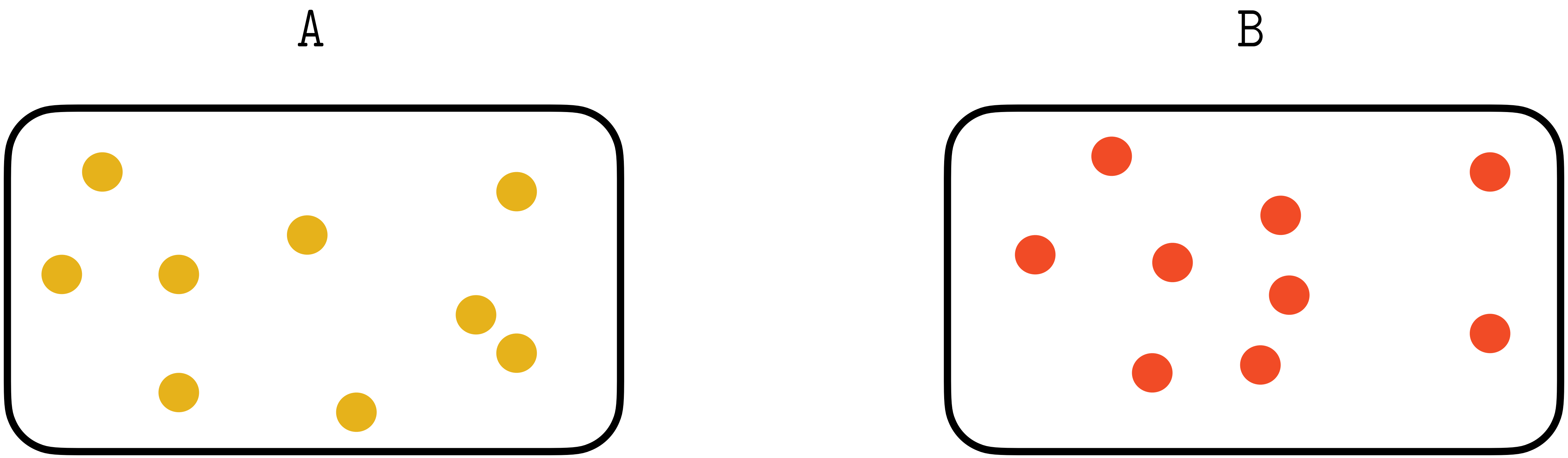

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Same probability distributions in the classical setting.

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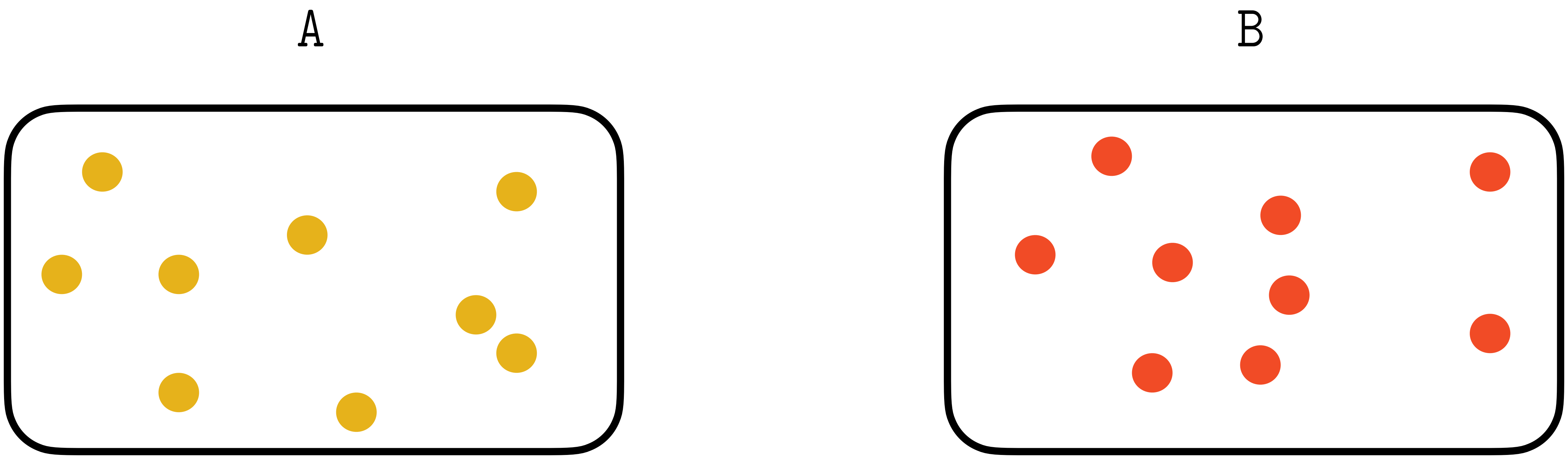

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Same probability distributions in the classical setting.

What if the initial state is some arbitrary $\rho^{\mathtt{AB}}$ with thermal marginals?

Three reasons to consider KD distributions

… in the context of thermodynamics:

(i) Avoiding disturbance

(ii) "KD averages" equal quantum expectation values

(iii) No-go theorems

(i) Avoiding disturbance

General $\rho^{\mathtt{AB}}$ with thermal marginals.

Dephasing in the energy eigenbasis:

$$\rho^{\mathtt{AB}} \to \sum_{j,k} \left(\Pi^{\mathtt{A}}_{E_j} \otimes \Pi^{\mathtt{B}}_{E_k}\right) \rho^{\mathtt{AB}} \left(\Pi^{\mathtt{A}}_{E_j} \otimes \Pi^{\mathtt{B}}_{E_k}\right)$$

(i) Avoiding disturbance

To avoid the disturbance, we may weakly measure the initial energy.

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Strong measurements lead to the probability distribution

$$p(E_{i_{\mathtt{A}}}, E_{i_{\mathtt{B}}} \to E_{f_{\mathtt{A}}}, E_{f_{\mathtt{B}}}) = \mathrm{Tr}(\Pi_{f_{\mathtt{A}}, f_{\mathtt{B}}} U \Pi_{i_{\mathtt{A}}, i_{\mathtt{B}}} \rho^{\mathtt{AB}} \Pi_{i_{\mathtt{A}}, i_{\mathtt{B}}} U^{\dagger}) \ .$$

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Weak measurements lead to the Kirkwood-Dirac distribution

$$q^{\rho}(E_{i_{\mathtt{A}}}, E_{i_{\mathtt{B}}} \to E_{f_{\mathtt{A}}}, E_{f_{\mathtt{B}}}) = \mathrm{Tr}(U^{\dagger} \Pi_{f_{\mathtt{A}}, f_{\mathtt{B}}} U \Pi_{i_{\mathtt{A}}, i_{\mathtt{B}}} \rho^{\mathtt{AB}}) \; .$$

(ii) "KD averages" = quantum expectation values

Classically, Q is a random variable.

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The average of Q is

$$\langle Q \rangle = \sum_{E_{i_\mathtt{A}}, E_{i_\mathtt{B}}, E_{f_\mathtt{A}}, E_{f_\mathtt{B}}} p(E_{i_\mathtt{A}}, E_{i_\mathtt{B}} \to E_{f_\mathtt{A}}, E_{f_\mathtt{B}}) Q = \sum_{E_{i_\mathtt{A}}, E_{i_\mathtt{B}}, E_{f_\mathtt{A}}, E_{f_\mathtt{B}}} p(E_{i_\mathtt{A}}, E_{i_\mathtt{B}} \to E_{f_\mathtt{A}}, E_{f_\mathtt{B}})(E_{f_\mathtt{B}} - E_{i_\mathtt{B}})$$

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The quantum expectation value can be expressed via the KD distribution:

$$\langle Q \rangle = \mathrm{Tr}(U^\dagger H^{\mathtt{AB}} U \rho^{\mathtt{AB}}) - \mathrm{Tr}(H^{\mathtt{AB}} \rho^{\mathtt{AB}}) = \sum_{f_\mathtt{A}, f_\mathtt{B}, i_\mathtt{A}, i_\mathtt{B}} \mathrm{Tr}(U^\dagger \Pi_{f_\mathtt{A}, f_\mathtt{B}} U \Pi_{i_\mathtt{A}, i_\mathtt{B}} \rho^{\mathtt{AB}}) (E_{f_\mathtt{B}} - E_{i_\mathtt{B}})$$

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$$\neq \sum_{f_\mathtt{A}, f_\mathtt{B}, i_\mathtt{A}, i_\mathtt{B}} \underline{\mathrm{Tr}(\Pi_{f_\mathtt{A}, f_\mathtt{B}} U \Pi_{i_\mathtt{A}, i_\mathtt{B}} \rho^{\mathtt{AB}} \Pi_{i_\mathtt{A}, i_\mathtt{B}} U^\dagger)}(E_{f_\mathtt{B}} - E_{i_\mathtt{B}})$$

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Classically, Q is a random variable.

The average of Q is

$$\langle Q \rangle = \sum_{E_{i_A}, E_{i_B}, E_{f_A}, E_{f_B}} p(E_{i_A}, E_{i_B} \to E_{f_A}, E_{f_B}) Q = \sum_{E_{i_A}, E_{i_B}, E_{f_A}, E_{f_B}} p(E_{i_A}, E_{i_B} \to E_{f_A}, E_{f_B})(E_{f_B} - E_{i_B})$$

The quantum expectation value can be expressed via the KD distribution:

$$\langle Q \rangle = \mathrm{Tr}(U^\dagger H^{AB} U \rho^{AB}) - \mathrm{Tr}(H^{AB} \rho^{AB}) = \sum_{f_A, f_B, i_A, i_B} \mathrm{Tr}(U^\dagger \Pi_{f_A, f_B} U \Pi_{i_A, i_B} \rho^{AB})(E_{f_B} - E_{i_B})$$

$$\neq \sum_{f_A, f_B, i_A, i_B} \mathrm{Tr}(\Pi_{f_A, f_B} U \Pi_{i_A, i_B} \rho^{AB} \Pi_{i_A, i_B} U^\dagger)(E_{f_B} - E_{i_B})$$

Marginals agree with the Born rule:

$$\sum_{i_A, i_B} q^\rho = \mathrm{Tr}(\Pi_{f_A, f_B} U \rho^{AB} U^\dagger), \quad \sum_{f_A, f_B} q^\rho = \mathrm{Tr}(\Pi_{i_A, i_B} \rho^{AB}), \quad \text{and} \quad \sum_{i_A, i_B, f_A, f_B} q^\rho = 1$$

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Impossibility of probabilistic descriptions and quantum thermodynamic processes.

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There exist no probability distributions that satisfy these requirements and also describe fluctuations of heat.

[Perarnau-Llobet et al., PRL 118, 070601 (2017)]

[Lostaglio et al., Quantum 7, 1128 (2023)]

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Kirkwood-Dirac distributions satisfy both requirements.

Thermodynamic applications

- Negative and nonreal KD quasiprobabilities signal nonclassical heat and work flows.

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- Featured in the analogue of a thermodynamic fluctuation theorem.

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- An extended KD distribution characterizes noncommuting quantities' fluctuations.

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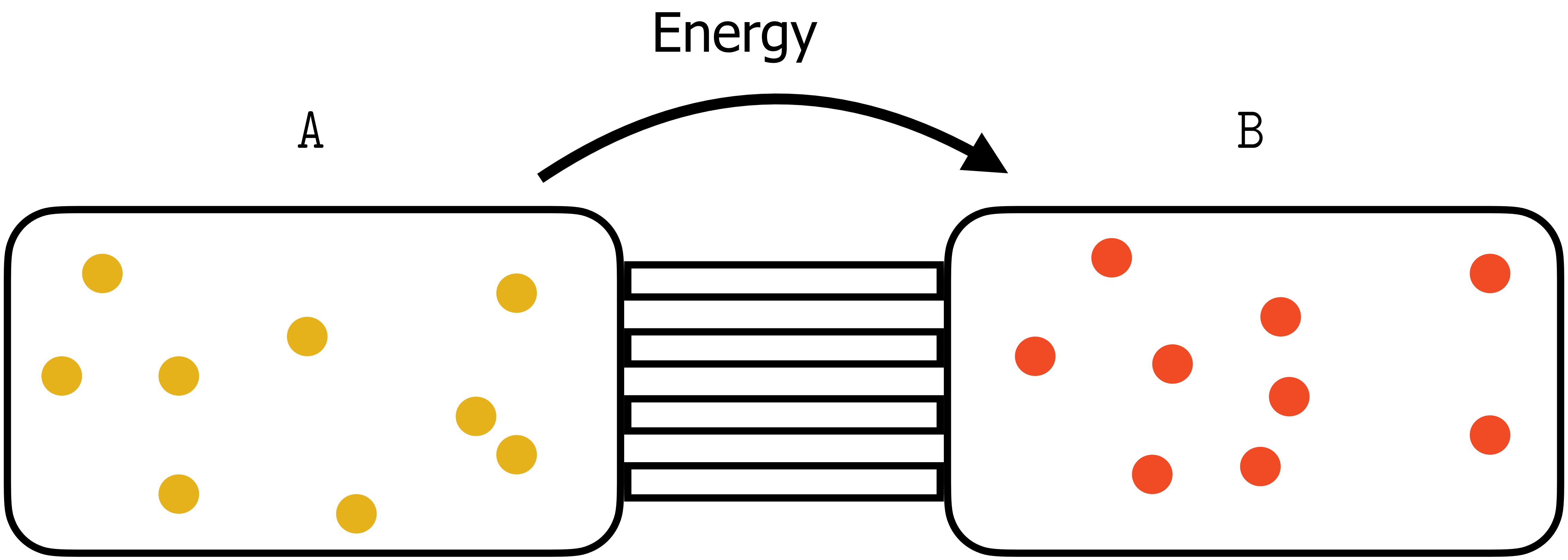

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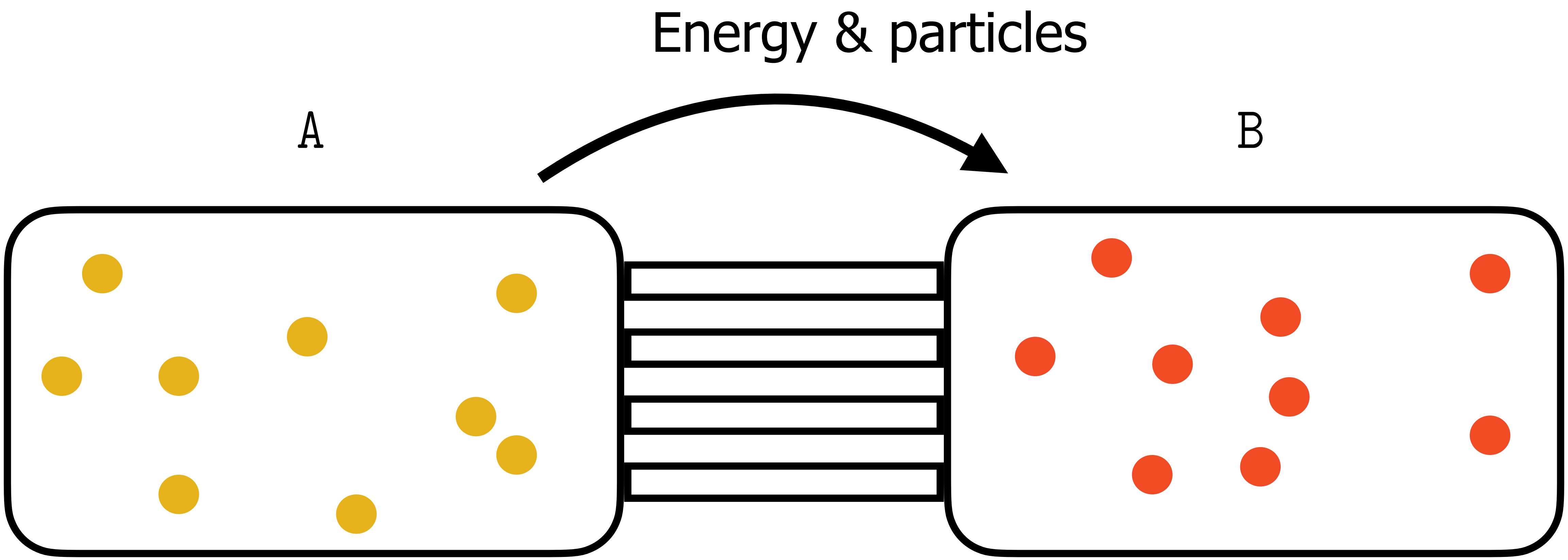

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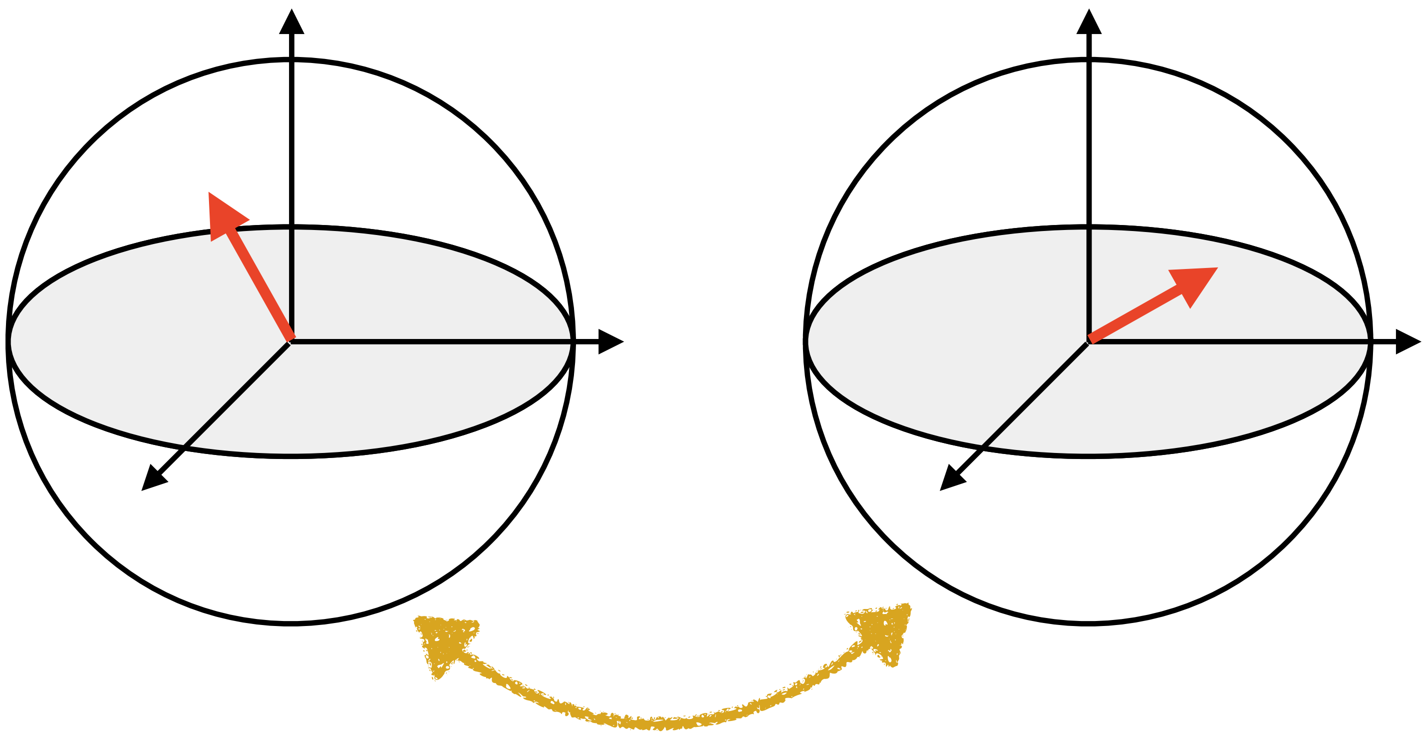

$\sigma_{\alpha=x,y,z}$

[Majidy et al., Nat. Rev. Phys. (2023)]

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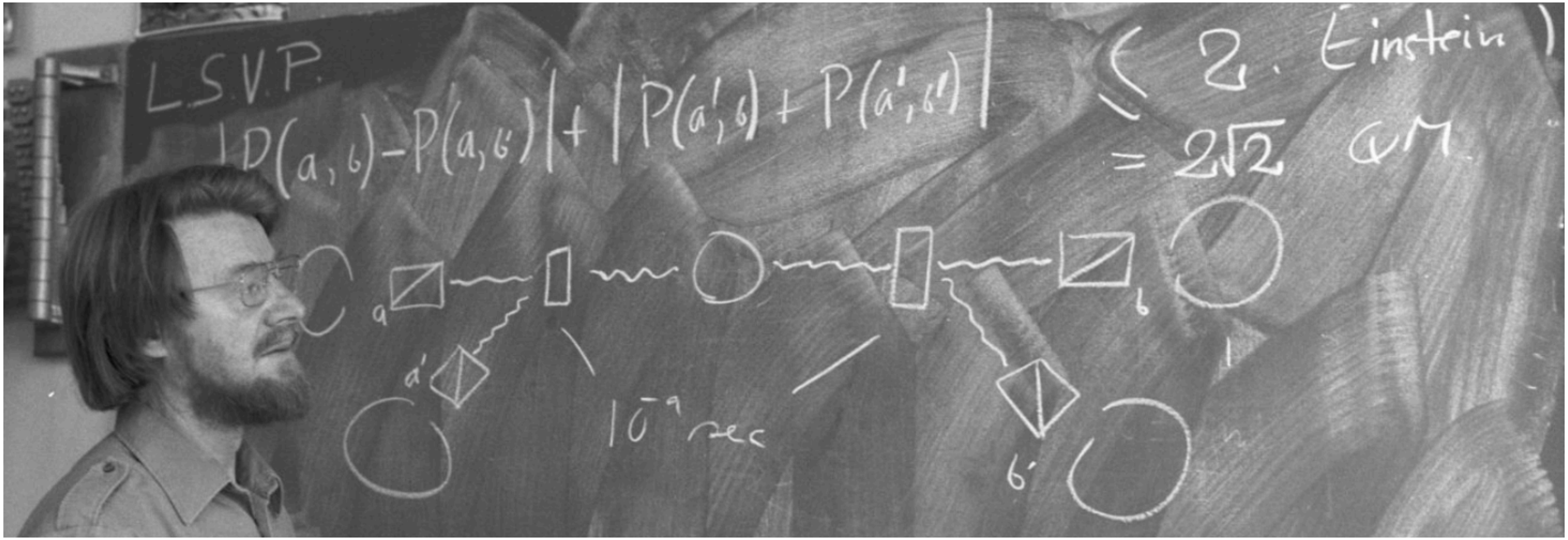

Where we are going

(i) A type of realist model: ontological model

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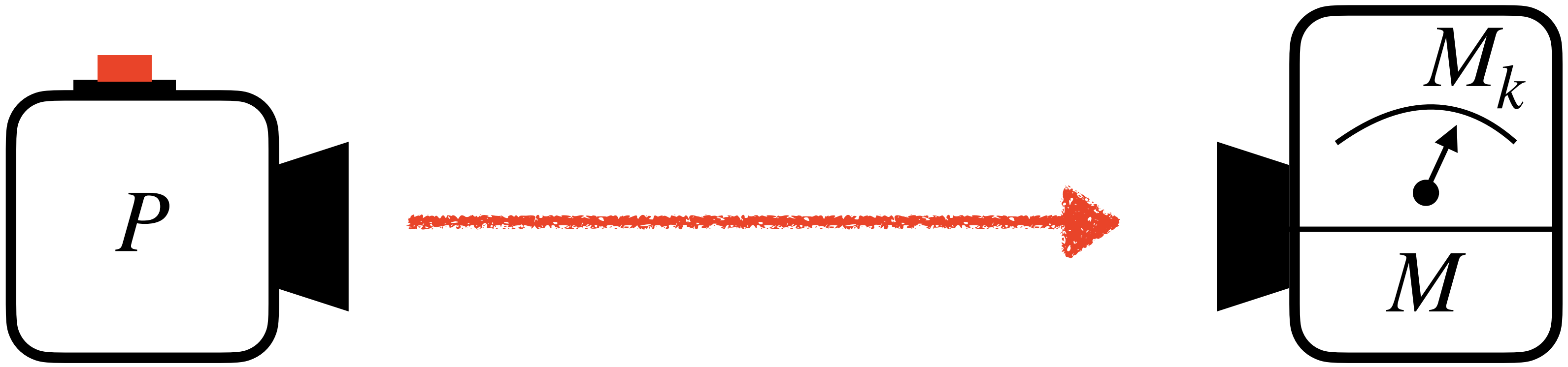
(iii) Kirkwood-Dirac negativity and nonreality imply contextuality

[Spekkens, PRA 71, 052108 (2005)]

[Pusey, PRL 113, 200401 (2014)]

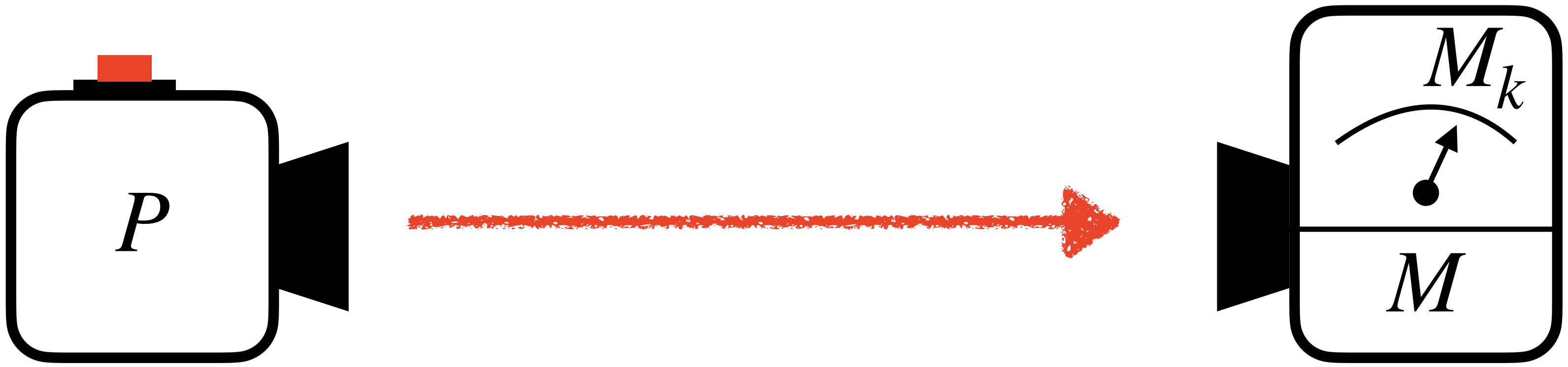
[Kunjwal, Lostaglio, and Pusey, PRA 100, 042116 (2019)

Ontological Models



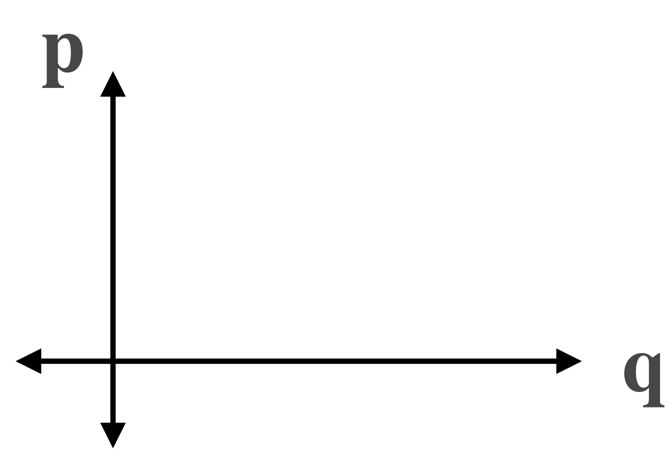
Theory independent!

Ontological Models



Introduce the classical/ontic state space Λ with states $\lambda \in \Lambda$.

Examples:



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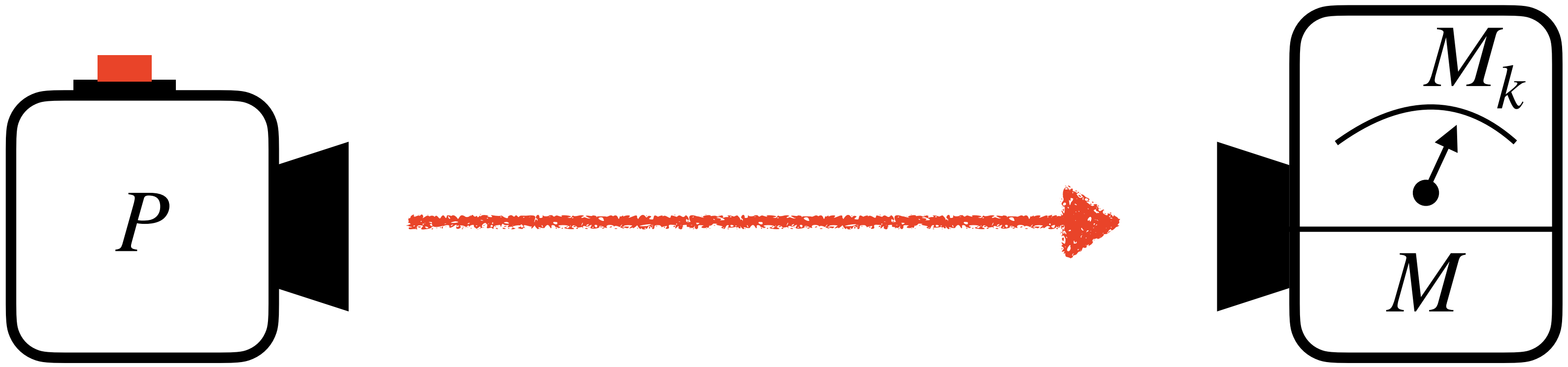

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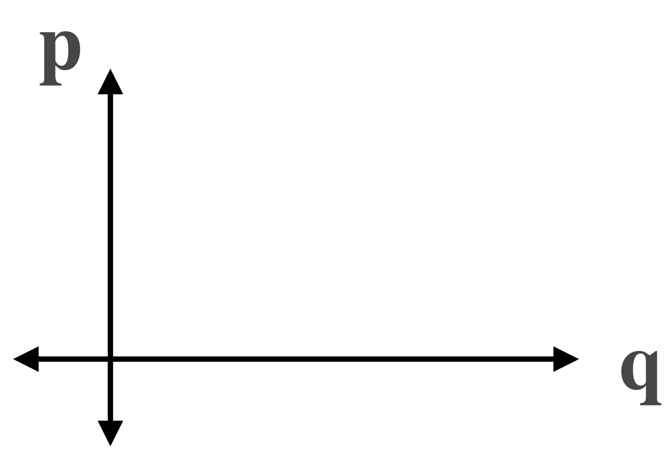

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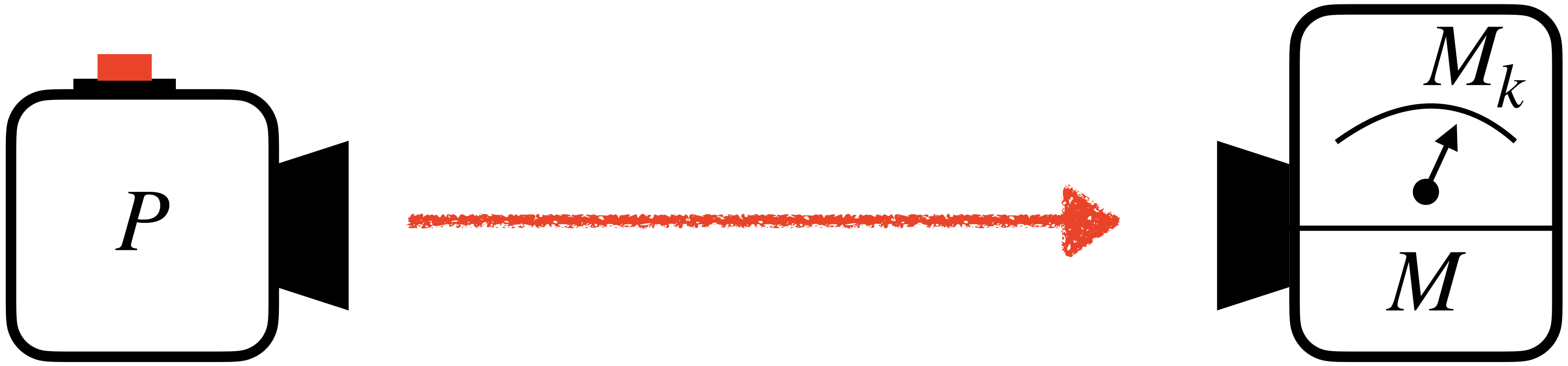

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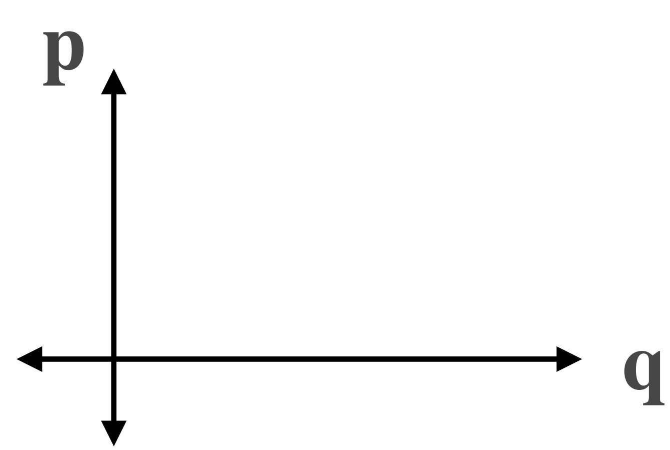

Example: response function for outcome

“the coin is heads up.”


	H	T
(euro coin)	1	0
(penny)	1	0

Ontological Models

Ontological model summary:

- ontic state space Λ with states $\lambda \in \Lambda$
- map $\rho \to p(\lambda \mid \rho)$
  - $\sum_{\lambda} p(\lambda \mid P) = 1$
- map $M_k \to r(M_k \mid \lambda)$ such that
  - for all M_k, $r(M_k \mid \lambda) \geq 0$
  - $\sum_{k} r(M_k \mid \lambda) = 1$

[Spekkens, PRA 71, 052108 (2005)]

Ontological Models

The outcome statistics are $p(M_k \,|\, P) = \sum_\lambda r(M_k \,|\, \lambda)\; p(\lambda \,|\, P)$.

Quantum measurements: positive operator-valued measure

$$\{\hat{M}_k\} \quad \text{such that} \quad \sum_k \hat{M}_k = I$$

Modeling a quantum experiment: $\mathrm{Tr}(\hat{M}_k \rho) = \sum_\lambda r(\hat{M}_k \,|\, \lambda)\; p(\lambda \,|\, \rho)$.

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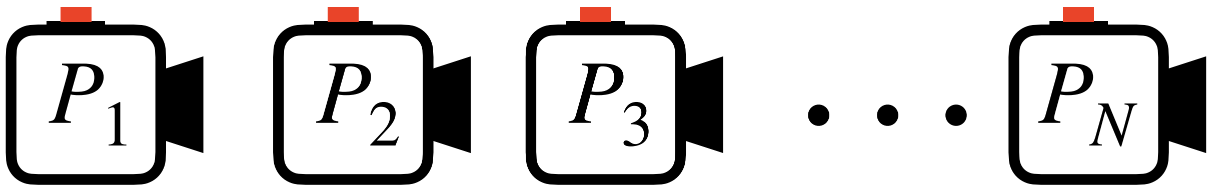
Noncontextuality



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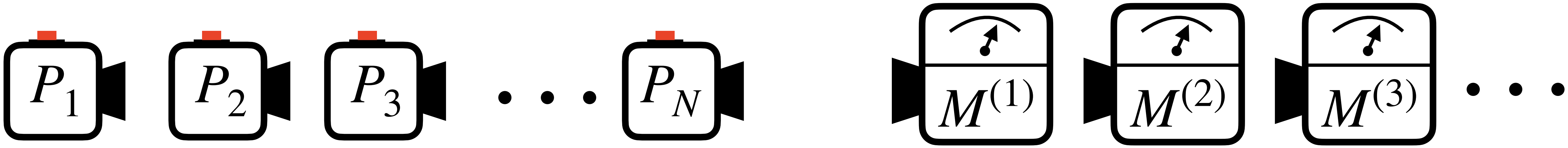

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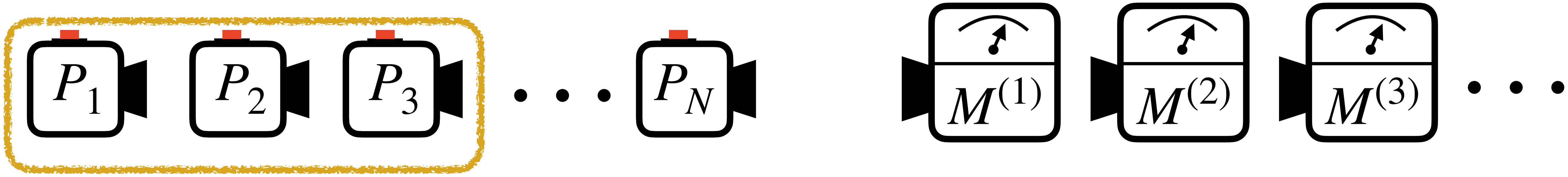

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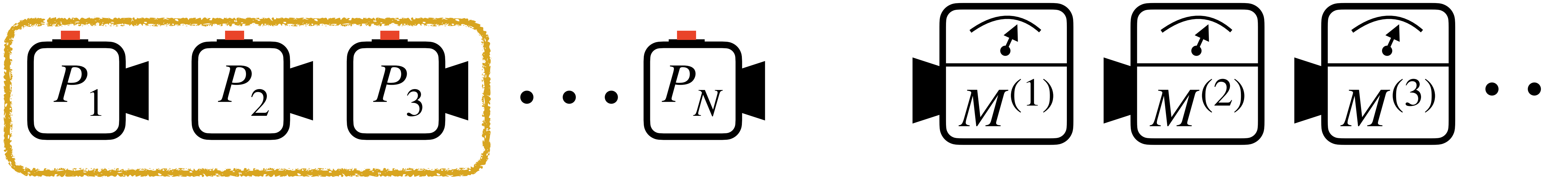

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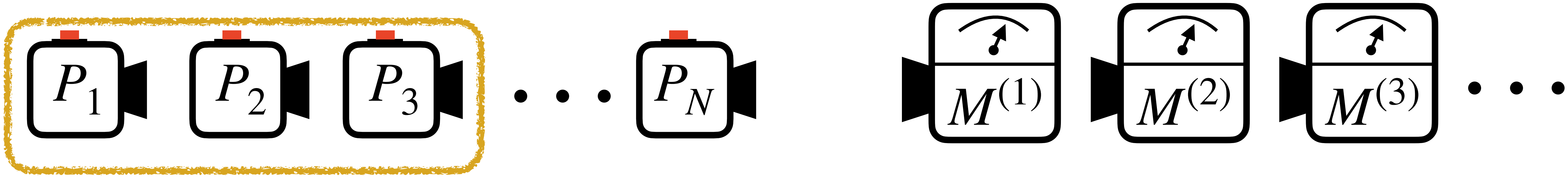

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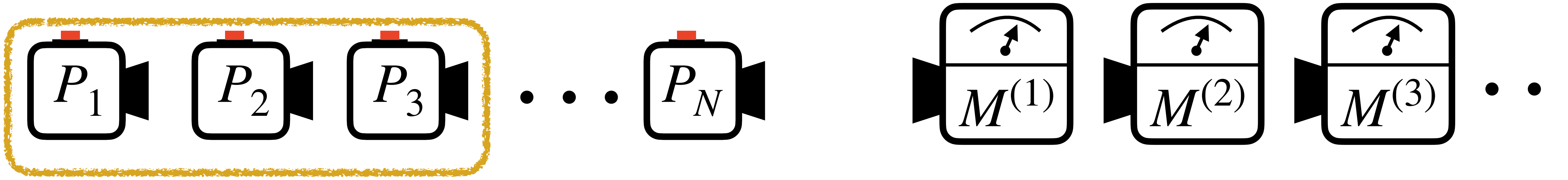

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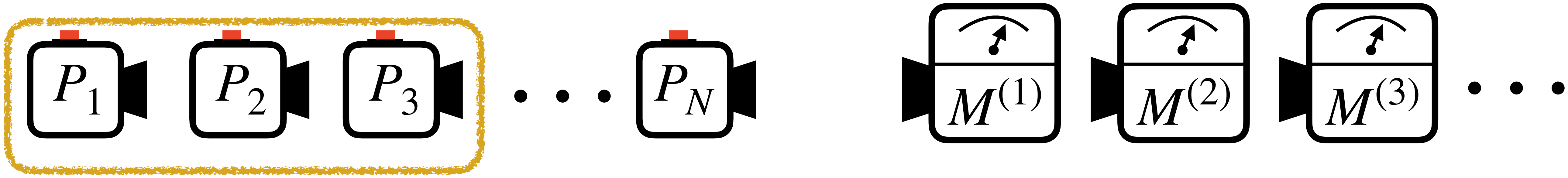

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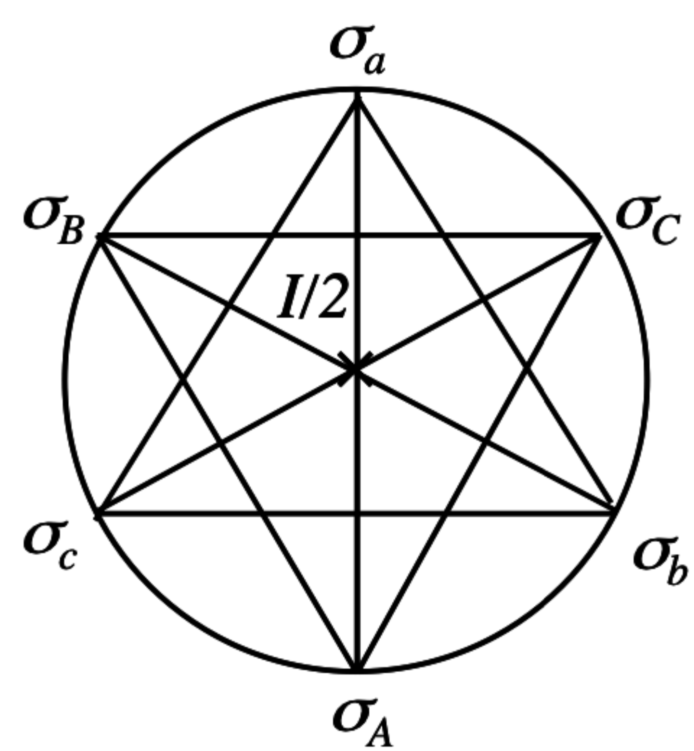

Kirkwood-Dirac contextuality proof

$$\mathrm{Re}(q^{\rho}_{a_j,f_k}) = \mathrm{ReTr}\left(\Pi_{f_k}\Pi_{a_j}\rho\right) < 0$$

$\Longrightarrow$ one experiment is contextual.

[Pusey, PRL 113, 200401 (2014)]

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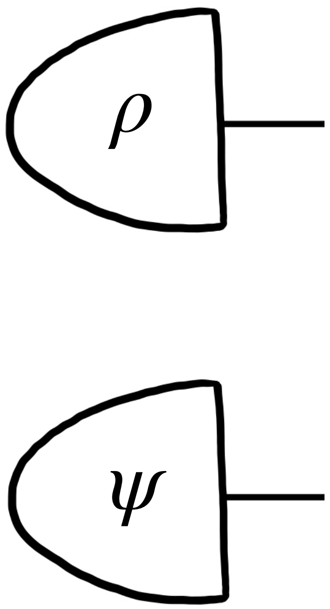

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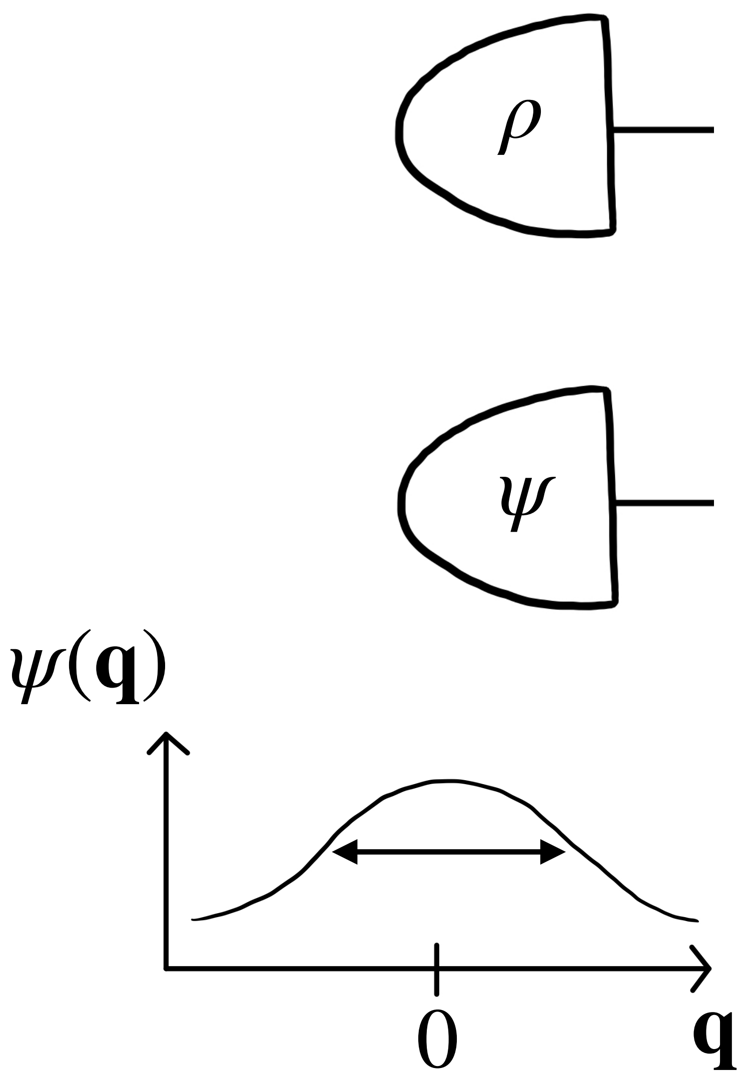

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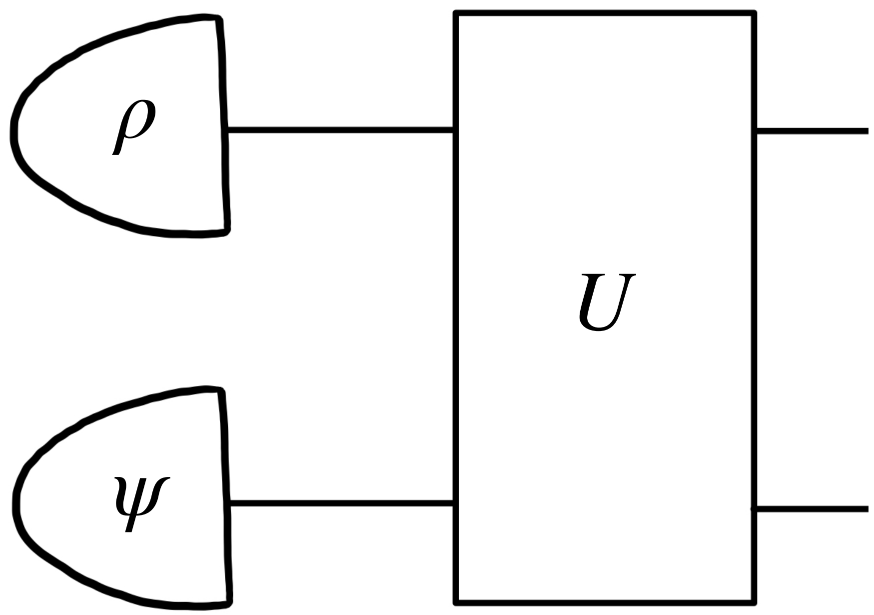

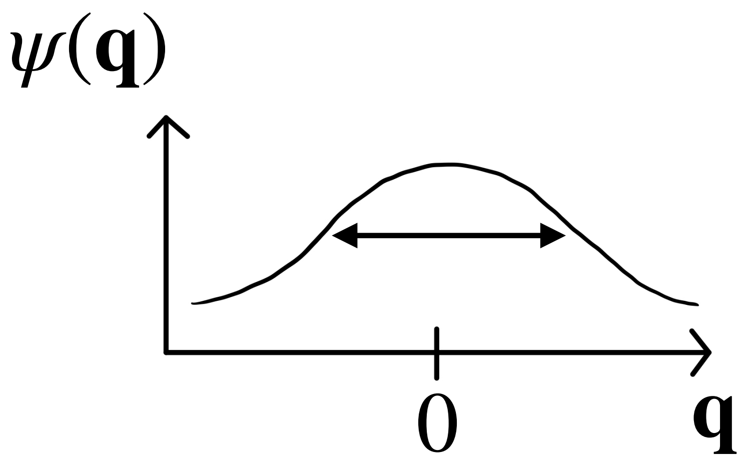

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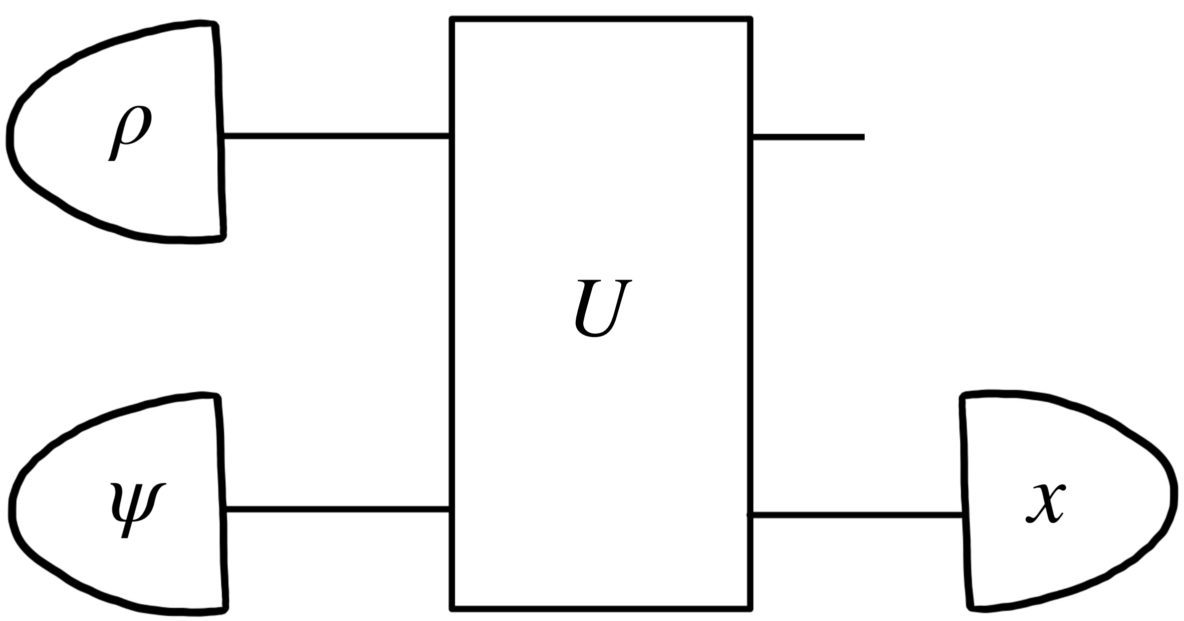

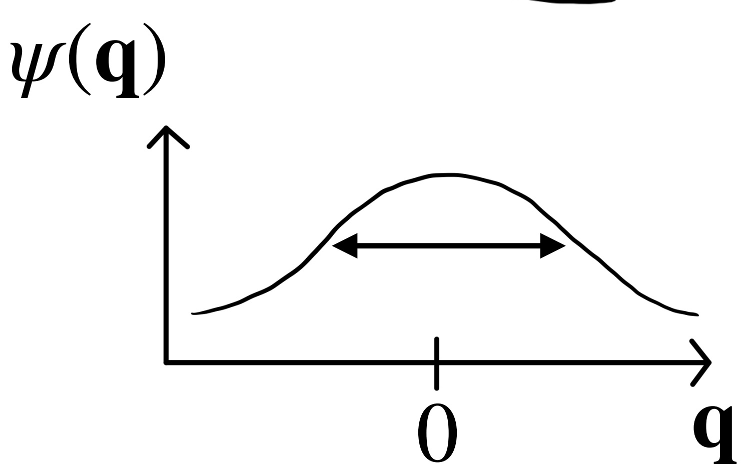

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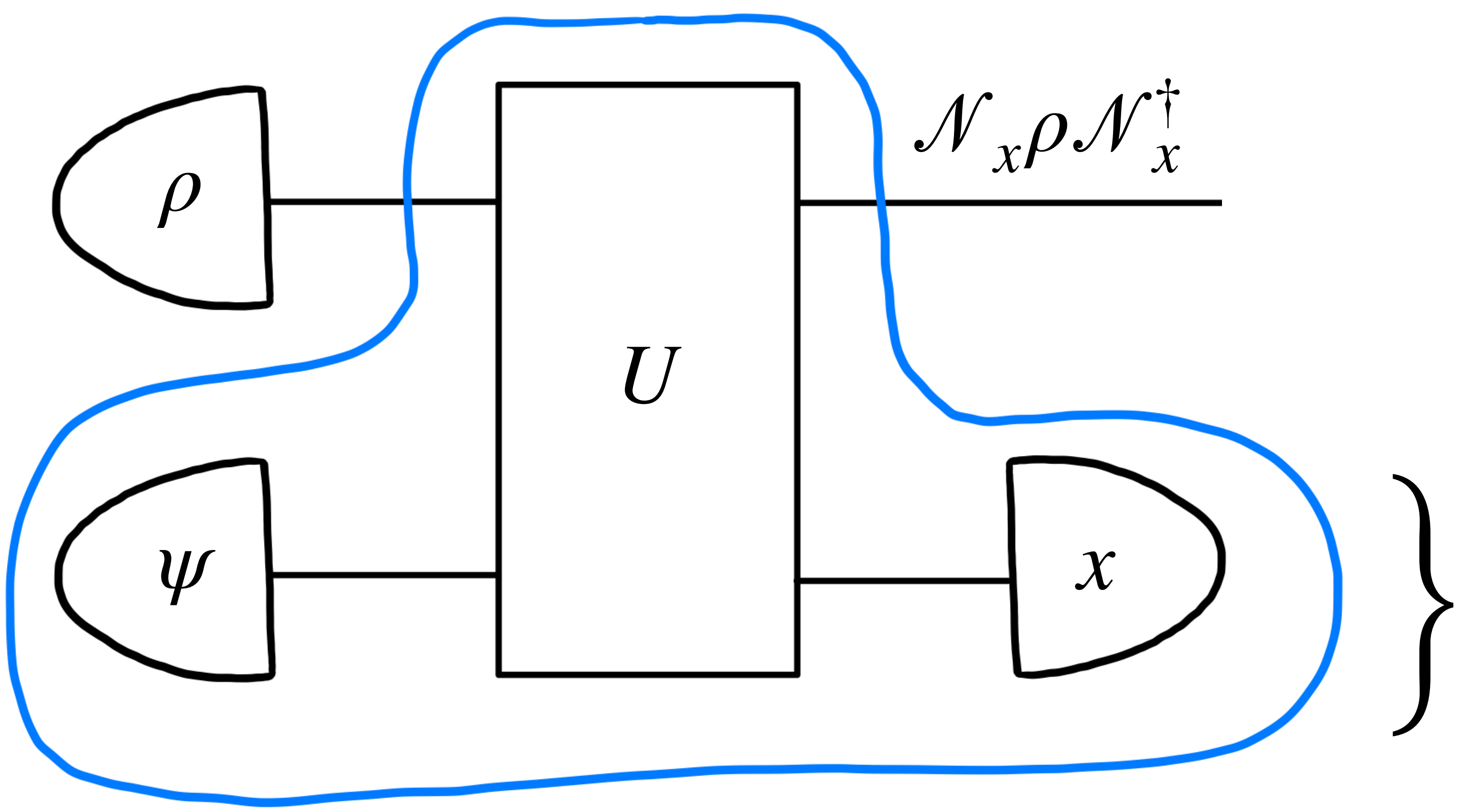

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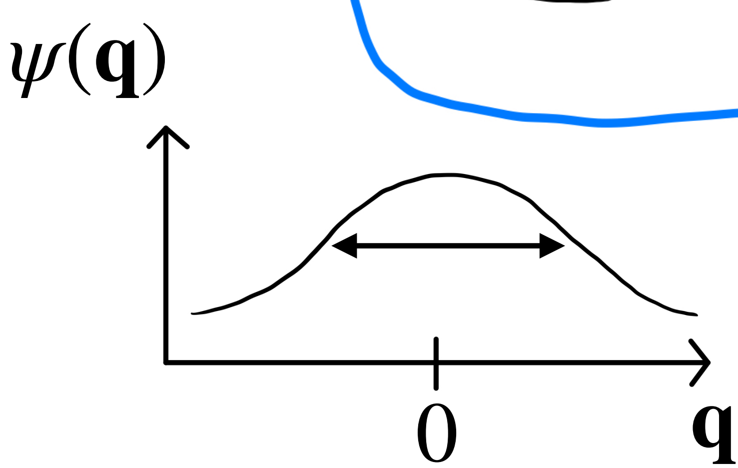

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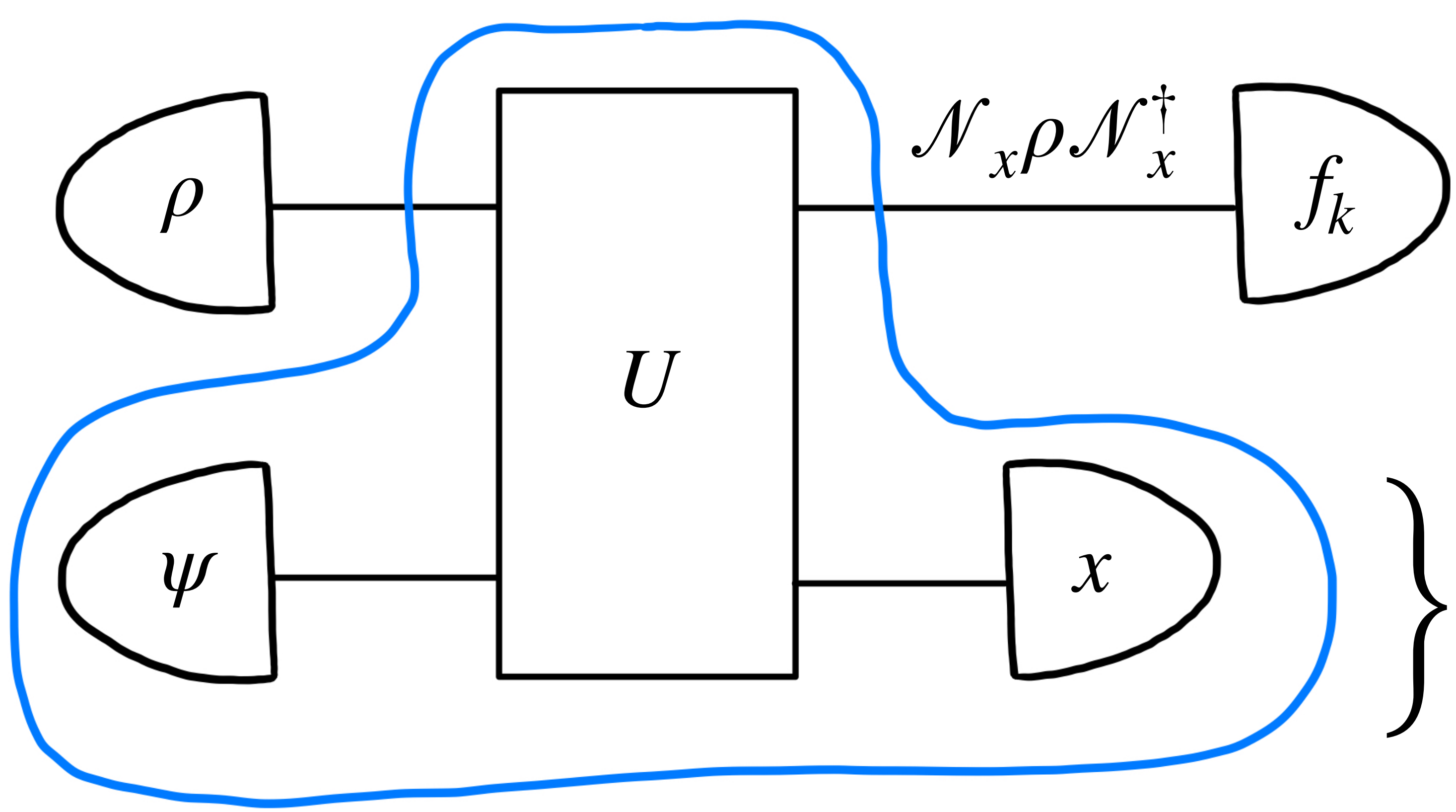

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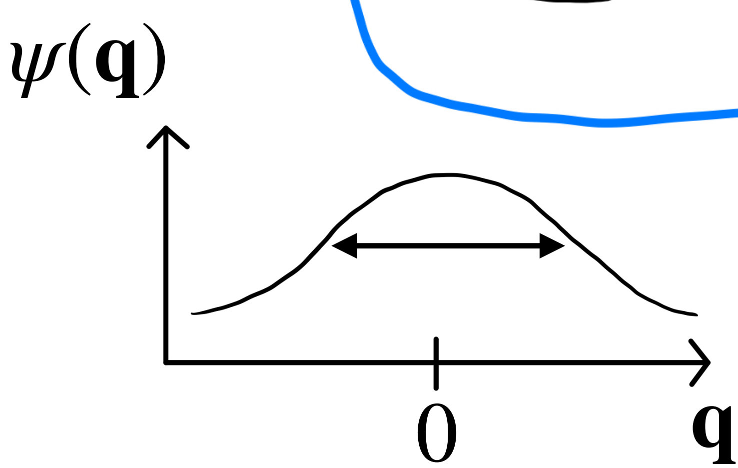

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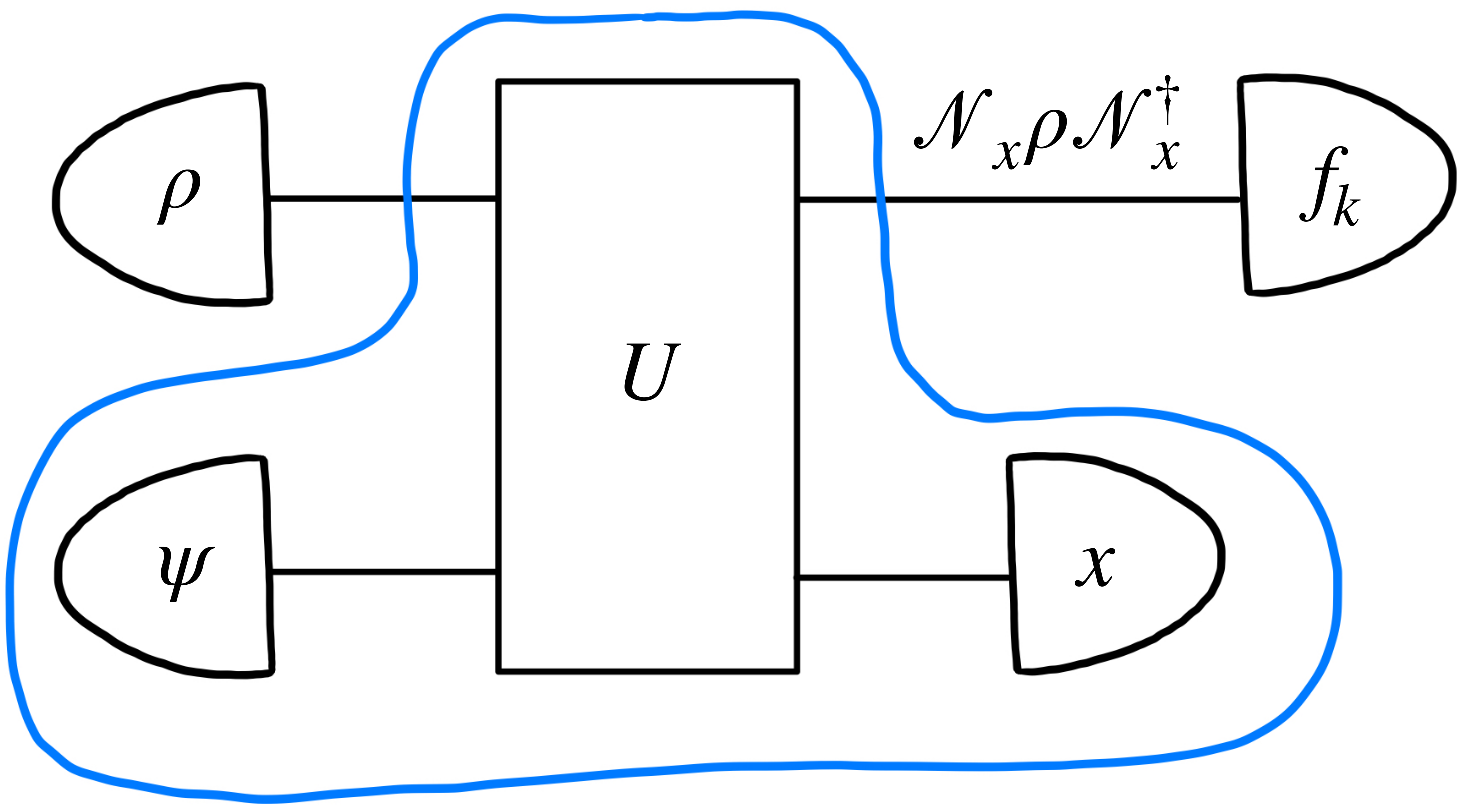

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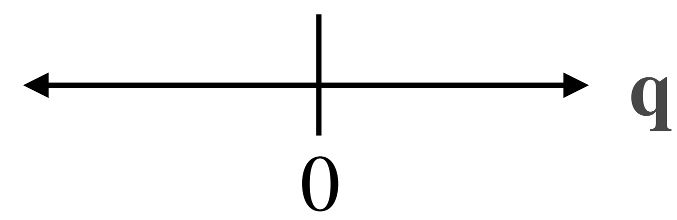

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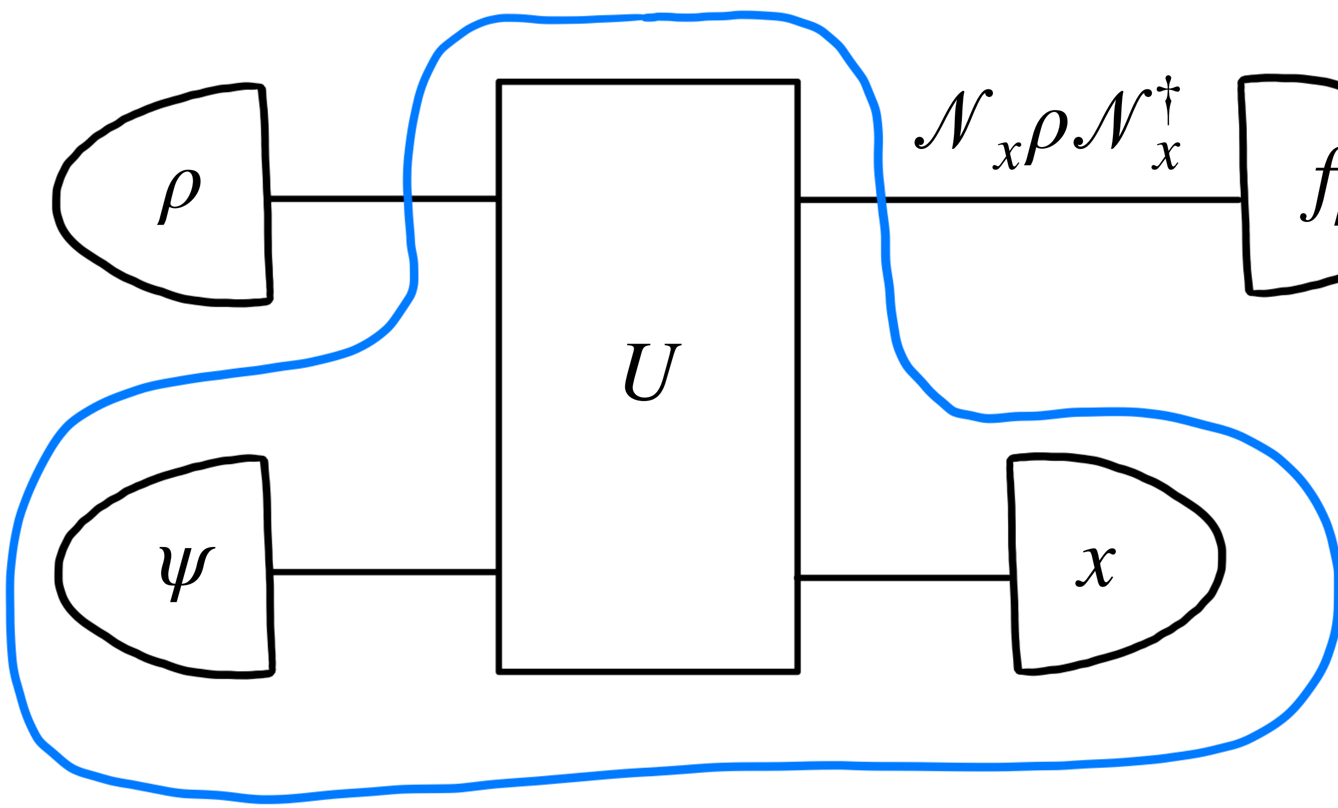

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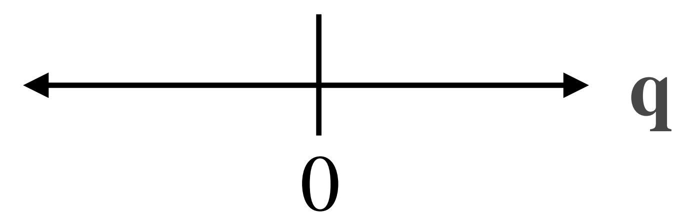

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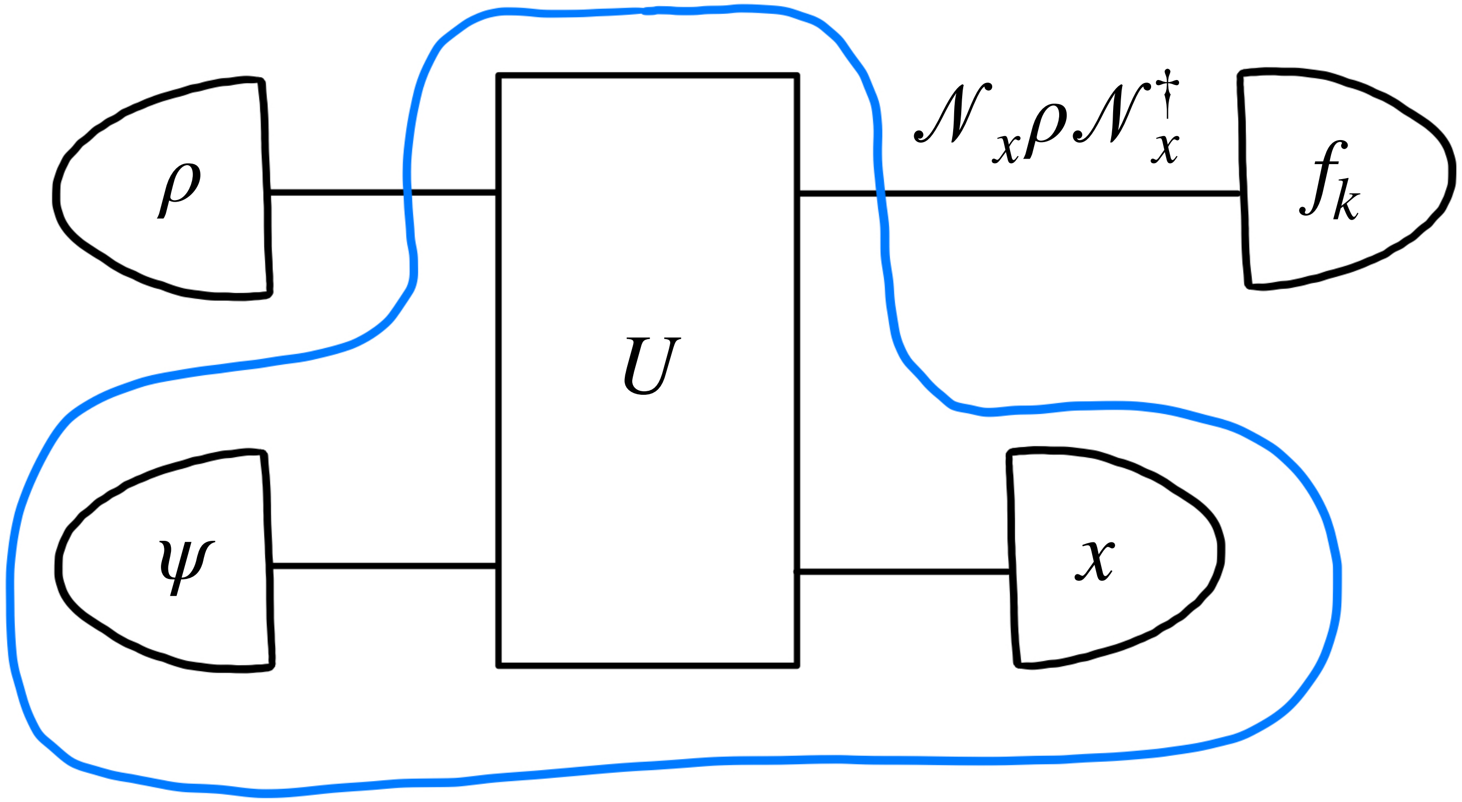

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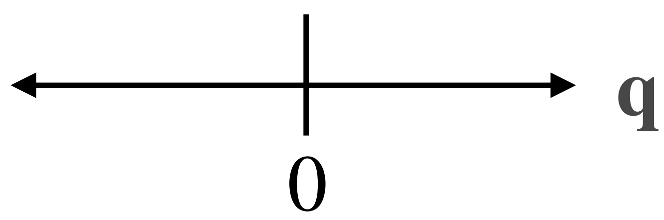

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$$p_-^{\text{NOM}} \leq \frac{p_F}{2} + p_d = \frac{p_F}{2} + o(1/s)$$

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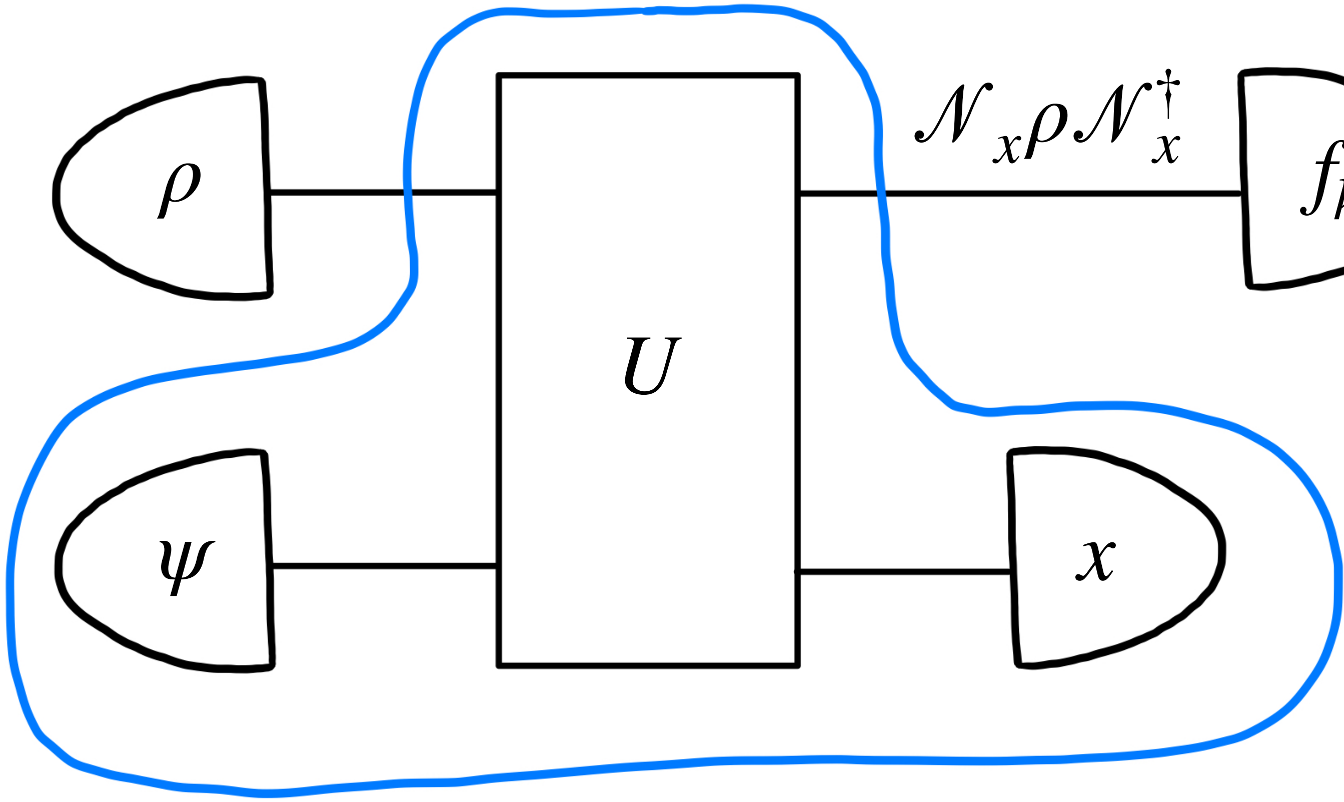
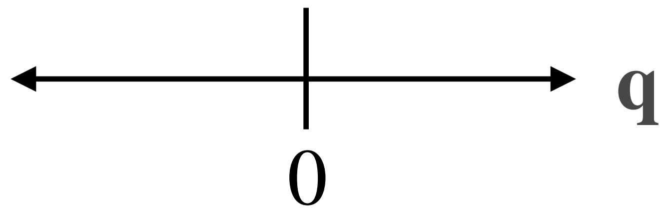


Final pointer position:



$$p_-^{\text{ideal}} = \int_{-\infty}^{0} dx\ \mathrm{Tr}(\Pi_{f_k} \mathcal{N}_x \rho \mathcal{N}_x^\dagger) = \frac{p_F}{2} - \frac{\mathrm{ReTr}(\Pi_{f_k} \Pi_{a_j} \rho)}{\sqrt{\pi s}} + \mathrm{o}(1/s)$$

$$p_-^{\text{NOM}} \leq \frac{p_F}{2} + p_d = \frac{p_F}{2} + \mathrm{o}(1/s)$$

KD negativity implies contextuality.
Also holds for KD nonreality.

[Kunjwal, Lostaglio, and Pusey, PRA 100, 042116 (2019)]

Summary

Kirkwood-Dirac distributions…

- enable the quantization of results in stochastic thermodynamics
- provide a rigorous witness of nonclassicality

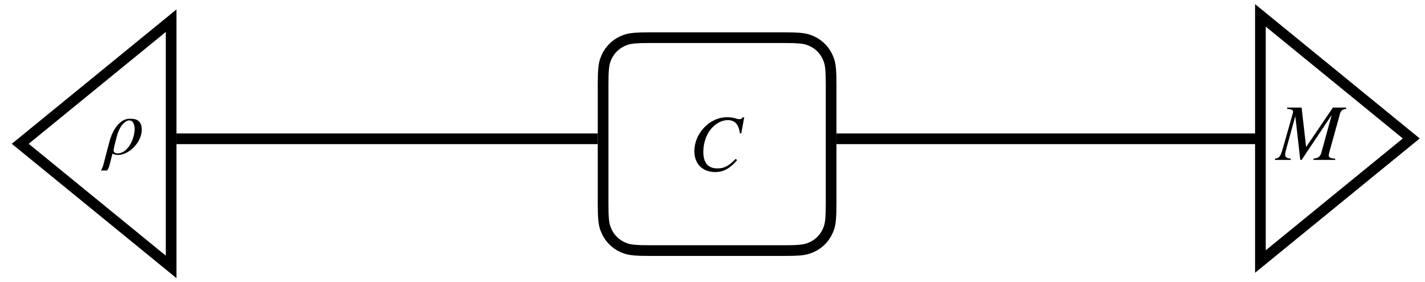
Thanks for your attention!

[Upadhyaya, Braasch, Landi, Yunger Halpen, arXiv:2305.15480 (2023)]

Noncontextuality and positive quasiprobabilities

Quasiprobability distributions are defined over measurable spaces.

Quantum experiment:

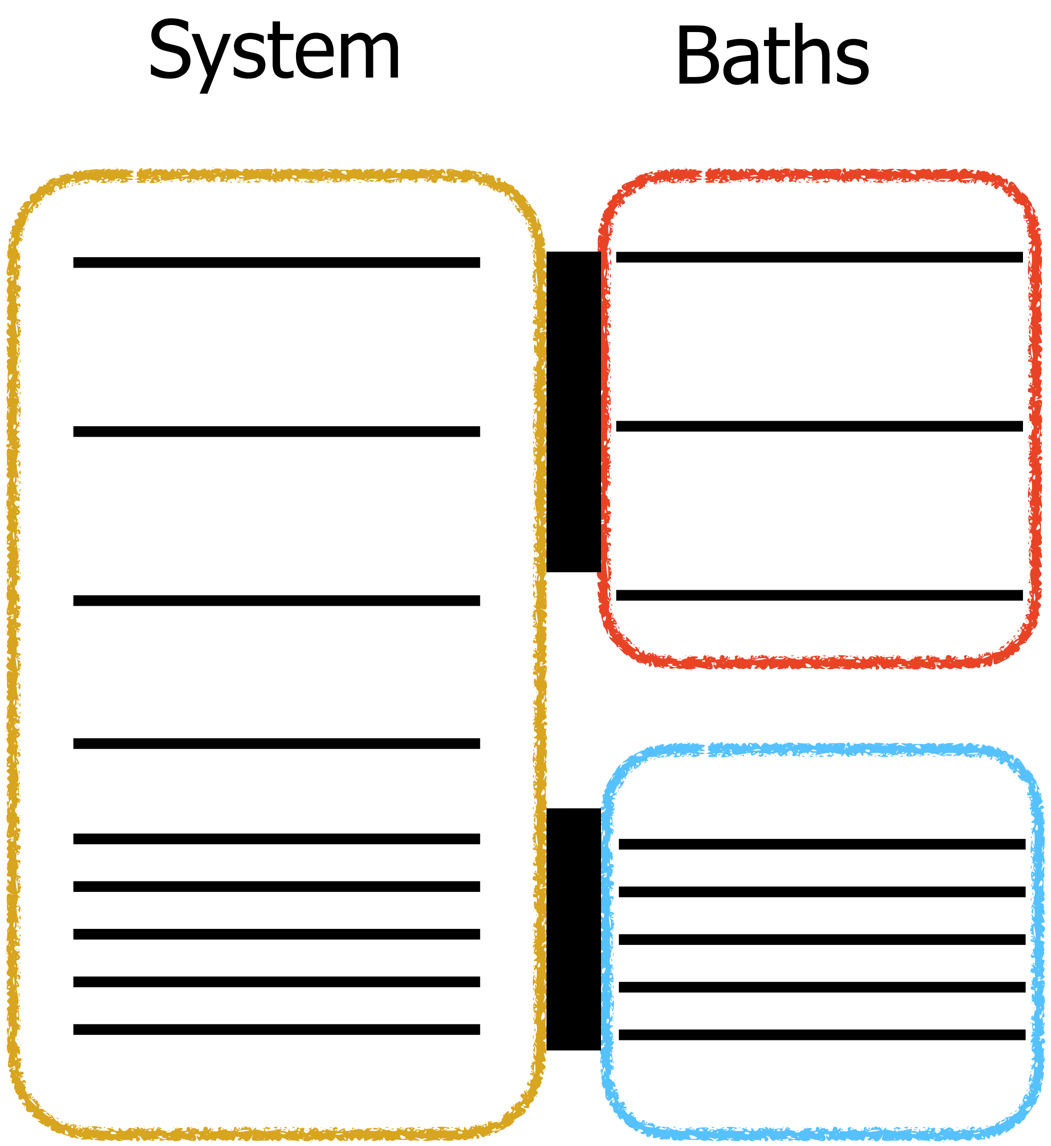


Nonnegative quasiprobability rep.: $p(\lambda\,|\,P)$ $p(\lambda'\,|\,\lambda, C)$ $p(M_k\,|\,\lambda')$

This implies that contextuality is equivalent to negative or nonreal quasiprobabilities in **every** representation of an experiment.

Nonclassicality in a thermodynamic setting

Nonclassical work extraction.



Two-stroke cycle:

- Prepare nonequilib. steady-state ρ
- Disconnect baths and implement $U(\tau)$, generated by $H_0 + gV(t)$

The work extracted in one cycle is the change of the energy's expectation value:

$$W^Q = \frac{2g\tau}{\hbar}\mathrm{Im}\mathrm{Tr}(\rho X H_0) + \mathcal{O}(g^2)$$

where $X := (1/\tau)\int_0^\tau V_I(t)dt$.

For small enough g, the averaged KD distribution $\mathrm{Im}\mathrm{Tr}(\rho X H_0)$ is not compatible with that in every NOM.

[Lostaglio2020certifying]