Quantum Bayesian Networks

Experimental determination and applications in quantum thermodynamics

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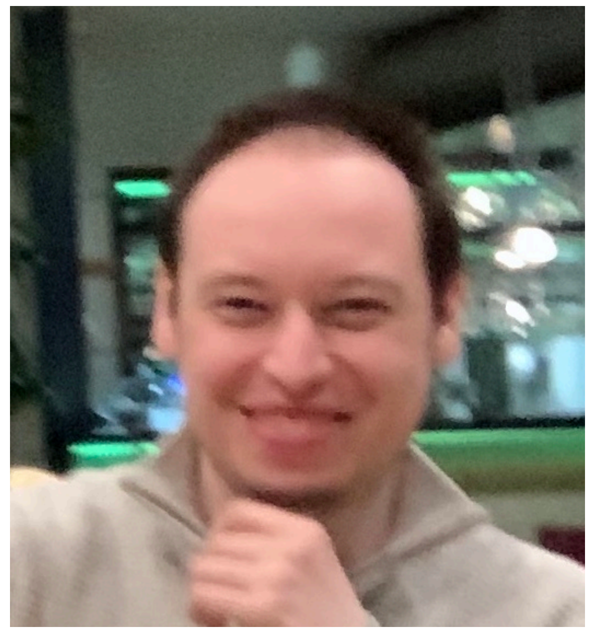
Overview

- Thermodynamics deals with **processes**, not states.
- In quantum systems that can be an issue:
  - Measurement invasiveness.
    - ***Processes become extrinsic.***

Prof. Eric Lutz

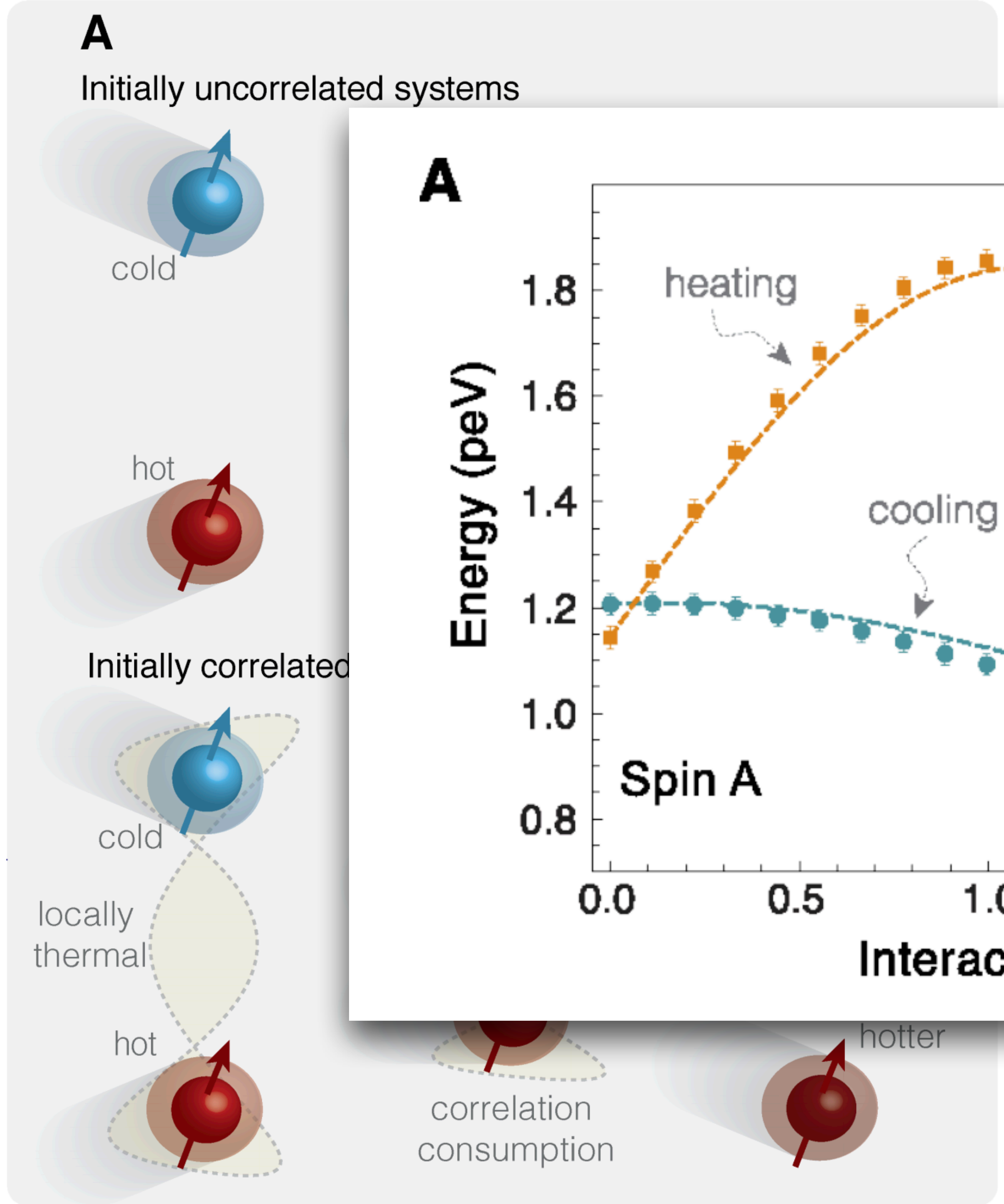


Dr. Kaonan Micadei

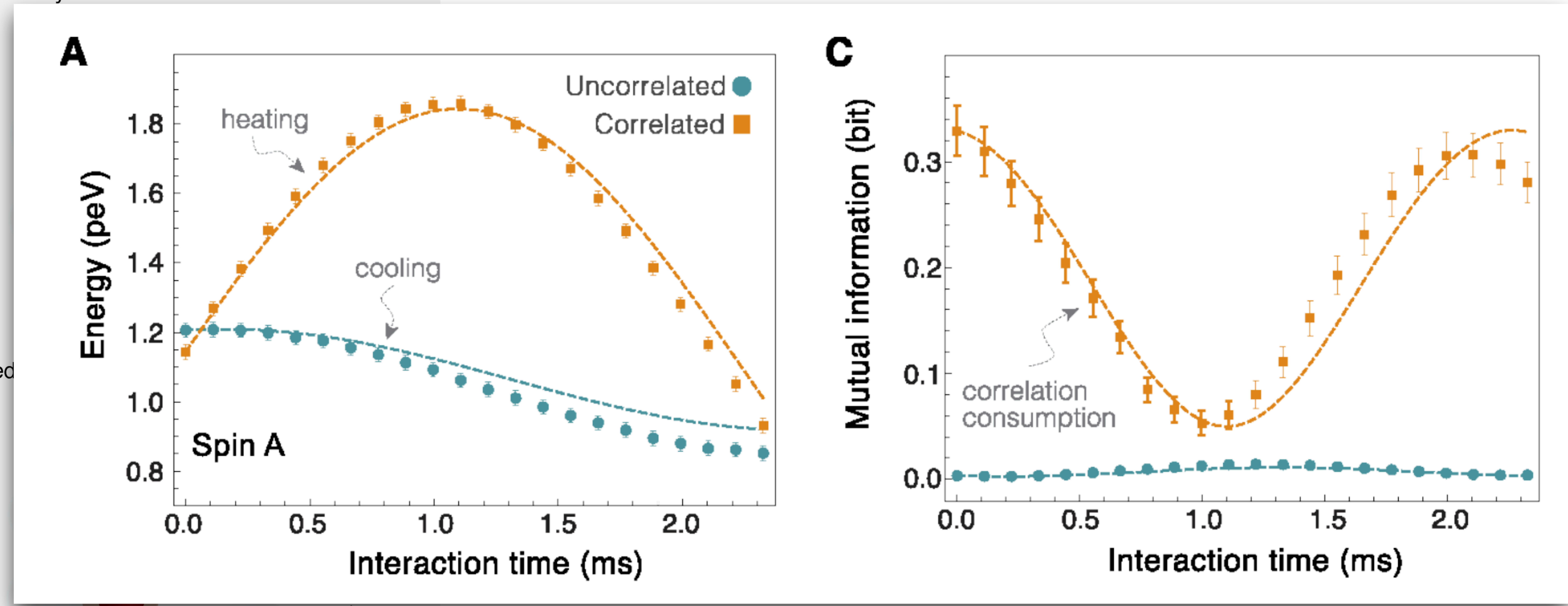
Quantum Bayesian Networks (QBNs)

1. “Reversing the direction of heat flow using quantum correlations”, *Nature Communications* **10**, 2456 (2019).
2. “Quantum fluctuation theorems beyond two-point measurements”, *Phys. Rev. Lett.* **124**, 090602 (2020).
3. “Experimental validation of fully quantum fluctuation theorems”, arXiv:2012.06294.
4. “Extracting Bayesian networks from multiple copies of a quantum system”, arXiv:2103.14570.
5. “Quantum mean-square predictors of work”, arXiv:2104.07132.

Reversing the direction of heat flow using quantum correlations



Two qubits: *locally thermal but globally correlated.*



ase.

Modified 2nd law: $(\beta_A - \beta_B)Q \geqslant \Delta I(A:B)$.

Partovi, M. H., *Phys. Rev. E,* **77**, 021110 (2008)
Jennings, D. & Rudolph, T., *Phys. Rev. E,* **81,** 061130 (2010)
Horodecki, M. & Oppenheim, J., *Nat. Comm.*, **4**, 2059 (2013).
Brandão, F., et. al., *Phys. Rev. Lett.,* **111**, 250404 (2013).

Issue

$$\rho_{AB} = \begin{pmatrix} (1-p_a)(1-p_b) & 0 & 0 & 0 \\ 0 & (1-p_a)p_b & \alpha & 0 \\ 0 & \alpha^* & p_a(1-p_b) & 0 \\ 0 & 0 & 0 & p_a p_b \end{pmatrix}$$

$$\Downarrow$$

$$\rho_{AB} = \begin{pmatrix} (1-p_a)(1-p_b) & 0 & 0 & 0 \\ 0 & (1-p_a)p_b & 0 & 0 \\ 0 & 0 & p_a(1-p_b) & 0 \\ 0 & 0 & 0 & p_a p_b \end{pmatrix}$$

- How to actually measure the heat?
  - We did it using full tomography.
    - Not very satisfactory.
- Heat refers to the process, not the state:

$$Q = E_{a'} - E_a = -\left(E_{b'} - E_b\right)$$

- Standard protocol: two-point measurement (TPM).
  - Measure in the energy basis before and after the unitary.
- **Problem:** 1st measurement destroys coherences.

Alternatives:
- Operator of work.
- Quasiprobabilities.
- Quantum Bayesian Networks.

Talkner, P., Lutz, E., & Hänggi, P. *Phys. Rev. E*, **75**, 050102 (2007)

Quantum Bayesian Networks

- Basic idea: global system evolves unitarily.

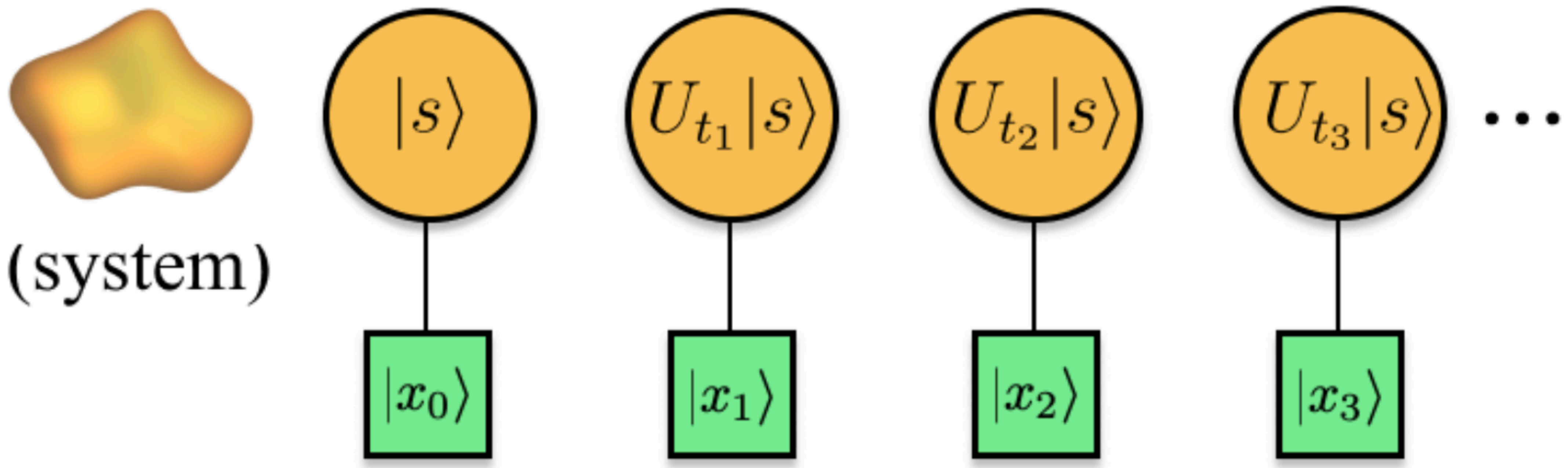
$$\rho = \sum_s P_s |s\rangle\langle s| \quad \rightarrow \quad \rho(t) = U_t \rho U_t^\dagger = \sum_s P_s U_t |s\rangle\langle s| U_t^\dagger$$

- For a given set of instants $t_0 = 0,\ t_1, t_2, \ldots$ we build the **conditional probability**

$$p(x_t | s_t) = |\langle x_t | U_t | s\rangle|^2 \qquad \text{for arbitrary basis sets } \{|x_t\rangle\}$$

- The Bayesian Network distribution for a path $|x_0\rangle \rightarrow |x_1\rangle \rightarrow |x_2\rangle \rightarrow \ldots$ is then

$$P(x_0, x_1, x_2, \ldots) = \sum_s P_s p(x_0 | s_0) p(x_1 | s_1) p(x_2 | s_2).$$

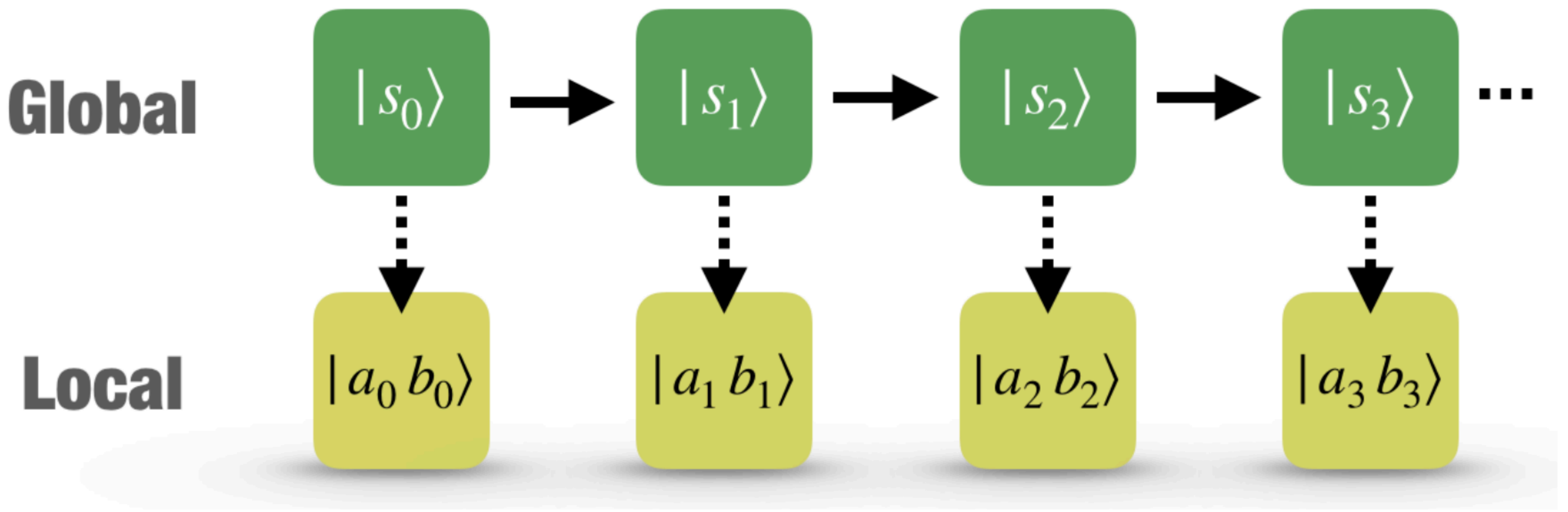


Interpretation

- Always produces a valid (strictly non-negative) distribution.
- Marginalizing leads to non-back-acted distributions.
- Corresponds to the outcomes of an actual experiment (involving multiple copies).
- Choice of path $|x_0\rangle \to |x_1\rangle \to |x_2\rangle \to \ldots$ is absolutely general:
  - e.g. global vs. local.
    - Heat is defined as before: $Q = E_{a_1} - E_{a_0} = -\left(E_{b_1} - E_{b_0}\right)$
- But now the heat distribution can be computed as

$$P(Q) = \sum_{a_0,b_0,a_1,b_1} \delta(Q - (E_{a_1} - E_{a_0}))P(a_0, b_0, a_1, b_1)$$

- Avoids any measurement backaction.



Comparison with TPM

- Heat-exchange QBN (2-step process):

$$P(a_0, b_0, a_1, b_1) = \sum_s P_s p(a_0, b_0 \,|\, s_0) p(a_1, b_1 \,|\, s_1)$$

$$= \sum_s P_s \,|\langle a_1, b_1 \,|\, U_t \,|\, s\rangle|^2 \,|\langle a_0, b_0 \,|\, s\rangle|^2$$

- Marginalizing over a_0, b_0:

$$P(a_1, b_1) = \sum_s P_s \,|\langle a_1, b_1 \,|\, U_t \,|\, s\rangle|^2 = \langle a_1, b_1 \,|\, U_t \rho U_t^\dagger \,|\, a_1, b_1\rangle \quad \text{(no backaction)}$$

- In contrast, the distribution from performing a TPM reads

$$P_{\mathrm{TPM}}(a_0, b_0, a_1, b_1) = \sum_s P_s \,|\langle a_1, b_1 \,|\, U_t \,|\, a_0, b_0\rangle|^2 \,|\langle a_0, b_0 \,|\, s\rangle|^2$$

- Marginalizing over a_0, b_0:

$$P_{\mathrm{TPM}}(a_1, b_1) = \sum_s P_s \langle a_1, b_1 \,|\, U_t \mathbb{D}(\rho) U_t^\dagger \,|\, a_1, b_1\rangle \quad \text{where} \quad \mathbb{D}(\rho) = \sum_{a_0, b_0} |a_0, b_0\rangle\langle a_0, b_0 \,|\, \rho \,|\, a_0, b_0\rangle\langle a_0, b_0|$$

Fluctuation theorems

Fundamental symmetries about thermodynamic trajectories

- Heat-exchange QBN (2-step process):

$$P_f(s, a_0, b_0, a_1, b_1) = P_s p(a_0, b_0 | s_0) p(a_1, b_1 | s_1)$$

- Reverse trajectory:

$$P_r(s^*, a_0, b_0, a_1, b_1) = P_{s^*} \bar{p}(a_1, b_1 | s_0^*) \bar{p}(a_0, b_0 | s_1^*)$$

where $\bar{p}$ involve $U^\dagger$ instead of U.

- Their ratio satisfy the detailed fluctuation theorem:

$$\frac{P_f}{P_r} = \exp\left\{ \Delta\beta\, Q + I_0 - I_1 - \Sigma_A - \Sigma_B + \gamma \right\}$$

Here:

$$I_0 = \ln P_s / P_{a_0} P_{b_0}$$

$$I_1 = \ln P_{s^*} / \mathscr{P}(a_1) \mathscr{P}(b_1)$$

$$\Sigma_A = \ln \mathscr{P}(a_1) / P_{a_1}$$

$$\Sigma_B = \ln \mathscr{P}(b_1) / P_{b_1}$$

$$\gamma = \ln p(a_0, b_0 | s_0) p(a_1, b_1 | s_1) / \bar{p}(a_1, b_1 | s_0^*) p(a_0, b_0 | s_1^*)$$

- Detailed FT implies Integral FT:

$$\langle e^{\Delta\beta Q + I_0 - I_1 - \Sigma_A - \Sigma_B + \gamma} \rangle = 1$$

- But, in addition, some quantities also individually satisfy integral FTs:

$$\langle e^{-I_i} \rangle = \langle e^{-\Sigma_i} \rangle = \langle e^{-\gamma} \rangle = 1$$

- We can also further split $I_i = J_i + C_i$ where

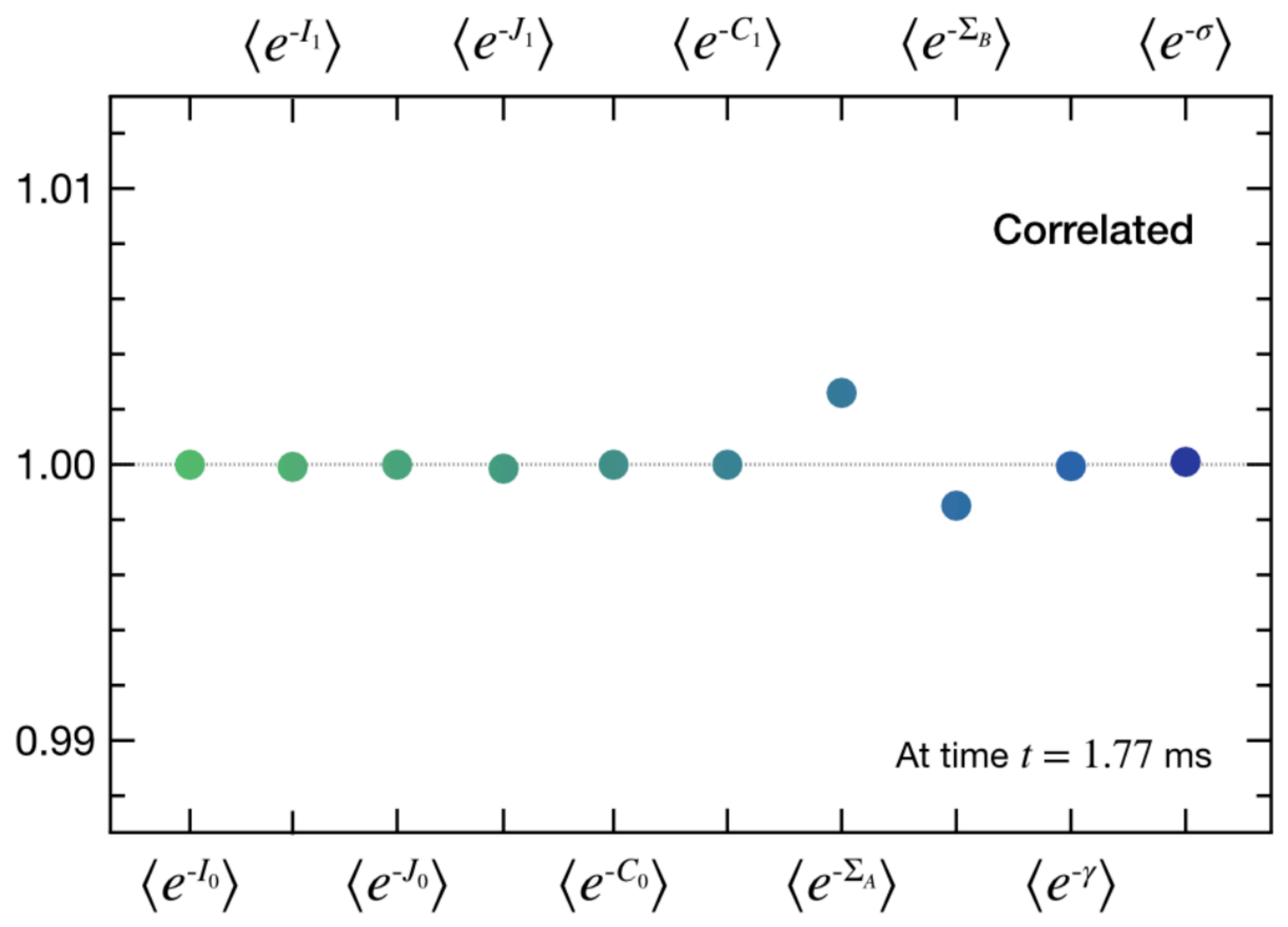
$J_i = \ln P_{a_i,b_i} / P_{a_i} P_{b_i}$ = stochastic classical information

and

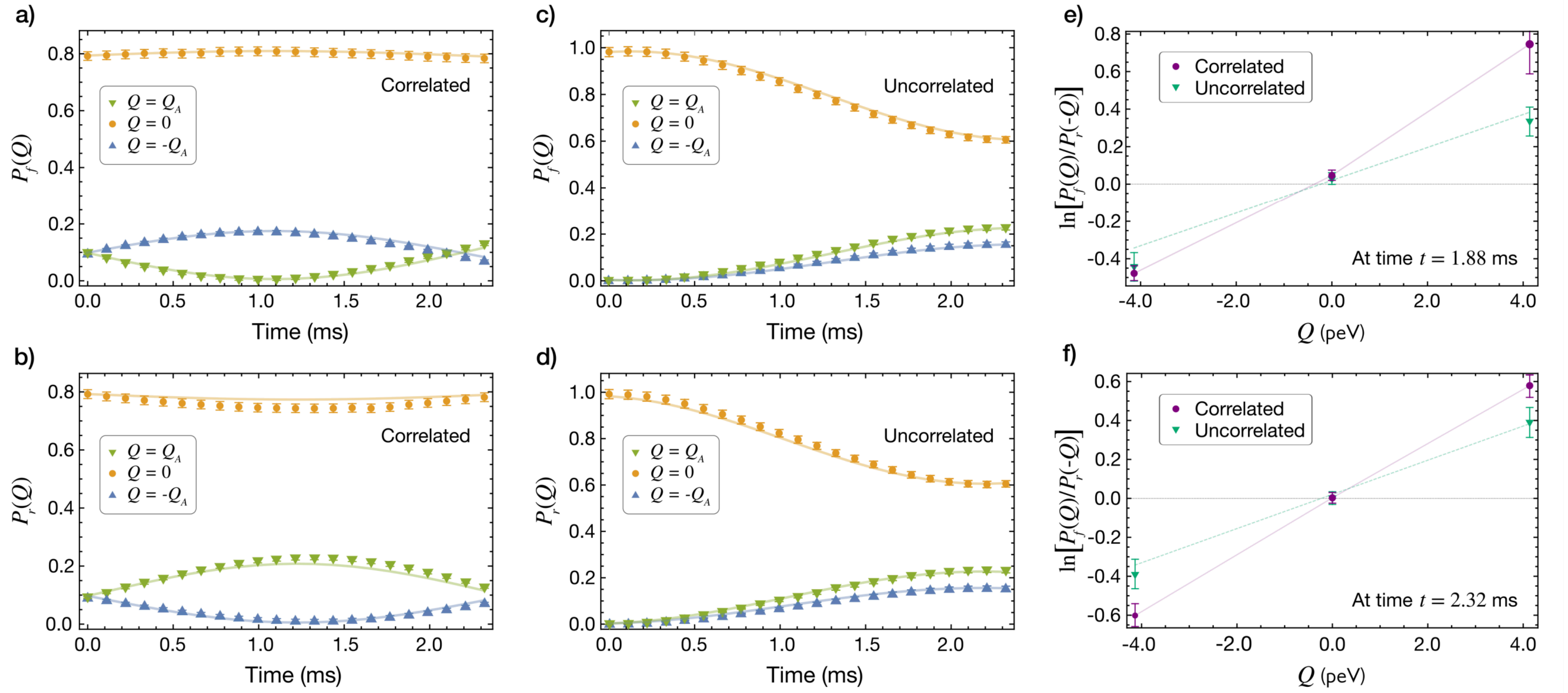
$C_i = \ln P_s / P_{a_i,b_i}$ = stochastic discord.

- These quantities also satisfy integral FTs:

$$\langle e^{-J_i} \rangle = \langle e^{-C_i} \rangle = 1$$



arXiv 2012.06294



$$\frac{P_f(Q)}{P_r(-Q)} = \frac{e^{\Delta\beta\, Q}}{\Psi(Q)}$$ where $\Psi(Q) \neq 1$ when the systems are correlated.

Jarzynski, C., & Wójcik, D. K. *Physical Review Letters*, **92**, 230602 (2004)

Extracting Bayesian Networks from multiple copies

- QBNs have nice properties.
- But in our experiment, we had to reconstruct them from full tomography data.
  - *Can QBNs be associated with the actual outcomes of an experiment?*
- Using a single system, this is impossible, because any measurement would cause backaction (this is the whole point of QBNs).
  - But this can be done using identical copies of a quantum system.

Post-selection

- To illustrate the procedure, consider the 2-point QBN:

$$P(x_0, x_1) = \sum_s P_s p(x_1 | s_1) p(x_0 | s_0) = \sum_s P_s \, |\langle x_1 | U | s \rangle|^2 \, |\langle x_0 | s \rangle|^2$$

- Start with 2 copies $\rho \otimes \rho$ and apply the projective measurement $|s\rangle\langle s| \otimes |s'\rangle\langle s'|$.
  - Post-select only those systems with outcomes $s' = s$.
  - On these, apply the (product) POVM $M_x = |x_0\rangle\langle x_0| \otimes U_t |x_1\rangle\langle x_1| U_t^\dagger$.
    - Outcomes occur with prob. $P(x_0, x_1)$.

Work distribution in coherent processes

- Consider an isolated system undergoing a unitary protocol: $\rho' = U\rho U^\dagger$.
  - The unitary may involve work:

$$H_S = \sum_n E_n^i |n_i\rangle\langle n_i| \qquad \rightarrow \qquad H_S' = \sum_m E_m^f |m_f\rangle\langle m_f|$$

- The average work is $\langle W \rangle = \mathrm{tr}\left\{H_S'\rho' - H_S\rho\right\}$.
  - Requires measuring the system before and after U.
    - This is a problem if the system is initially coherent: $\rho = \sum_s P_s |s\rangle\langle s|$
    - TPM changes the process: $P_{\mathrm{TPM}} = \sum_s P_s \, |\langle m_f| U |n_i\rangle|^2 \, |\langle n_i|s\rangle|^2$

$$\rightarrow \langle W \rangle = \mathrm{tr}\left\{H_s' U \mathbb{D}(\rho) U^\dagger - H_S\rho\right\}$$

- QBNs preserve them:

$$P_{\text{QBN}}(n_i, m_f) = \sum_s P_s \, |\langle m_f | U | s \rangle|^2 \, |\langle n_i | s \rangle|^2 \quad \rightarrow \quad P(w) = \sum_{n_i, m_f} \delta\big(w - (E^f_m - E^i_n)\big) \, P_{\text{QBN}}(n_i, m_f)$$

- Yields $\langle W \rangle = \text{tr}\big\{H'_S \rho' - H_S \rho\big\}$.

- **NO-GO:** impossible to devise a POVM J_w such that the resulting distribution $P(w) = \text{tr}\big(J_w \rho\big)$ satisfies

(i) $\int dw \; w \; P(w) = \text{tr}\big\{H'_S \rho' - H_S \rho\big\}$

(ii) Reduces $P_{\text{TPM}}(w)$ when $[\rho, H_S] = 0$.

- With QBNs we can construct this:

$$J_w = \sum_{n_i, m_f, s} \delta\big(w - (E^f_m - E^i_n)\big) \frac{1}{P_s} M_x |ss\rangle\langle ss|$$

- Caveat: *what may J_w depend on?*

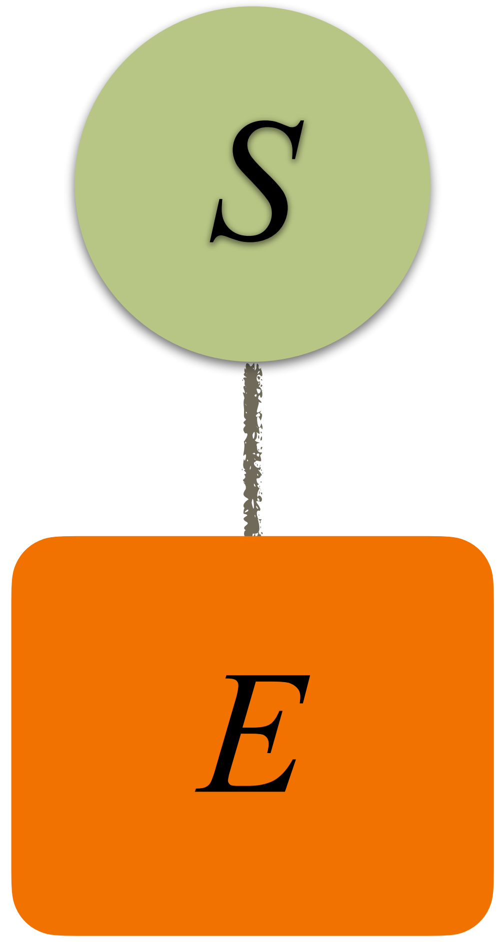
	Measurable	Fluctuation theorems	Coherent processes
Projective measurements	✓	✓	✗
Operators of work	✓	✗	✓
Quasiprobabilities	✗	✓	✓
Bayesian networks	✓	✓	✓

M. Perarnau-Llobet, *et. al., Phys. Rev. Lett.* **118**, 070601 (2017)

Predictors of work

- X: college admission exam.
- Y: physics 1 grades.
    - How to cook up a function $g(X)$ which best predicts Y given X?
        - Minimize mean-squared error $\Delta^2 = \langle \big(Y - g(X)\big)^2 \rangle$

- Consider a system interacting with a bath.
    - Bath is incoherent: we can do TPM.
    - System is coherent: we never measure it.
        - Given outcomes for the heat, what is the best possible *prediction* we can make about work?



TPM@E + QBN@S

- Distribution

$$P(n,m,\mu,\mu') = \sum_s P_s q_\mu \, |\langle n_i | s \rangle|^2 \, |\langle m_f, \mu' | U | s, \mu \rangle|^2$$

- where $|\mu\rangle, |\mu'\rangle$ are the eigenstates of the bath, and q_μ are the initial (thermal) probabilities.

- Question: create a function $\mathscr{W}(\mu,\mu')$ which minimizes the MSE

$$\Delta^2 = \left\langle \left(\mathscr{W}(\mu,\mu') - \left(E^f_m + \mathscr{E}_{\mu'} - E^i_n - \mathscr{E}_\mu \right) \right)^2 \right\rangle$$

- Measuring the bath yields a specific set of Kraus operators for the system

$$\rho'_S = \sum_{\mu,\mu'} M_{\mu\mu'} \rho_S M^\dagger_{\mu\mu'}, \qquad M_{\mu\mu'} = q_\mu \langle \mu' | U | \mu \rangle$$

- Each trajectory occurs with probability $P(\mu,\mu') = \mathrm{tr}\left\{ M_{\mu\mu'} \rho_S M^\dagger_{\mu\mu'} \right\}$

- Optimal mean-squared predictor:

$$\mathscr{W}(\mu,\mu') = \mathscr{E}_{\mu'} - \mathscr{E}_\mu + \frac{1}{P(\mu,\mu')} \left\langle M^\dagger_{\mu\mu'} H'_S M_{\mu\mu'} - \frac{1}{2} \left\{ M^\dagger_{\mu\mu'} M_{\mu\mu'}, \mathscr{D}_{\rho_S}(H_S) \right\} \right\rangle_{\rho_S}$$

Minimal qubit model

- Simplification: $U = U_h(I_S \otimes U_w)$: first we do work, then we interact with the bath.
- Consider a qubit with $H_S = H'_S = \omega \,|\,1\rangle\langle 1\,|$.
  - Perform work with $U_w = \sigma_x$
- Interact with bath: also a qubit, with $H_E = \omega\,|\,1\rangle\langle 1\,|$ and $\rho_E = (1-f)\,|\,0\rangle\langle 0\,| + f\,|\,1\rangle\langle 1\,|$.
  - U_h = SWAP.
- Initial state:

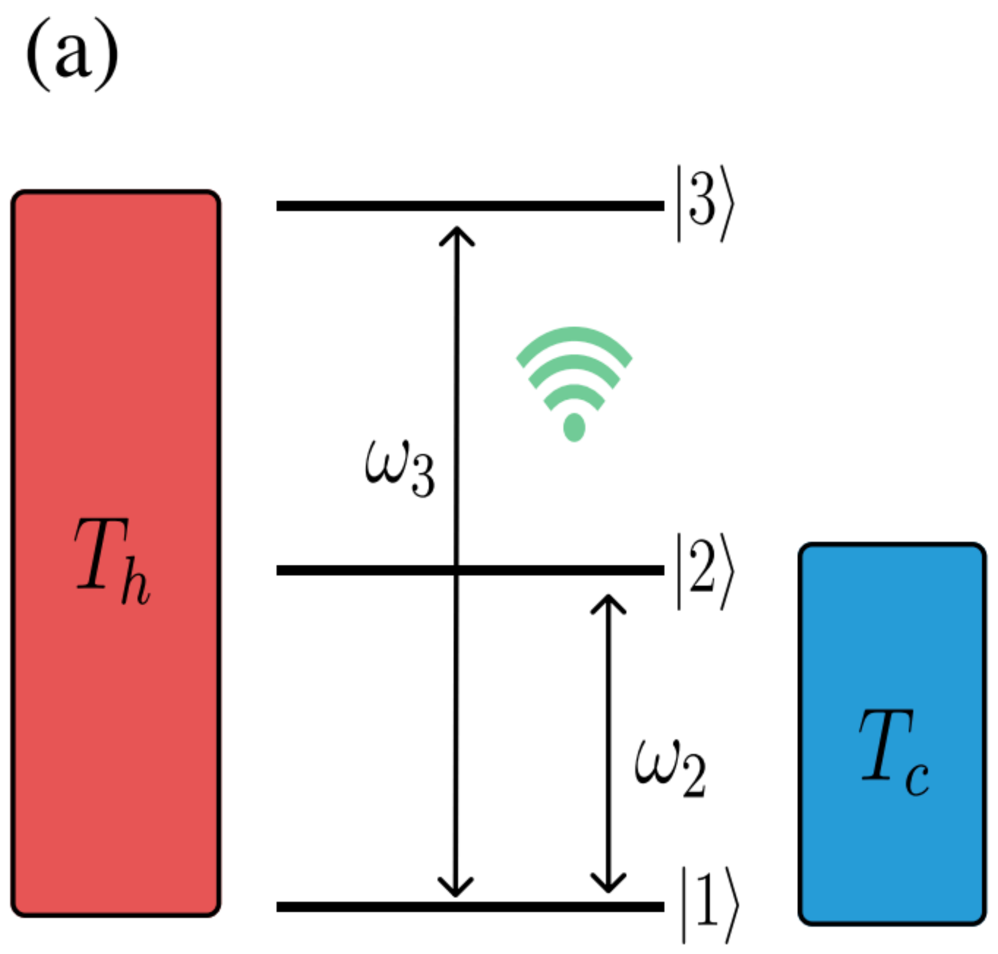
$$\rho_S = \frac{1}{2}\begin{pmatrix} 1 + s\cos\theta & s\sin\theta \\ s\sin\theta & 1 - s\cos\theta \end{pmatrix}$$

J. P. Pekola, P. Solinas, A. Shnirman, and D. V. Averin, *NJP,* **15**, 115006 (2013)

$\mu \to \mu'$	$n \to m' \to n'$	$P[\gamma]$	$Q[\gamma]$	$\mathcal{W}_{\text{opt}}[\gamma](\theta = 0)$	$\mathcal{W}_{\text{opt}}[\gamma]$	$W[\gamma, n, n']$
$0 \to 0$	$1 \to 0 \to 0$	$(1-f)(1-s\cos\theta)/2$	0	$-\omega\left(\frac{1+s}{1-s}\right)$	$-\frac{\omega}{4}\left(\frac{3+4s\cos\theta+\cos(2\theta)}{4(1-s\cos\theta)}\right)$	$-\omega$
$0 \to 1$	$0 \to 1 \to 0$	$(1-f)(1+s\cos\theta)/2$	ω	ω	$\omega\left(1-\frac{\sin^2\theta}{2(1+s\cos\theta)}\right)$	ω
$1 \to 0$	$1 \to 0 \to 1$	$f(1-s\cos\theta)/2$	$-\omega$	$-\omega$	$-\omega\left(1-\frac{\sin^2\theta}{2(1-s\cos\theta)}\right)$	$-\omega$
$1 \to 1$	$0 \to 1 \to 1$	$f(1+s\cos\theta)/2$	0	$\omega\left(\frac{1-s}{1+s}\right)$	$\frac{\omega}{4}\left(\frac{3-4s\cos\theta+\cos(2\theta)}{4(1+s\cos\theta)}\right)$	ω

Conclusions and outlook

- Quantum Bayesian Networks: *statistics of multi-time quantities without measurement backaction.*
  - Relevant for **coherent** systems and processes.
- Can be obtained directly from experiments in multiple **copies** of a system.
- Meaningful in quantum thermodynamics:
  - Satisfy **fluctuation theorems.**
- Can be used to construct experimentally relevant **estimation schemes.**
- Potential applications:
  - Continuous-time heat engines & Quantum transport.
  - Beyond thermo: metrology, others (?)



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THANK YOU!

Quantum Thermodynamics Quantum Transport

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