THERMODYNAMIC UNCERTAINTY RELATIONS AND THEIR CONNECTION WITH FLUCTUATION THEOREMS

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Quantum thermodynamics

quantum transport

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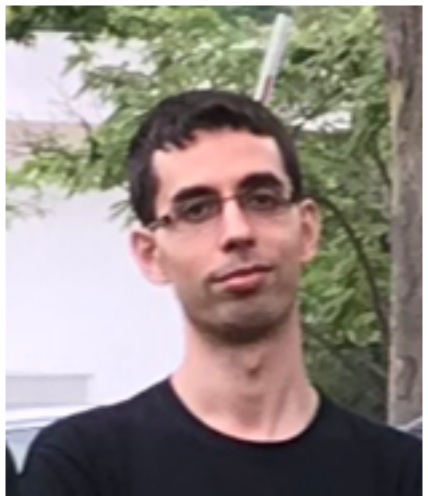
summary



I. Entropy production.

II. Thermodynamic uncertainty relations (TURs).

III. TURs and fluctuation theorems.

IV. Applications to quantum heat engines.

André M. Timpanaro, Giacomo Guarnieri, John Goold, GTL,
"**Thermodynamic uncertainty relations from exchange fluctuation theorems**".
Accepted in PRL.
arXiv 1904.07574

Entropy production ≠ entropy

- Entropy does not satisfy a continuity equation: $\Delta S = \Sigma + \frac{Q}{T}, \qquad \Sigma \geq 0$

- 1st and 2nd laws for a system coupled to two baths:

$$\frac{dU}{dt} = \dot{Q}_h + \dot{Q}_c + \dot{W}$$

$$\frac{dS}{dt} = \dot{\Sigma} + \frac{\dot{Q}_h}{T_h} + \frac{\dot{Q}_c}{T_c}$$

- Example: if there is no work involved,

$$\dot{\Sigma} = \left(\frac{1}{T_c} - \frac{1}{T_h}\right)\dot{Q}_h \geq 0$$

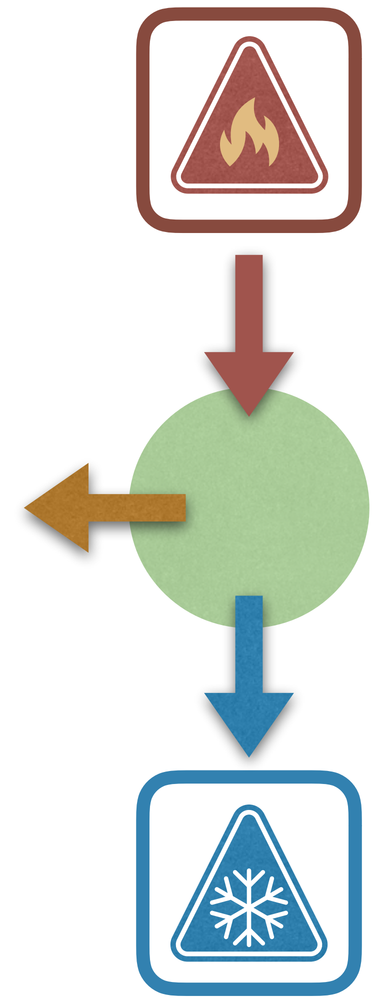
- *Heat flows from hot to cold.*

Why entropy production matters

- 1st and 2nd laws for a system coupled to two baths:

$$\frac{dU}{dt} = \dot{Q}_h + \dot{Q}_c + \dot{W} = 0$$

$$\frac{dS}{dt} = \dot{\Sigma} + \frac{\dot{Q}_h}{T_h} + \frac{\dot{Q}_c}{T_c} = 0$$



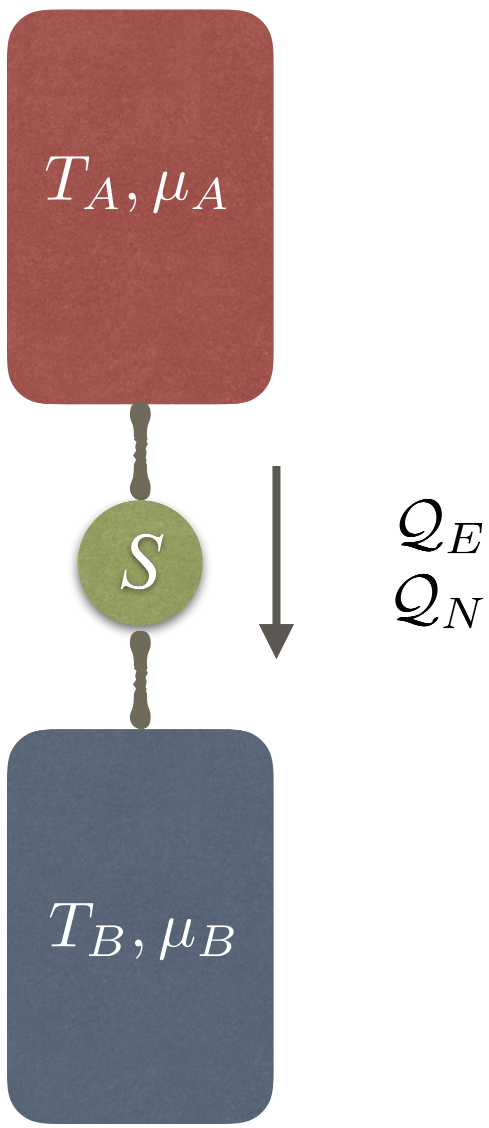
- The efficiency of the engine may then be written as

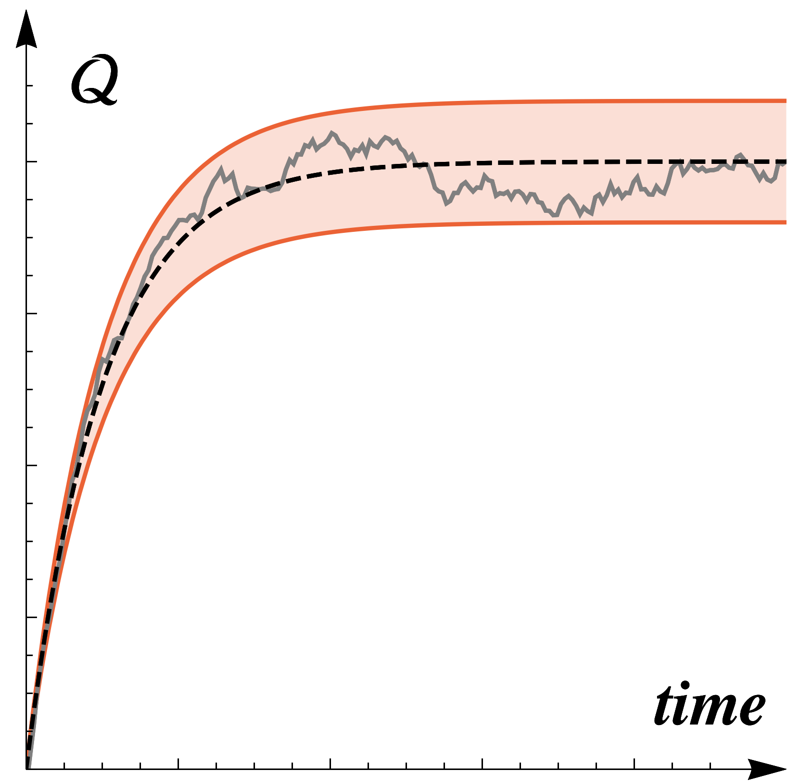
$$\eta = -\frac{\dot{W}}{\dot{Q}_h} = 1 + \frac{\dot{Q}_c}{\dot{Q}_h} = 1 - \frac{T_c}{T_h} - \frac{T_c}{\dot{Q}_h}\dot{\Sigma}$$

- *Entropy production is therefore the reason the efficiency is smaller than Carnot:*

$$\eta = \eta_C - \frac{T_c}{\dot{Q}_h}\dot{\Sigma}$$

Thermodynamic Uncertainty Relations (TURs)





$$\frac{\mathrm{var}(\mathcal{Q})}{\langle \mathcal{Q} \rangle^2} \geq \frac{2}{\langle \Sigma \rangle}$$

- Proved for classical Markov processes.
- Physical origins are rather obscure.
- Regimes of validity?
- Quantum effects?

A. C. Barato, U. Seifert, "Thermodynamic Uncertainty Relation for Biomolecular Processes", *Physical Review Letters*, **114**, 158101 (2015)

Implications for mesoscopic engines

- In an autonomous engine the output power is defined by $P = \dot{W}$
- The TUR in this case then reads

$$\frac{\mathrm{var} P}{\langle P \rangle^2} \geq \frac{2}{\langle \dot{\Sigma} \rangle}$$

- But $\langle \dot{\Sigma} \rangle = \frac{\langle \dot{Q}_h \rangle}{T_c}(\eta_C - \eta)$, which gives

$$\frac{\mathrm{var} P}{\langle P \rangle^2} \geq \frac{2T_c}{\dot{Q}_h} \frac{1}{\eta_C - \eta}$$

$$\eta = \eta_C - \frac{T_c}{\dot{Q}_h} \dot{\Sigma}$$

- Finally, we note that $\eta = \frac{\langle P \rangle}{\langle \dot{Q}_h \rangle}$. Whence

$$\mathrm{var} P \geq 2T_c \langle P \rangle \frac{\eta}{\eta_C - \eta}$$

P. Pietzonka and U. Seifert, *Phys. Rev. Lett.*, **120**, 190602 (2017)

Connection with fluctuation theorems

André M. Timpanaro, Giacomo Guarnieri, John Goold, GTL,
"**Thermodynamic uncertainty relations from exchange fluctuation theorems**".
Accepted in PRL.
arXiv 1904.07574

Fluctuation theorems

- Fluctuation theorems describe the stochastic behavior of the entropy production:

$$\frac{P_F(\sigma)}{P_B(-\sigma)} = e^{\sigma}$$

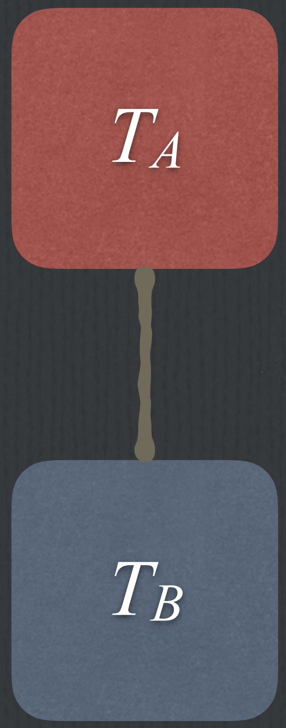
- The most famous one is the Crooks fluctuation theorem:

$$\frac{P_F(W)}{P_B(-W)} = e^{\beta(W-\Delta F)}$$

- Jarzynski-Wójcik Exchange Fluctuation Theorem
(Phys. Rev. Lett. 92, 230602 (2004)

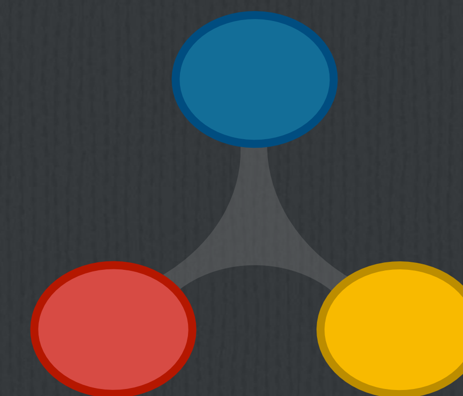
$$\frac{P(Q)}{P(-Q)} = e^{\delta\beta Q}$$

Stronger symmetry!



Extension to multiple charges

- Can be generalized to an arbitrary number of systems and an arbitrary number of currents:



$$\frac{P(\mathcal{Q}_1, \ldots, \mathcal{Q}_n)}{P(-\mathcal{Q}_1, \ldots, -\mathcal{Q}_n)} = e^{\sum_i A_i \mathcal{Q}_i}$$

- e.g.: two systems, but with particle and energy flow:

$$\frac{P(\Delta E_1, \Delta E_2, \Delta N_1)}{P(-\Delta E_1, -\Delta E_2, -\Delta N_1)} = e^{\beta_1 \Delta E_1 + \beta_2 \Delta E_2 + \delta\beta\mu \Delta N_1}$$

$$\delta\beta\mu = \beta_1 \mu_1 - \beta_2 \mu_2$$

- In general $\Delta E_1 \neq -\Delta E_2$: this means there is work involved; e.g.,

$$\frac{P(Q_H, W)}{P(-Q_H, -W)} = e^{(\beta_H - \beta_C) Q_H + \beta_C W}$$

TUR de force

- Our mai
- Conside
- For fixed ... ariance that Z can attai

Theorem (*"TUR de force"*). *For fixed finite* $\langle\Sigma\rangle$ *and* $\langle Z\rangle$, *the probability distribution* $P(\Sigma, Z)$ *satisfying* $P(\Sigma, Z)/P(-\Sigma, -Z) = e^{\Sigma}$, *with the smallest possible variance (the minimal distribution) is the distribution*

$$P_{min}(\Sigma, Z) = \frac{1}{2\cosh(a/2)}\Big\{e^{a/2}\delta(\Sigma - a)\,\delta(Z - b) + e^{-a/2}\delta(\Sigma + a)\,\delta(Z + b)\Big\}, \quad (1)$$

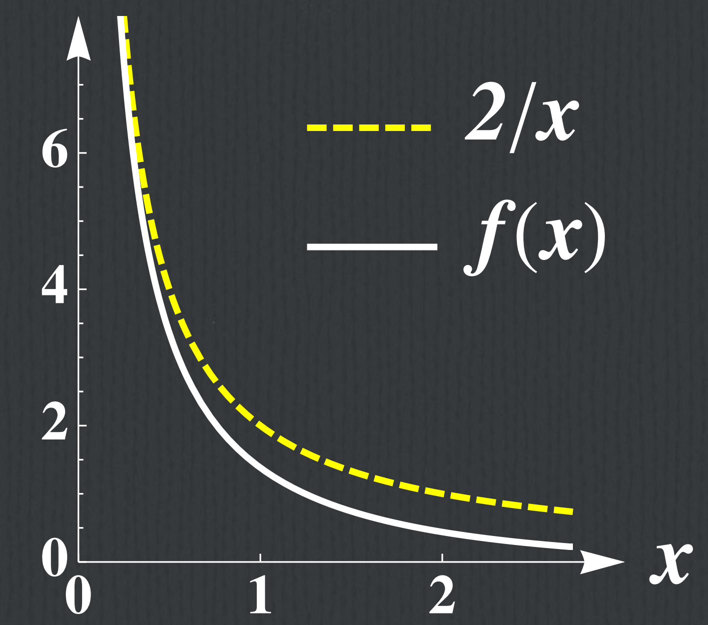
where the values of a *and* b *are fixed by* $\langle\Sigma\rangle = a\tanh(a/2)$ *and* $\langle Z\rangle = b\tanh(a/2)$. *For this distribution*

$$\mathrm{Var}(Z)_{min} = \langle Z\rangle^2 f(\langle\Sigma\rangle), \quad (2)$$

where $f(x) = csch^2(g(x/2))$, $csch(x)$ *is the hyperbolic cosecant and* $g(x)$ *is the function inverse of* $x\tanh(x)$.

- As a consequence, for any other distribution, one must have

$$\mathrm{var}(Z) \geq \langle Z \rangle^2 f(\langle \Sigma \rangle)$$



- ✓ This is the *tighest* (saturable) bound possible for this scenario.

- ✓ And we know which distribution saturates this bound.

- Similar papers appeared at the same time, but all deriving a looser bound (which is thus never tight):

$$f(x) = \frac{2}{e^x - 1}$$

Hasegawa & Vu 1902.06376.
Proesman & Horowitz 1902.07008.
Potts & Samuelsoon 1904.04913.

- Consider now a general TUR $\dfrac{P(\mathcal{Q}_1,\ldots,\mathcal{Q}_n)}{P(-\mathcal{Q}_1,\ldots,-\mathcal{Q}_n)} = e^{\sum_i A_i \mathcal{Q}_i}$

- Define $\Sigma = \sum_i A_i \mathcal{Q}_i \qquad Z = \sum_i z_i \mathcal{Q}_i, \qquad \forall z_i$

- Then $\dfrac{P(\Sigma, Z)}{P(-\Sigma, -Z)} = e^{\Sigma} \implies \mathrm{var}(Z) \geq \langle Z \rangle^2 f(\langle \Sigma \rangle)$

- But $\langle Z \rangle = \sum_i z_i q_i, \qquad q_i = \langle \mathcal{Q}_i \rangle$

$$\mathrm{var}(Z) = \sum_{ij} \mathcal{C}_{ij} z_i z_j, \qquad \mathcal{C}_{ij} = \mathrm{cov}(\mathcal{Q}_i, \mathcal{Q}_j)$$

- Thus $z^{\mathrm{T}} \left(\mathcal{C} - f \boldsymbol{q}\boldsymbol{q}^{\mathrm{T}} \right) z \geq 0$

$$\mathcal{C} - f \boldsymbol{q}\boldsymbol{q}^{\mathrm{T}} \geq 0$$

- When a matrix is positive semi-definite, all the diagonal entries must be non-negative:

$$\frac{\mathrm{var}(\mathcal{Q}_i)}{\langle \mathcal{Q}_i \rangle^2} \geq f(\langle \Sigma \rangle)$$

$$\mathcal{C} - f\boldsymbol{q}\boldsymbol{q}^{\mathrm{T}} \geq 0$$

- With our framework, we can also go further and say something about the covariances.

- If G is psd, any 2x2 sub-matrix must also be psd: $-\sqrt{G_{ii}G_{jj}} \leq G_{ij} \leq \sqrt{G_{ii}G_{jj}}$

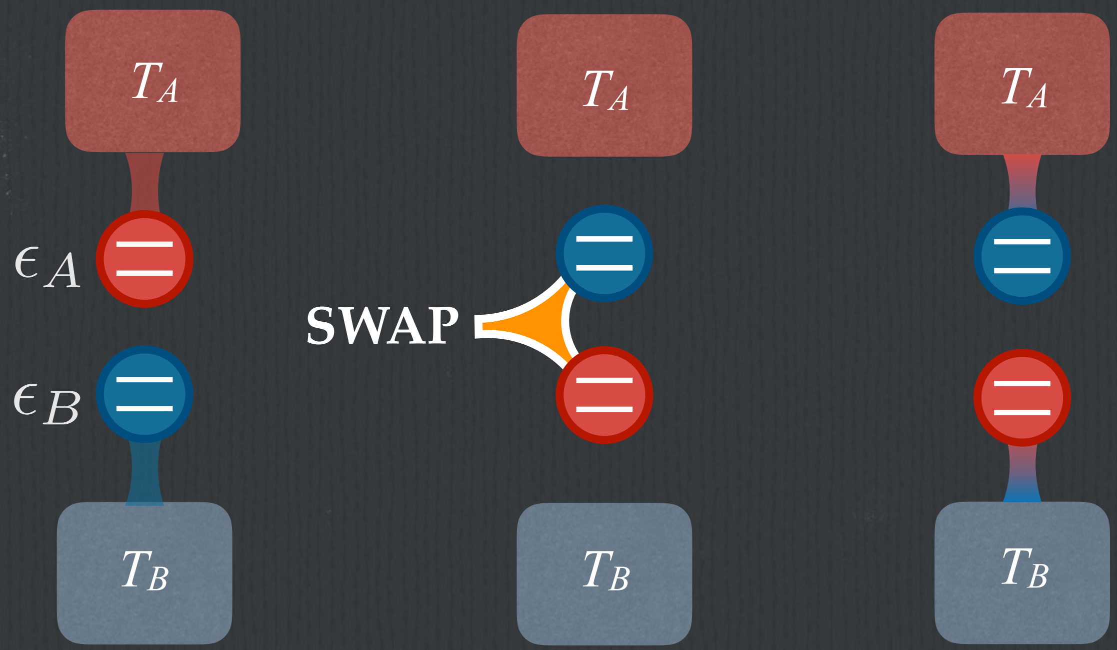
- Whence:

$$f q_i q_j - M_{ij} \leq C_{ij} \leq f q_i q_j + M_{ij}, \qquad M_{ij} = \sqrt{(\mathrm{var}(\mathcal{Q}_i) - f q_i^2)(\mathrm{var}(\mathcal{Q}_j) - f q_j^2)}$$

- Particularly interesting are the signs of the covariance:

$$\frac{q_i^2}{\mathrm{var}(\mathcal{Q}_i)} + \frac{q_j^2}{\mathrm{var}(\mathcal{Q}_j)} \geq \frac{1}{f(\langle \Sigma \rangle)} \qquad \Longrightarrow \qquad \mathrm{sign}(C_{ij}) = \mathrm{sign}(q_i q_j)$$

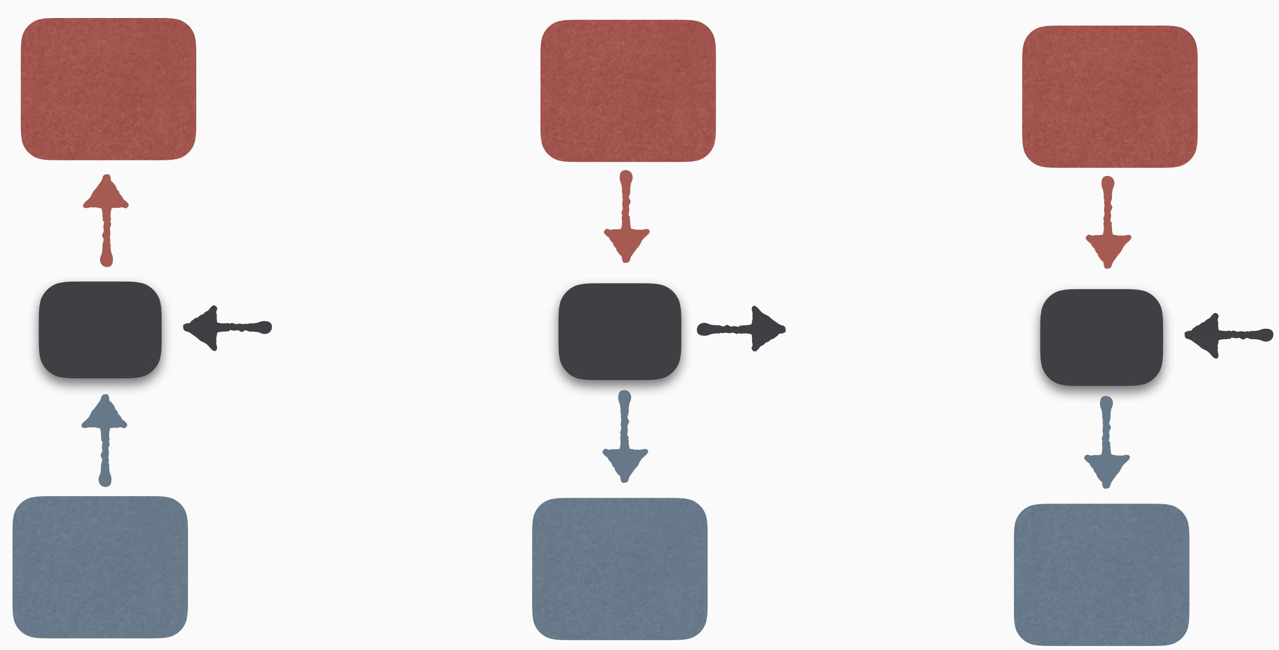
SWAP engine



$$\langle Q_h \rangle = \epsilon_A (f_A - f_B)$$

$$\langle Q_c \rangle = -\epsilon_B (f_A - f_B) \qquad f_i = \frac{1}{e^{\beta_i \epsilon_i} + 1}$$

$$\langle W \rangle = -(\epsilon_A - \epsilon_B)(f_A - f_B)$$



Refrigerator

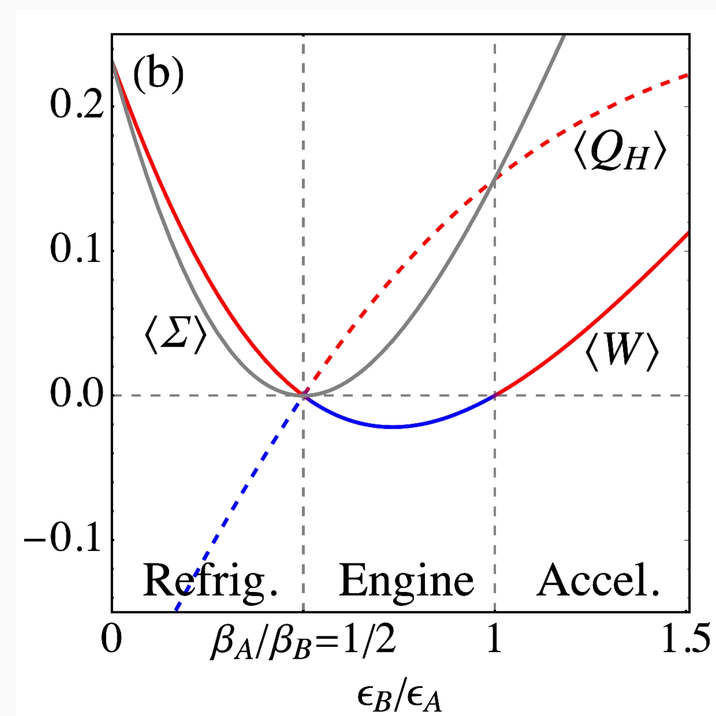
$$\frac{\epsilon_B}{\epsilon_A} < \frac{\beta_A}{\beta_B}$$

Engine

$$\frac{\beta_A}{\beta_B} < \frac{\epsilon_B}{\epsilon_A} < 1$$

Heat pump

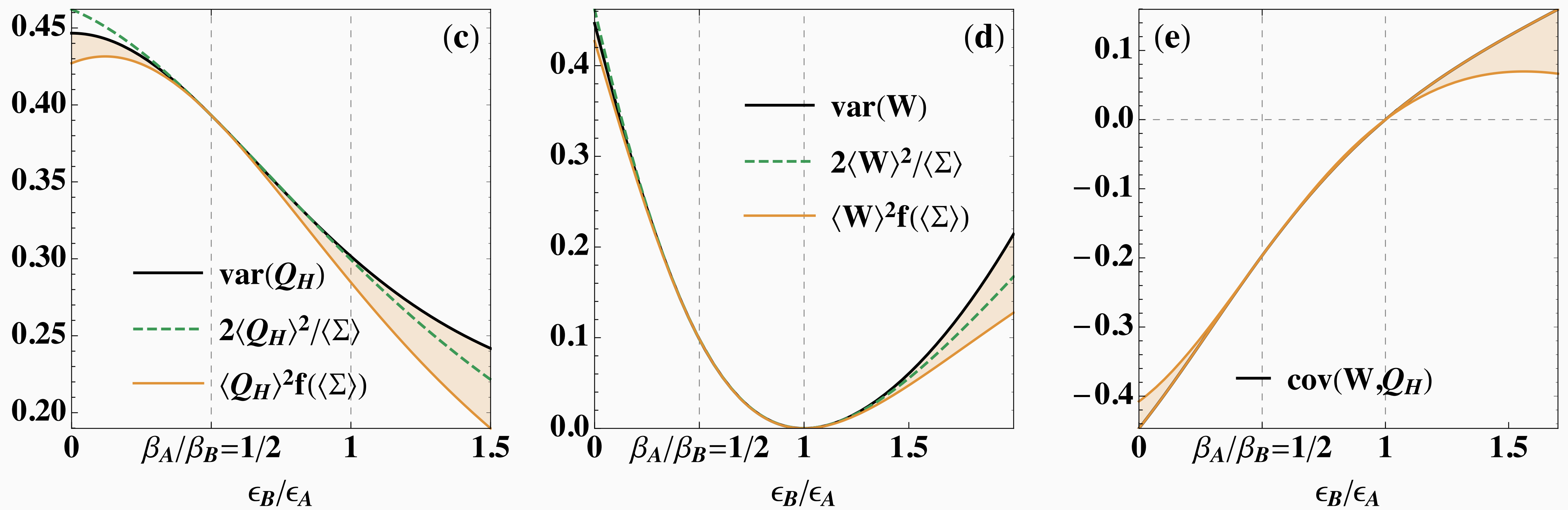
$$1 < \frac{\epsilon_B}{\epsilon_A}$$



M. Campisi, J. Pekola, R. Fazio, NJP, 17, 035012 (2015)

SWAP engine

$$\frac{P(Q_H, W)}{P(-Q_H, -W)} = e^{(\beta_B - \beta_A)Q_H + \beta_B W}$$



Conclusions

Acknowledgements:
IFUSP, FAPESP, CNPq

- TURs: simple but with enormous predictive power.
- A dynamical TUR can be derived as a *consequence* of Fluctuation Theorems.
- Our TUR is matrix valued:
  - Bounds all variances;
  - as well as *co*variances.
- It is the tightest bound pos

Quantum thermodynamics
QT^2
quantum transport
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Violations of the TUR in the quantum regime

- The classical TUR can be violated in quantum transport problems.

We have recently shown that close to linear response the bound is 1/2 looser:

$$\frac{\mathrm{var}(\mathcal{Q})}{\langle \mathcal{Q} \rangle^2} \geq \frac{1}{\langle \Sigma \rangle}$$

This is a consequence of the Fisher information metric and Quantum Cramer-Rao bound.

G. Guarnieri, G. T. Landi, S. R. Clark, J. Goold, arXiv 1902.10428

- This has bee ce.
- A violation could be exploited to utput power.

K. Ptaszyński, K. *Phys. Rev. B,* **98**, 085425 (2018)
B. Agarwalla, D. Segal, *Phys. Rev. B.*, **98**, 155438 (2018)