SUPPORT OPTIMIZATION FOR THERMODYNAMIC PROCESSES

Gabriel T. Landi

Instituto de Física da Universidade de São Paulo

Nottingham University.

Jan. 27th, 2020

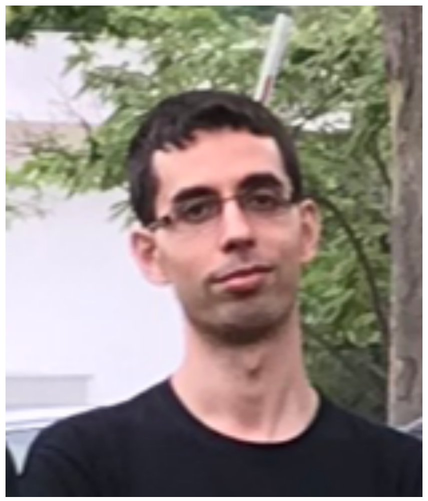
Quantum thermodynamics

quantum transport

IFUSP

www.fmt.if.usp.br/~gtlandi

Summary

André M. Timpanaro, Giacomo Guarnieri, John Goold, GTL,
"**Thermodynamic uncertainty relations from exchange fluctuation theorems**".
Phys. Rev. Lett. **123**, 090604 (2019) (arXiv 1904.07574)

GTL, Giacomo Guarnieri, John Goold and André M. Timpanaro,
"**Optimal support for thermodynamic processes**"
(in preparation)

BOUNDS AND OPTIMIZATION

- *MaxEnt principle*: which distribution maximizes the entropy for a fixed energy?

$$\tilde{S}[\boldsymbol{p}] = S[\boldsymbol{p}] + \alpha\left(1 - \sum_n p_n\right) + \beta\left(U - \sum_n E_n p_n\right) \qquad S[\boldsymbol{p}] = -\sum_n p_n \ln p_n$$

- Answer: the equilibrium distribution: $p_n^{\mathrm{eq}} = e^{-\beta E_n}/Z$
- The optimization also leads to a *bound*: $S[\boldsymbol{p}] \leq S[\boldsymbol{p}_{\mathrm{eq}}]$

- *Landauer's principle*: what is the minimum amount of heat required to erase some information?

$$\Delta Q_{\mathrm{env}} \geq -T\Delta S_{\mathrm{sys}}$$

- The optimal way of accomplishing this is through a reversible process.

OPTIMAL SUPPORT

The support of a distribution $P(x)$ is defined as the set of points x_i at which $P(x_i) \neq 0$.

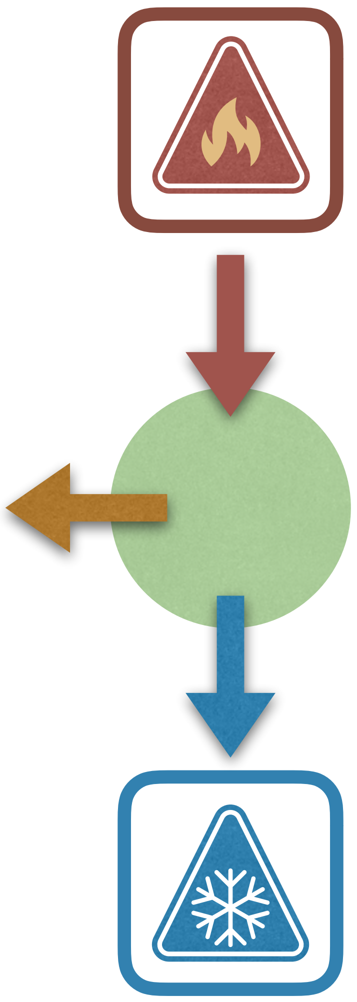
- Entropy does not care about support: it is a function only of the distribution.

- An example of a quantity that cares about the support is the variance

$$\mathrm{var}(X) = \sum_i \Big(x_i - \mathbb{E}(X) \Big)^2 P(x_i)$$

- By changing the support, one can *increase* the variance and simultaneously *decrease* the entropy.

OPTIMIZATION vs. SUPPORT OPTIMIZATION



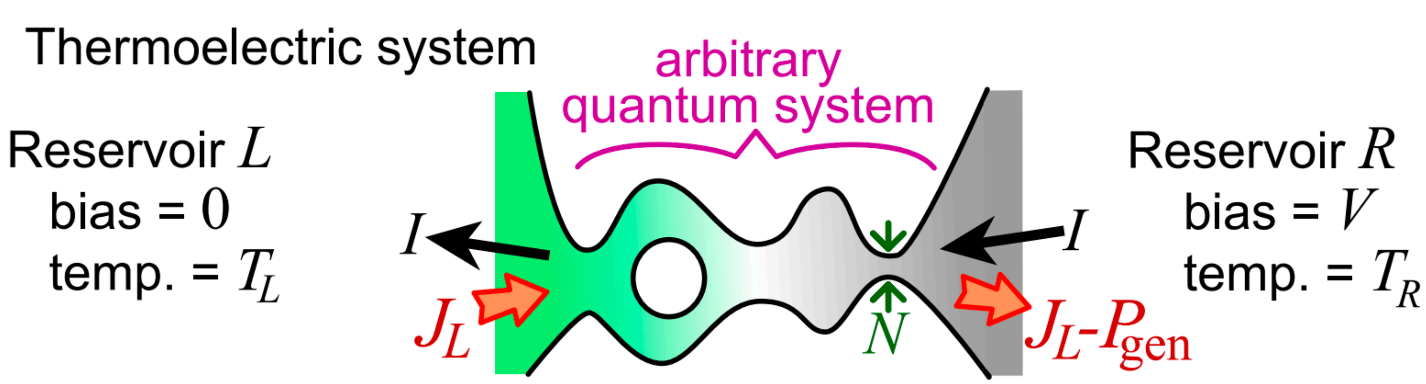
- Suppose we wish to optimize a heat engine.
  - e.g., maximize the efficiency for a fixed output power.
- *Optimization* means tweaking the parameters of the engine.
- *Support optimization* means choosing the best working fluid.
  - i.e., change the energy levels of the system.

EXAMPLE: THERMOELECTRIC ENGINE

- In a thermoelectric the "working fluid" is characterized by a transmission function instead:

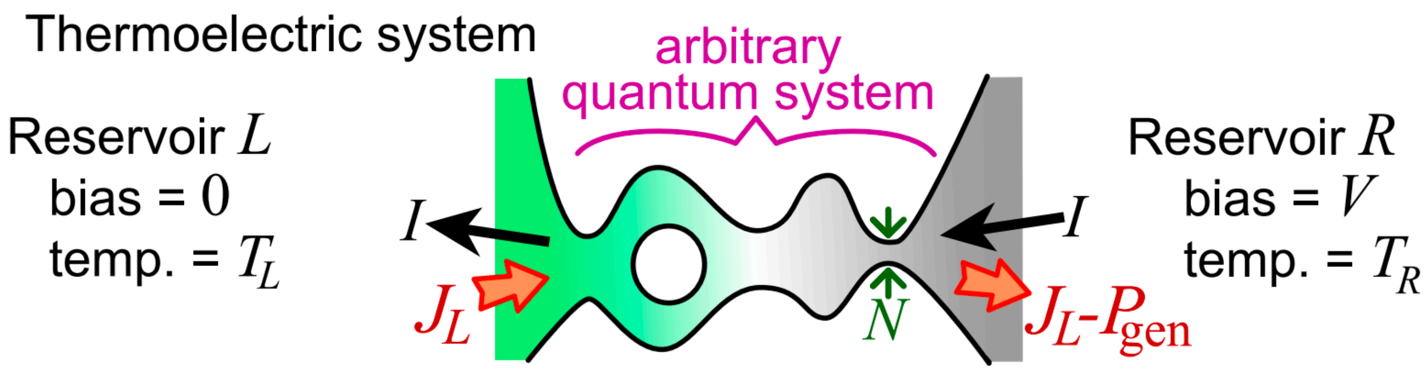
$$J_L = \int d\epsilon\, \mathcal{T}(\epsilon)\epsilon \Big[f_L(\epsilon) - f_R(\epsilon) \Big] \qquad\qquad P_{\mathrm{gen}} = \int d\epsilon\, \mathcal{T}(\epsilon) V \Big[f_L(\epsilon) - f_R(\epsilon) \Big]$$

- Which thermoelectric has the best possible efficiency $\eta = P_{\mathrm{gen}}/J_L$?
- *Answer*: a deltatransmission function $\mathcal{T}(\epsilon) = N\,\delta\Big(\epsilon - V(1 - T_R/T_L)\Big)$
- It operates at Carnot efficiency, $\eta = 1 - T_R/T_L$, but with *zero power*.

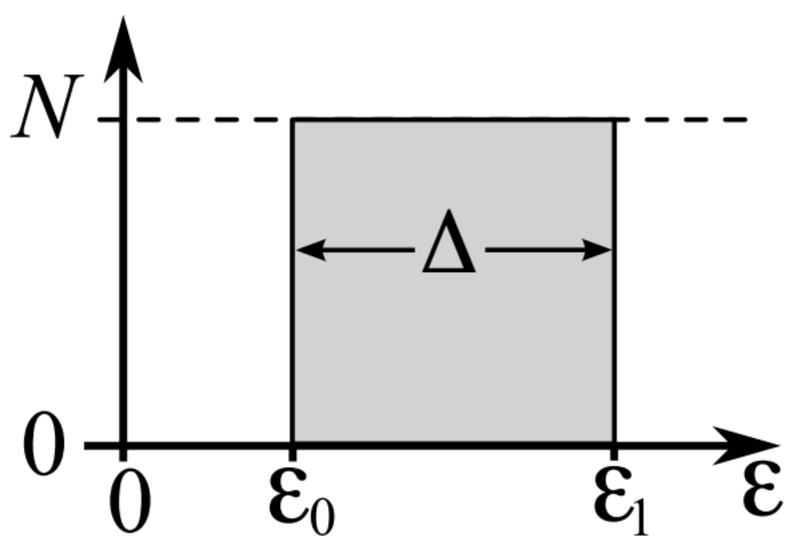


Taken from R. Whitney, *PRL* **112**, 130601 (2014)

G. D. Mahan and J. O. Sofo, *PNAS*, **93**, 7436 (1996)



- Which thermoelectric has the best possible efficiency for a fixed output power P_{gen}?
- The answer is a boxcar function



$$\mathcal{T}(\epsilon) = N\ \theta(\epsilon-\epsilon_0)\theta(\epsilon_1-\epsilon)$$

$$\epsilon_0 = V(1-T_R/T_L)$$

$$\epsilon_1 \text{ determined by } P_{\mathrm{gen}}$$

R. Whitney, *PRL* **112**, 130601 (2014)

EXAMPLE: OPTIMAL WORK EXTRACTION

- Consider the *single-shot* extraction of work from a thermodynamic system.

- This process is stochastic and thus must be characterized by a work distribution *P(W)*, restricted by the Jarzynski equality

$$\mathbb{E}\big(e^{-\beta W}\big) = e^{-\beta \Delta F}$$

- *Which kind of system/process allows me to extract the maximum amount of work?*

- Since we are at the single-shot level, this is best formulated as:

  - Which process maximizes $P(W \geq \Lambda)$, for some given Λ?

V. Cavina, A. Mari and V. Giovannetti, *Scientific Reports*, **6**, 29282 (2016).

- This question turns out to be ill-posed:
  - The Jarzynski equality is not a strong enough constraint.
  - You can always extract an infinite amount of work in principle.
- But suppose we add the additional constraint that $P(W < W_{\min}) = 0$
- Cavina *et. al.* found that

$$P(W \geq \Lambda) = \frac{e^{-\beta \Delta F} - e^{\beta W_{\min}}}{e^{\beta \Lambda} - e^{\beta W_{\min}}}$$

- In the unrestricted regime $W_{\min} \to \infty$ this reduces to

$$\boxed{P(W \geq \Lambda) = e^{-\beta(\Delta F - \Lambda)}}$$

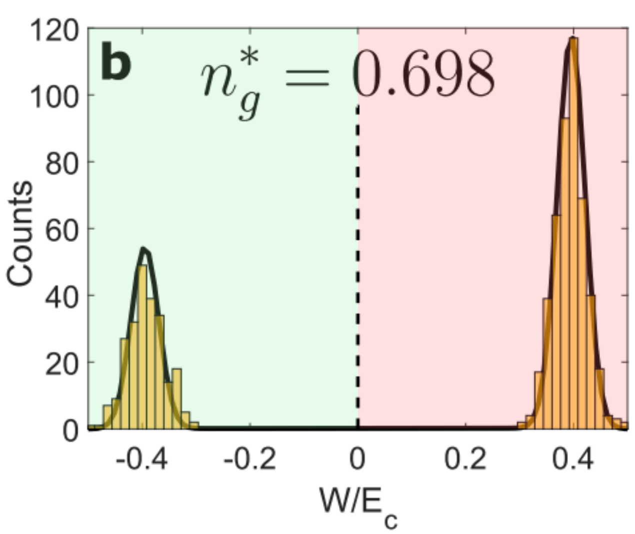
V. Cavina, A. Mari and V. Giovannetti, *Scientific Reports*, **6**, 29282 (2016).

$$P(W \geq \Lambda) = e^{-\beta(\Delta F - \Lambda)}$$

- This result is pretty cool.
  - It implies that in the single-shot scenario, the probability of extracting work above ΔF is exponentially small.
- This bound was already known since 2008. The novel result of Cavina *et. al.* is that they also found the *optimal process:*

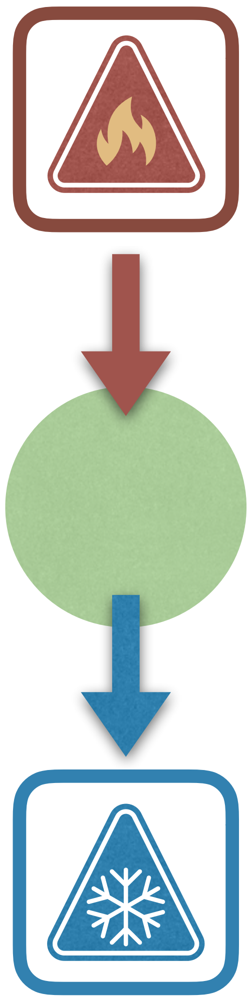
$$P(W) = p\delta(W - \Lambda) + (1-p)\delta(W - W_{\min})$$

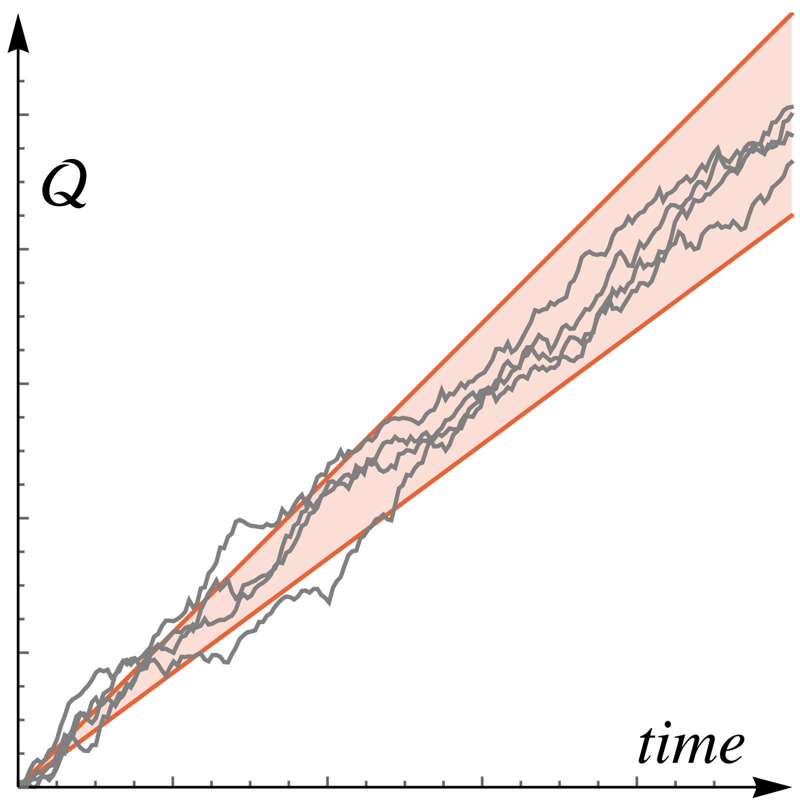
$$p = \frac{e^{-\beta\Delta F} - e^{\beta W_{\min}}}{e^{\beta\Lambda} - e^{\beta W_{\min}}}$$



C. Jarzynski, *European Physical Journal B*, **64**, 331 (2008).
O. Maillet, *PRL*, **122**, 150604 (2019)

Thermodynamic Uncertainty Relations (TURs)





$$\frac{\mathrm{var}(\mathcal{Q})}{\mathbb{E}(\mathcal{Q})^2} \geq \frac{2}{\mathbb{E}(\Sigma)}$$

$\Sigma = \delta\beta\ \mathcal{Q}$ (in the simplest case)

- Simple, elegant and powerful.
- Counterintuitive: To reduce the fluctuations, the process should be *more irreversible*.

- Derived only for the steady-state of classical Markov chains.
- Can be violated in many relevant scenarios (e.g. thermoelectrics).

A. C. Barato, U. Seifert, *Physical Review Letters*, **114**, 158101 (2015)

FLUCTUATIONS IN A HEAT ENGINE

- As an example of the applicability of TURs, Pietzonka and Seifert showed that the output power in a heat engine is bounded by

$$\mathrm{var}(P_{\mathrm{gen}}) \geq 2T_c P_{\mathrm{gen}} \frac{\eta}{\eta_C - \eta}$$

- For a fixed *average* power, the fluctuations go up if we approach Carnot efficiency.
  - To reduce fluctuations, one should operate away from Carnot efficiency.

Fluctuations therefore appear as an additional property to take into account when optimizing heat devices.

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

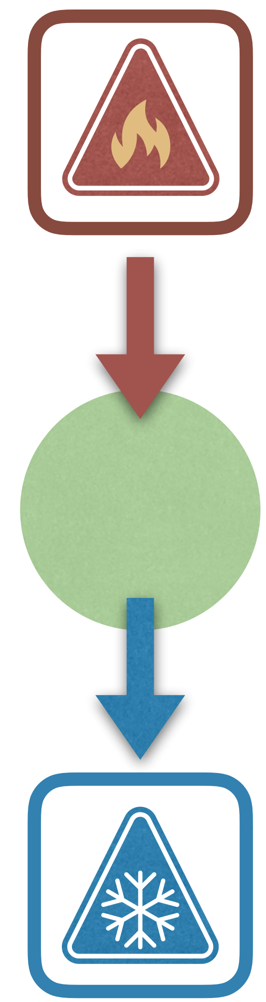
TUR from fluctuation theorems

André M. Timpanaro, Giacomo Guarnieri, John Goold, GTL,
"**Thermodynamic uncertainty relations from exchange fluctuation theorems**".
Phys. Rev. Lett. **123**, 090604 (2019) (arXiv 1904.07574)

EXCHANGE FLUCTUATION THEOREM

- Fluctuation theorems for thermodynamic processes usually have the form

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



- e.g. Crooks theorem for work: $\Sigma = \beta(W - \Delta F)$
- FTs, however, compare a *forward* with a *backward* process.
- In some systems, both coincide. These are called *Exchange FTs:*

$$\boxed{\frac{P(\Sigma)}{P(-\Sigma)} = e^{\Sigma}}$$

- This is *much stronger*: it is a symmetry on a single probability distribution.
- Example: direct heat exchange: $\Sigma = \delta\beta Q$

- Motivated by this, we proved the following theorem:

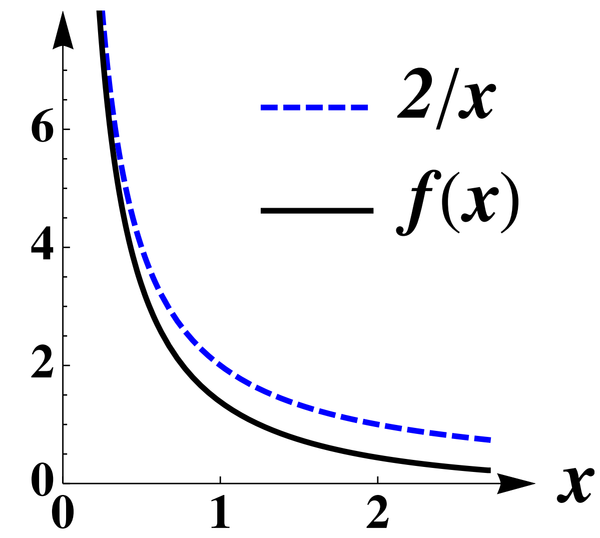
Theorem (*"TUR de force"*). *For fixed finite $\mathbb{E}(\Sigma)$, the probability distribution $P(\Sigma)$ satisfying $P(\Sigma)/P(-\Sigma) = e^{\Sigma}$, with the smallest possible variance (the minimal distribution) is*

$$P_{min}(\Sigma) = \frac{1}{2\cosh(a/2)}\left\{e^{a/2}\delta(\Sigma - a) + e^{-a/2}\delta(\Sigma + a)\right\},$$

where the value of a is fixed by $\mathbb{E}(\Sigma) = a\tanh(a/2)$. For this distribution

$$\mathrm{Var}(\Sigma)_{min} = \mathbb{E}(\Sigma)^2 f(\mathbb{E}(\Sigma)),$$

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



For any other distribution we must then have:

$$\frac{\mathrm{var}(\Sigma)}{\mathbb{E}(\Sigma)^2} \geq f(\mathbb{E}(\Sigma))$$

TUR de force IS TIGHT

- Our TUR is the tighest (saturable) bound for this scenario.
- And we know which thermodynamic process saturates it.
- This is relevant because, around the same time, similar papers appeared.
  - But all derived a looser bound with

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

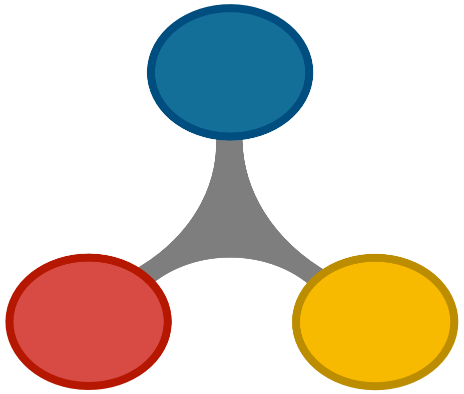
- This bound, however, is never tight.

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

EXTENSION TO MULTIPLE CHARGES

- We can also generalize our framework to Exchange FTs involving multiple charges:

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



- The entropy production in this case is $\Sigma = \sum_i A_i \mathcal{Q}_i$

- ex: heat engine FT:

$$\frac{P(Q_h, W)}{P(-Q_h, -W)} = e^{(\beta_h - \beta_c) Q_h + \beta_c W}$$

- In this case we obtain the matrix bound

$$\boxed{\mathcal{C} - f(\mathbb{E}(\Sigma)) \boldsymbol{q}\boldsymbol{q}^{\mathrm{T}} \geq 0}$$

$$q_i = \mathbb{E}(\mathcal{Q}_i)$$

$$\mathcal{C}_{ij} = \mathrm{cov}(\mathcal{Q}_i, \mathcal{Q}_j)$$

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

$$\mathcal{C} - f(\mathbb{E}(\Sigma))\boldsymbol{q}\boldsymbol{q}^{\mathrm{T}} \geq 0$$

$$q_i = \mathbb{E}(\mathcal{Q}_i)$$

$$\mathcal{C}_{ij} = \mathrm{cov}(\mathcal{Q}_i, \mathcal{Q}_j)$$

- This says that the matrix above is positive semi-definite.

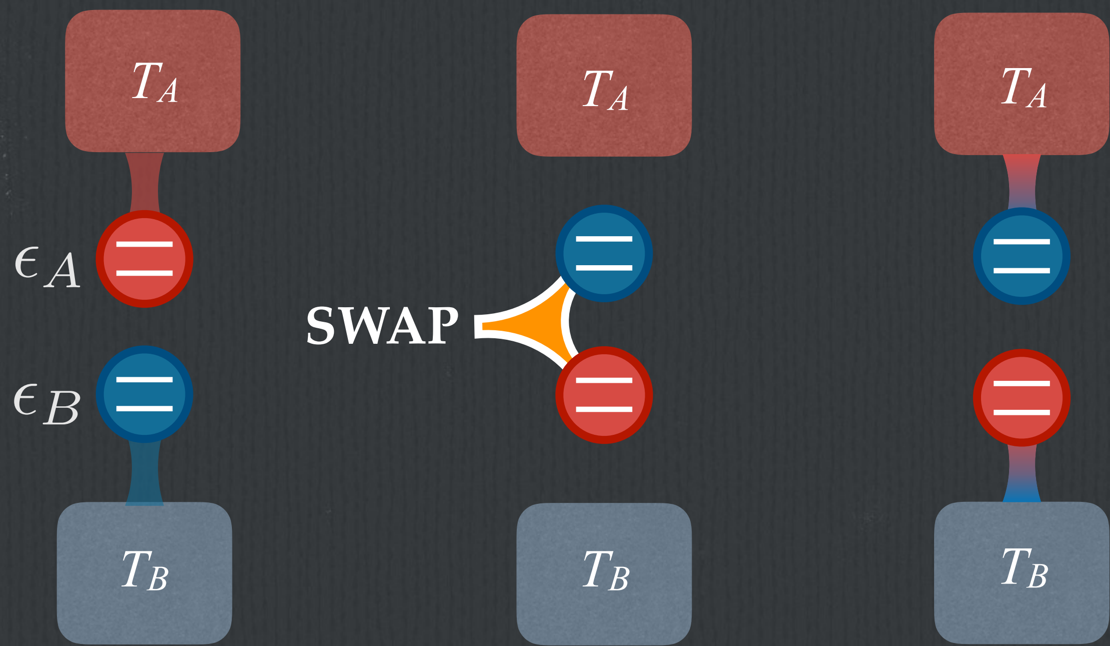
- As a consequence, all diagonal entries must be positive, which implies an individual TUR for each charge:

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

- In addition, it also places restrictions on the covariances:

  - If *G* is psd then $G_{ij}^2 \leq G_{ii}G_{jj}$

- Correlations between thermodynamic quantities has so far been largely unexplored.

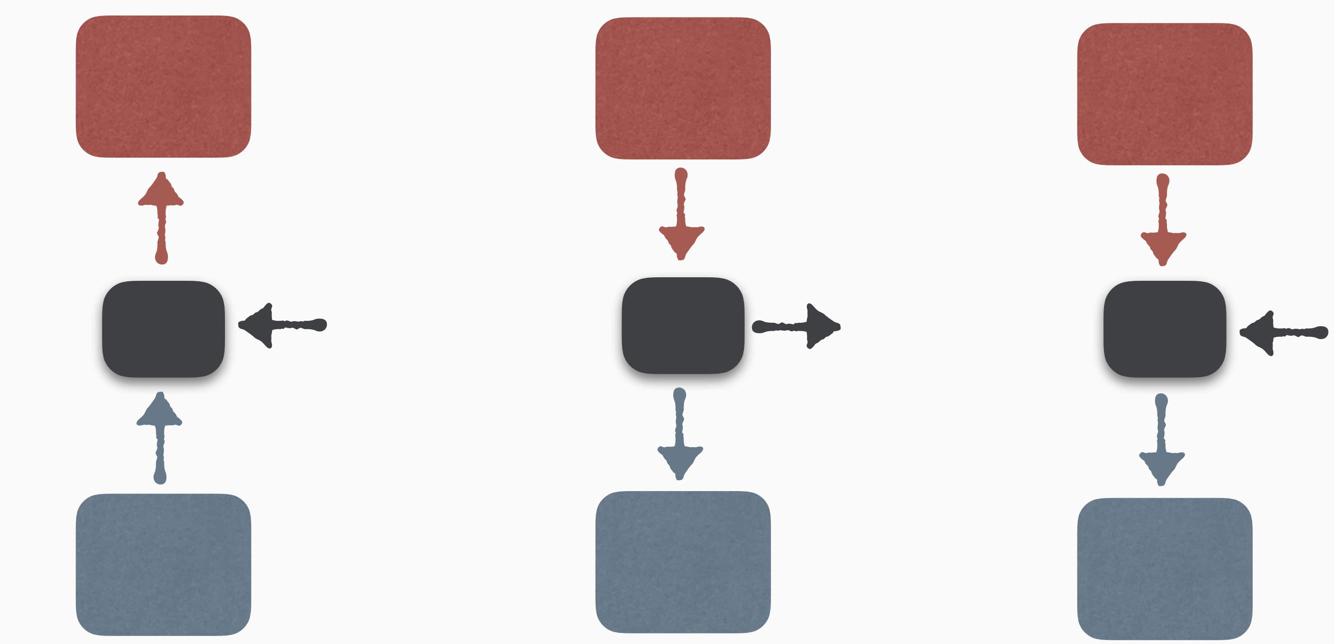


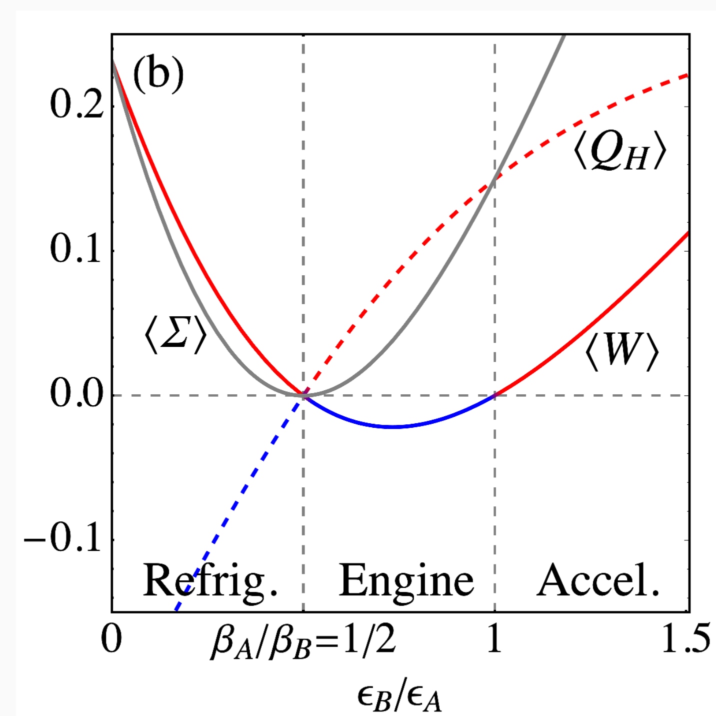
SWAP engine

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

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

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





Refrigerator

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

Engine

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

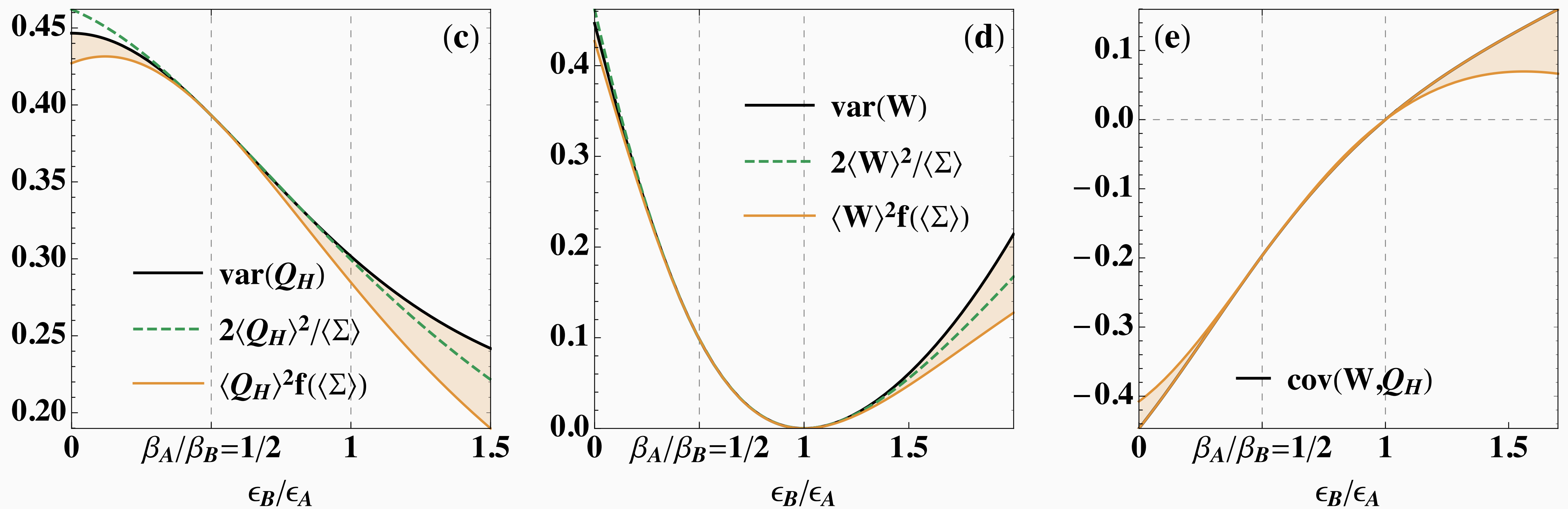
Accelerator

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

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

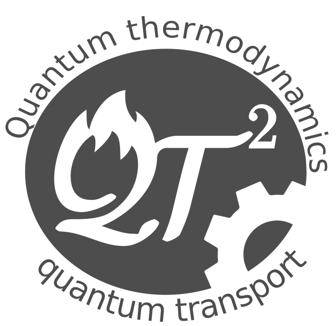
- In this talk I tried to discuss the idea of **optimizing the support in thermodynamic processes**.

- I feel that this is important because it sheds light on:

  a. What are the ultimate lin

  b. Which sorts of processes

  c. What are the ideal proce machine;



Quantum thermodynamics
quantum transport
IFUSP

www.fmt.if.usp.br/~gtlandi