FINITE TIME STOCHASTIC THERMODYNAMICS AND OPTIMAL MASS TRANSPORT

Krzysztof Gawedzki, Lyon, June 2012

"Time is the longest distance between two places"

Tennessee Williams, "The Glass Menagerie"

Stochastic Thermodynamics :

- In classical version it describes dynamics of mesoscopic systems (colloids, polymers, biomolecules, etc.) in contact with heat bath(s) modeled by random noise
- Subject with long history starting with **Einstein**, **Smoluchowski**, **Langevin**
- More recently revived in the context of theoretical study of **fluctuation relations**: **Kurchan**, **Lebowitz-Spohn**, **Jarzynski**, **Crooks**, **Sekimoto**, **Hatano**, **Sasa**, **Maes**, **Seifert**, ...

- A simple set-up for studying interplay between thermodynamical and statistical concepts away from equilibrium
- In quantum version it uses **Markovian** modelization of the dynamics of open nanoscopic systems
- Lends itself to experimental verifications, e.g. in experiments by Stuttgart (**Bechinger**), Lyon (**Ciliberto**), Barcelone (**Ritort**), Berkeley (**Bustamante**), Notre Dame (**Orlov**), ... groups

The simplest classical model: overdamped **Langevin** equation

$$\frac{d\boldsymbol{x}}{dt} \;=\; -M\boldsymbol{\nabla}U(t,\boldsymbol{x}) \;+\; \boldsymbol{\eta}(t)$$

with constant **mobility** matrix $M = (M^{ij}) > 0$ and the **white noise**

$$\left\langle\, \eta^i(s)\, \eta^j(t) \,\right\rangle \;=\; 2\boxed{k_B T\, M^{ij}}\,\delta(s-t)$$

Einstein relation

1st Law of Stochastic Thermodynamics

- fluctuating **work** performed in time interval $[0, t_f]$:

$$W = \int_0^{t_f} \partial_t U(t, \boldsymbol{x}(t))\, dt$$

- fluctuating **heat** dissipation:

$$Q = -\int_0^{t_f} \partial_i U(t, \boldsymbol{x}(t)) \circ dx^i(t)$$

(with "$\circ$" marking the **Stratonovich** convention)

$$\boxed{W - Q = U(t_f, \boldsymbol{x}(t_f)) - U(0, \boldsymbol{x}(0)) \equiv \Delta U}$$

holds trajectory-wise, not only for the means ! (**Sekimoto** 1998)

2^{nd} Law of Stochastic Thermodynamics

The probability density

$$\rho(t,\boldsymbol{x}) \;=\; \big\langle\, \delta(\boldsymbol{x}-\boldsymbol{x}(t))\,\big\rangle \;\equiv\; \exp\Big[-\frac{R(t,\boldsymbol{x})}{k_B T}\Big]$$

evolves according to the **Fokker-Planck** equation that may be written as the advection equation

$$\partial_t \rho \;+\; \boldsymbol{\nabla}\cdot(\rho\,\boldsymbol{v}) \;=\; 0$$

in the **current velocity** field (**Nelson** 1967)

$$\boldsymbol{v}(t,\boldsymbol{x}) \;=\; \frac{\big\langle\, \delta(\boldsymbol{x}-\boldsymbol{x}(t))\circ \frac{d\boldsymbol{x}}{dt}(t)\,\big\rangle}{\rho(t,\boldsymbol{x})} \;=\; M\boldsymbol{\nabla}(R-U)$$

(again with the **Stratonovich** convention)

2^{nd} Law of Stochastic Thermodynamics (cont'd)

- The fluctuating instantaneous **entropy** of the system is

$$S_{sys}(t) \;=\; -\,k_B\,\ln\rho(t,\boldsymbol{x}(t)) \;=\; \frac{1}{T}\,R(t,\boldsymbol{x}(t))$$

with the mean given by the **Gibbs-Shannon** formula

$$\left\langle\, S_{sys}(t)\,\right\rangle \;=\; -\,k_B\int \rho(t,\boldsymbol{x})\;\ln\rho(t,\boldsymbol{x})\;d\boldsymbol{x}$$

and the change along the trajectory

$$\Delta S_{sys} \;\equiv\; S_{sys}(t_f) - S_{sys}(0) \;=\; \frac{1}{T}\int_0^{t_f}\frac{d}{dt}\,R(t,\boldsymbol{x}(t))\,dt$$

- The change of entropy of the system is accompanied by the change of entropy of the thermal environment given by the thermodynamical relation

$$\Delta S_{env} \;=\; \frac{Q}{T} \;=\; -\,\frac{1}{T}\int_0^{t_f}\partial_i U(t,\boldsymbol{x}(t))\circ dx^i(t)$$

2^{nd} Law of Stochastic Thermodynamics (cont'd)

- The total change of fluctuating entropy

$$\Delta S_{tot} \quad = \quad \Delta S_{sys} + \Delta S_{env}$$

satisfies the **Jarzynski**-type **equality** (one of **Fluctuation Relations**)

$$\left\langle \, \mathrm{e}^{-\Delta S_{tot}/k_B} \, \right\rangle \; = \; 1 \qquad \text{(Seifert 2005)}$$

(an easy exercise based on **Girsanov** and **Feynman-Kac** formulae) implying by the **Jensen** inequality the $\mathbf{2}^{\text{nd}}$ **Law** stating that

$$\boxed{\left\langle \Delta S_{tot} \right\rangle \; \geq \; 0}$$

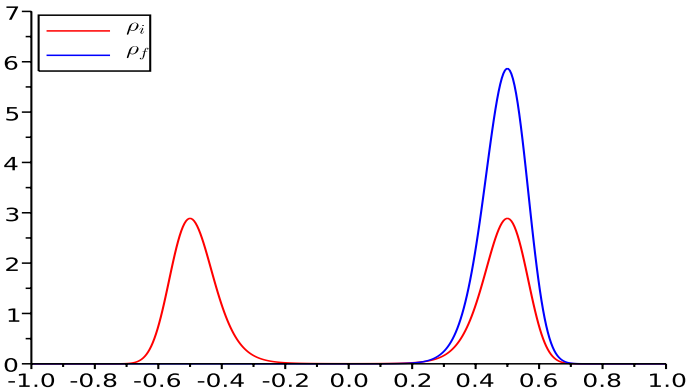
that also follows by a direct calculation giving

$$\left\langle \Delta S_{tot} \right\rangle \; = \; \frac{1}{T} \int_0^{t_f} dt \int \boldsymbol{v}(t,\boldsymbol{x}) \cdot M^{-1} \, \boldsymbol{v}(t,\boldsymbol{x}) \; \rho(t,\boldsymbol{x}) \; d\boldsymbol{x}$$

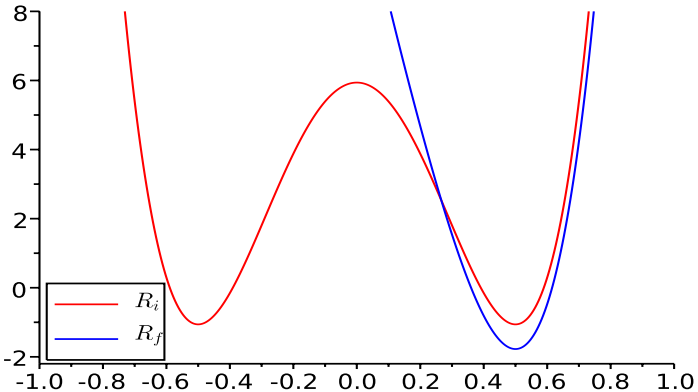
Landauer **Principle** (IBM Journal of Res. and Dev. **5:3** (1961))

> Erasure of one bit of memory in a computation in thermal environment requires dissipation of at least $k_B T \ln 2$ of heat (in mean)

Model: overdamped **Langevin** evolution from from the initial state $\rho_i = \frac{1}{Z_i} \mathrm{e}^{-\frac{R_i(\boldsymbol{x})}{k_B T}}$ to the final state $\rho_f = \frac{1}{Z_f} \mathrm{e}^{-\frac{R_f(\boldsymbol{x})}{k_B T}}$ with



ρ_i (red) and ρ_f (blue)



R_i (red) and R_f (blue)

- at the initial time $t = 0$, $\boldsymbol{x}(0)$ is either in the left or in the right potential well (1 bit of information)

- at the final time $t = t_f$, $\boldsymbol{x}(t_f)$ is in the right potential well with no memory of where it started

- The **Landauer** bound

$$\langle\, Q \,\rangle \;\geq\; k_B T \,\ln 2$$

is implied by the **2nd Law** rewritten as the bound

$$\langle\, Q \,\rangle \;\geq\; -\,T \,\langle \Delta S_{sys} \rangle$$

since here

$$\langle \Delta S_{sys} \rangle \;\approx\; -\,k_B \,\ln 1 \,+\, 2\,k_B \,(\ln \tfrac{1}{2})\,\tfrac{1}{2} \;=\; -\,k_B \,\ln 2$$

Finite-time Thermodynamics

- The **2nd Law** & **Landauer** bounds are saturated in quasi-stationary processes that take infinite time (if $\rho_i \neq \rho_f$)

- In computation, one wants to minimize dissipated heat but also to go fast

- This gives rise to the question:

> Given ρ_i, ρ_f and the length t_f of the time window, what is the minimal $\langle \Delta S_{tot} \rangle$?

- Problems studies in the thermal engineering theory from the 50' by **Novikov**, **Chambadal**, **Curzon-Ahlborn**, . . . , and, after the first oil crisis, by **Berry**, **Salamon**, **Andresen** . . . who coined the name of **Finite-Time Thermodynamics**

- In the context of **Stochastic Thermodynamics**, they were first addressed by **Schmiedl-Seifert** in 2007 for **Gaussian** processes

Main result: **Aurell-Mejìa-Monasterio-Muratore-Ginanneschi** (2011), **Aurell-G.-Mejìa-Monasterio-Mohayaee-Muratore-Ginanneschi** (2012)

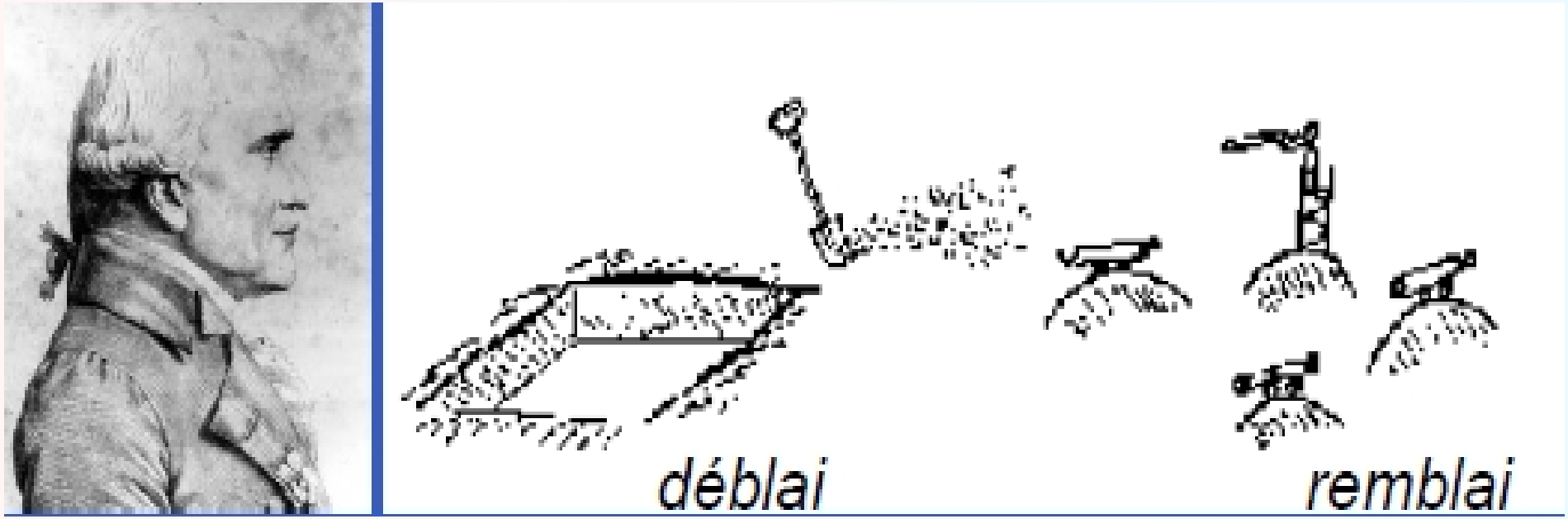
For fixed $\rho_i,\ \rho_f,\ t_f$ but otherwise arbitray control potentials $U(t,\boldsymbol{x})$,

$$\boxed{\left\langle \Delta S_{tot} \right\rangle_{min} \ = \ \frac{1}{t_f T}\ \mathcal{K}_{min}}$$

where $\mathcal{K}_{min} = \min\ \mathcal{K}[\boldsymbol{x}_f(\cdot)]$ over maps $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$ carring ρ_i to ρ_f, i.e. such that $\rho_i(\boldsymbol{x}_i)d\boldsymbol{x}_i = \rho_f(\boldsymbol{x}_f)d\boldsymbol{x}_f$, of the quadratic **cost function**

$$\mathcal{K}[\boldsymbol{x}_f(\cdot)] \ = \ \int (\boldsymbol{x}_f(x_i) - \boldsymbol{x}_i)\cdot M^{-1}\,(\boldsymbol{x}_f(x_i) - \boldsymbol{x}_i)\ \rho_i(\boldsymbol{x}_i)\ d\boldsymbol{x}_i$$

- Minimization of $\mathcal{K}[\boldsymbol{x}_f(\cdot)]$ over the maps $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$ that transport ρ_i to ρ_f is the celebrated **Monge** (1781) - **Kantorovich** (1942) **Optimal Mass Transport Problem**


déblai
remblai

Proof. A corollary of the result of **Benamou-Brenier** (1997) relating the optimal mass transport to the **Burgers** equation

- **Benamou-Brenier** minimize the functional

$$\mathcal{A}[\rho, \boldsymbol{v}] \;=\; \int_0^{t_f} dt \int (\boldsymbol{v} \cdot M^{-1} \boldsymbol{v})(t, \boldsymbol{x}) \; \rho(t, \boldsymbol{x}) \; d\boldsymbol{x}$$

over densities $\rho(t, \boldsymbol{x})$ and velocity fields $\boldsymbol{v}(t, \boldsymbol{x})$ satisfying advection equation $\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0$ and such that

$$\rho(0, \boldsymbol{x}) = \rho_i(\boldsymbol{x}) \,, \qquad \rho(t_f, \boldsymbol{x}) = \rho_f(\boldsymbol{x})$$

- The advection equation with the above initial conditions is solved by

$$\rho(t, \boldsymbol{x}) = \int \delta(\boldsymbol{x} - \boldsymbol{x}(t; \boldsymbol{x}_i)) \; \rho_i(\boldsymbol{x}_i) \; d\boldsymbol{x}_i$$

for the **Lagrangian** flow of $\boldsymbol{v}(t, \boldsymbol{x})$

$$\frac{d\boldsymbol{x}}{dt}(t; \boldsymbol{x}_i) = \boldsymbol{v}(t, \boldsymbol{x}(t; \boldsymbol{x}_i)) \,, \qquad \boldsymbol{x}(0; \boldsymbol{x}_i) = \boldsymbol{x}_i$$

- Inserting this solution to the expression for $\mathcal{A}$ gives:

$$\mathcal{A}[\rho, \boldsymbol{v}] \;=\; \int_0^{t_f} dt \int \big(\frac{d\boldsymbol{x}}{dt} \cdot M^{-1} \frac{d\boldsymbol{x}}{dt}\big)(t; \boldsymbol{x}_i)\; \rho_i(t, \boldsymbol{x}_i)\; d\boldsymbol{x}_i$$

- Minimizing first over the curves $[0, t_f] \ni t \mapsto \boldsymbol{x}(t; \boldsymbol{x}_i)$ keeping $\boldsymbol{x}(t_f; \boldsymbol{x}_i) = \boldsymbol{x}_f(\boldsymbol{x}_i)$ fixed, with the minima attained on straight lines

$$\boldsymbol{x}(t; \boldsymbol{x}_i) \;=\; \boldsymbol{x}_i + \frac{t}{t_f}\big(\boldsymbol{x}_f(\boldsymbol{x}_i) - \boldsymbol{x}_i\big) \;\equiv\; \boldsymbol{x}^{lin}(t; \boldsymbol{x}_i)\,,$$

with $\frac{d\boldsymbol{x}}{dt}(t, \boldsymbol{x}_i) = \frac{\boldsymbol{x}_f(\boldsymbol{x}_i) - \boldsymbol{x}_i}{t_f}$ one reduces the minimization of $\mathcal{A}$ to the optimal mass transport problem considered before:

$$\mathcal{A}_{min} \;=\; \frac{1}{t_f}\, \mathcal{K}_{min}$$

- The map $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$ that minimizes the quadratic cost function is of the gradient type:

$$\boldsymbol{x}_f(\boldsymbol{x}_i) \;=\; M \cdot \boldsymbol{\nabla} F(\boldsymbol{x}_i)$$

for a convex function F

- The velocity field $\boldsymbol{v}$ minimizing $\mathcal{A}$ has the linear **Lagrangian** flow $\boldsymbol{x}^{lin}(t;\boldsymbol{x}_i)$, and, as such, satisfies the inviscid **Burgers** equation

$$\partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\boldsymbol{\nabla})\boldsymbol{v} \;=\; 0\,,$$

- It is necessarily also of the gradient type **!**

$$\boldsymbol{v}(t,\boldsymbol{x}) \;=\; M\boldsymbol{\nabla}\Psi(t,\boldsymbol{x})$$

where Ψ satisfies

$$\partial_t \Psi \;+\; \frac{1}{2}\,\boldsymbol{\nabla}\Psi\cdot M\boldsymbol{\nabla}\Psi \;=\; 0$$

- It follows that $\boldsymbol{v} = M\boldsymbol{\nabla}\Psi$ minimizing $\mathcal{A}$ is the **current velocity** $= M\boldsymbol{\nabla}(R - U)$ for the overdamped **Langevin** process such that

$$\boxed{U(t, \boldsymbol{x}) = R(t, \boldsymbol{x}) - \Psi(t, \boldsymbol{x})}$$

for

$$R(t, \boldsymbol{x}) = -k_B T \ln \int \delta(\boldsymbol{x} - \boldsymbol{x}_f^{lin}(t; \boldsymbol{x}_i)) \ \rho_i(\boldsymbol{x}_i) \ d\boldsymbol{x}_i$$

- Since

$$\langle \Delta S_{tot} \rangle \ = \ \frac{1}{T} \mathcal{A}[\rho, \boldsymbol{v}]$$

for $\boldsymbol{v} = M\boldsymbol{\nabla}(R - U)$, we conclude that

$$\langle \Delta S_{tot} \rangle_{min} \ = \ \frac{1}{T} \mathcal{A}_{min} \ = \ \frac{1}{t_f T} \mathcal{K}_{min}$$

even if, *a priori*, $\mathcal{A}$ was minimized without assuming the gradient form of $\boldsymbol{v}$

- The optimal protocol $U(t, \boldsymbol{x})$ is given by the formulae on the top ■

Geometric interpretation *à la* **Jordan-Kinderlehrer-Otto** (1998)

- $\mathcal{K}_{min}$ is the square of the **Wasserstein distance** $d_W(\rho_i, \rho_f)$ corresponding to the formal **Riemannian** metric

$$\|\partial_t \rho\|_W^2 \;=\; \int (\partial_t \rho)\,(-\boldsymbol{\nabla}\cdot \rho\, M \boldsymbol{\nabla})^{-1} (\partial_t \rho)\, d\boldsymbol{x}$$

  on the space of densities ρ

- The **Fokker-Planck** equation describes the gradient flow corresponding to the **free energy** functional

$$\mathcal{F}_t[\rho] \;=\; \int U(t,\boldsymbol{x})\,\rho(\boldsymbol{x})\; d\boldsymbol{x} \;+\; k_B T \int \rho(\boldsymbol{x})\,\ln \rho(\boldsymbol{x})\; d\boldsymbol{x}$$

- One has

$$\big\langle \Delta S_{tot} \big\rangle \;=\; \frac{1}{T}\int_0^{t_f} \|\partial_t \rho(t,\cdot)\|_W^2\; dt \;\geq\; \frac{1}{t_f T}\, d_W(\rho_i,\rho_f)^2$$

- Optimal protocol gives the (shortest) **geodesics** joining ρ_i to ρ_f

Corollary (Finite-time refinement of the **2nd Law**)

- For overdamped **Langevin** process evolving in time interval $[0, t_t]$ with the initial probability density ρ_i and the final one ρ_f

$$\langle \Delta S_{tot} \rangle = \langle \Delta S_{sys} \rangle + \frac{1}{T} \langle \Delta Q \rangle \geq \frac{1}{t_f T} \mathcal{K}_{min} \geq 0$$

with the left lower bound saturated by the protocol with $U = R - \Psi$

- Equivalently

$$\langle Q \rangle \geq -T \langle \Delta S_{sys} \rangle + \frac{1}{t_f} \mathcal{K}_{min}$$

and for $\langle \Delta S_{sys} \rangle = -k_B \ln 2$ we obtain a finite time refinement of the **Landauer Principle**

Remarks

- The minimal cost $\mathcal{K}_{min}$ is independent of the time window so that $\langle \Delta S_{tot} \rangle_{min}$ is inversely proportional to its length t_f

- For the optimal transport map $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i) = M\boldsymbol{\nabla} F(\boldsymbol{x}_i)$, function F satisfies the **Monge-Ampère** equation

$$\rho_f(M\boldsymbol{\nabla} F(\boldsymbol{x}_i))\ \det\left(M\boldsymbol{\nabla}\boldsymbol{\nabla} F(\boldsymbol{x}_i)\right) = \rho_i(\boldsymbol{x})$$

- For the optimal protocol $U(t,\boldsymbol{x})$ and $\boldsymbol{x} = \boldsymbol{x}^{lin}(t;\boldsymbol{x}_i)$,

$$\boldsymbol{\nabla}(R-U)(t,\boldsymbol{x}) = \boldsymbol{\nabla}\Psi(t,\boldsymbol{x}) = M^{-1}\frac{\boldsymbol{x}_f(\boldsymbol{x}_i)-\boldsymbol{x}_i}{t_f}$$

so that if $\rho_i \neq \rho_f$ then for <u>no times</u> in $[0,t_f]$ the densities $\rho(t,\boldsymbol{x})$ coincide with the **Gibbsian** ones for the control potentials $U(t,\boldsymbol{x})$

- In particular, the potential has to jump at the initial time if ρ_i was prepared by long evolution in a time-independent potential **!**

Remarks (cont'd)

- The optimal map $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$ may be approximated by optimal permutations π assigning to N points $\boldsymbol{x}_{i,n}$, distributed with density ρ_i, N points $\boldsymbol{x}_{f,n}$, distributed with density ρ_f, in a way minimizing the quadratic cost function

$$\frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{x}_{f,\pi(n)} - \boldsymbol{x}_{i,n})\, M^{-1}(\boldsymbol{x}_{f,\pi(n)} - \boldsymbol{x}_{i,n}) \;\equiv\; \mathcal{K}_N$$

  and the optimal π may be found by an **Auction Algorithm** based on the steepest descend with polynomially growing time $\propto N^{\gamma}$, $\gamma \approx 2.3$

- The numerical algorithms are not very efficient in regions where the densities are very small - when the latter are not strictly positive, the optimal transport map may be discontinuous

Remarks (cont'd)

- In one dimension, the optimal map $x_i \mapsto x_f(x_i)$ may be found from the equation

$$\int_{-\infty}^{x_f(x_i)} \rho_f(x)\, dx = \int_{-\infty}^{x_i} \rho_i(x)\, dx$$

- Numerically, the optimal assignment between $x_{i,n}$ and $x_{f,n}$ may be found by sorting both 1D sequences in increasing order

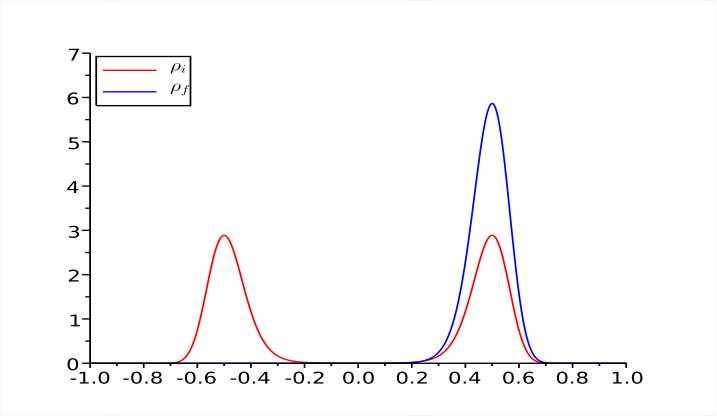
- If R_i and R_f are polynomials of the same even degree then $x_f(x_i) - x_i$ may be expanded in powers of x_i^{-1} for large $|x_i|$

Experiment-Motivated Example

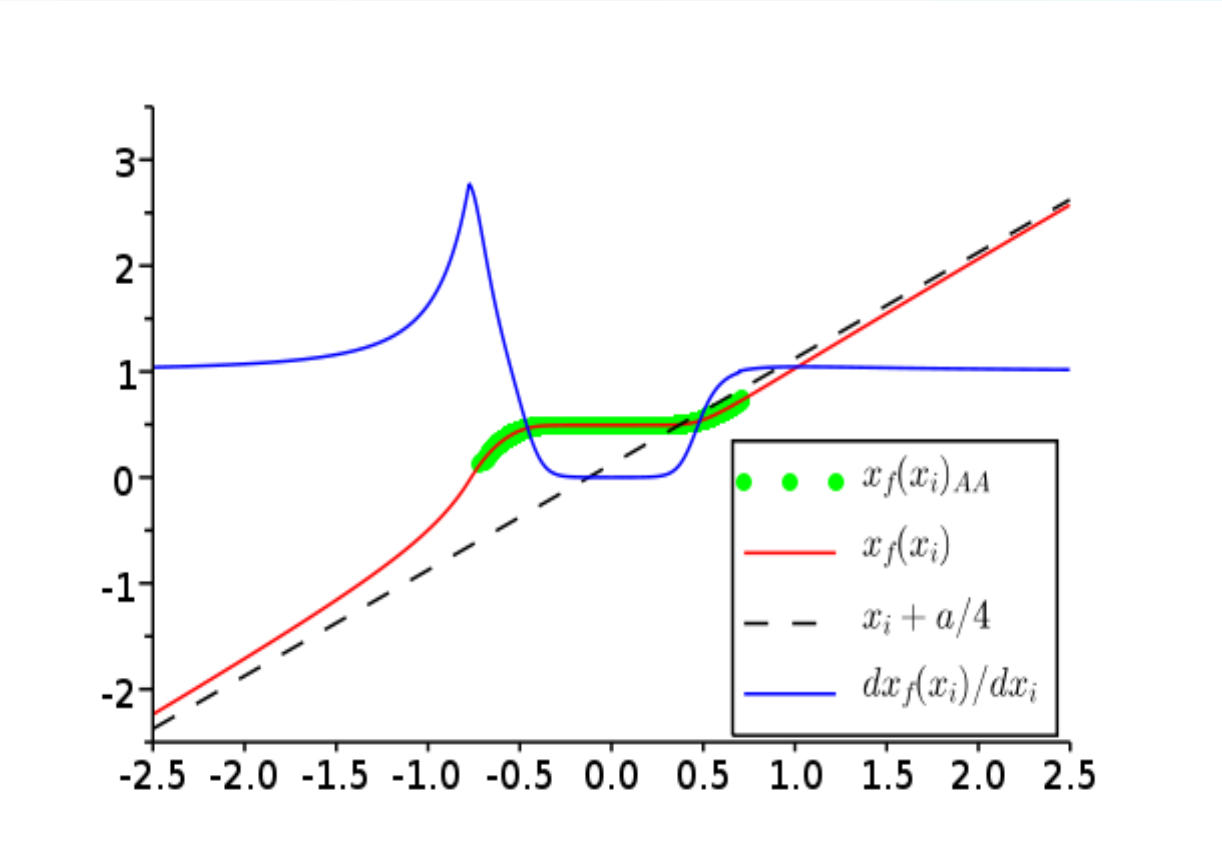
- Consider the memory erasure 1D example where the initial bimodal distribution evolves to its right branch with

$$\rho_i(x) = \frac{1}{Z_i} \exp\left[-\frac{A}{k_B T}(x^2 - \alpha^2)^2 \right]$$
$$\rho_f(x) = \frac{1}{Z_f} \exp\left[-\frac{A}{k_B T}(x-\alpha)^2((x-\alpha)^2 + 3\alpha(x-\alpha) + 4\alpha^2) \right]$$

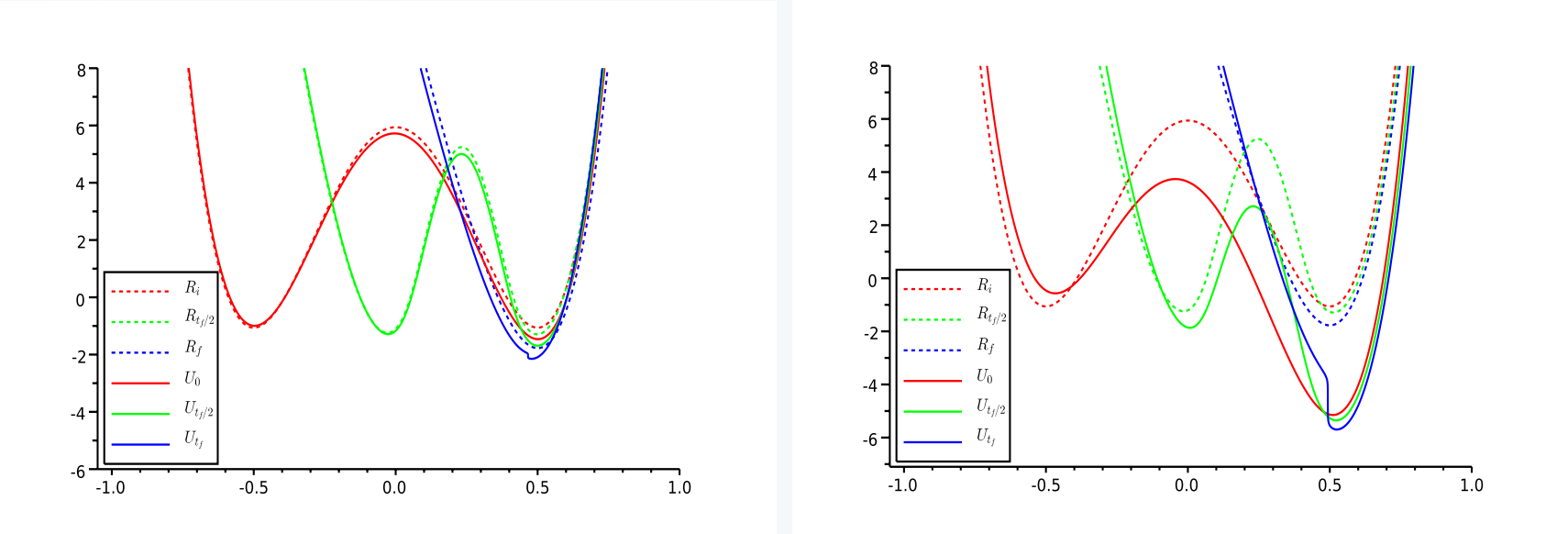
for $A = 112\, k_B T\, \mu m^{-4}$, $\alpha = 0.5\, \mu m$, and x expressed in μm's



- Numerical simulations combined with asymptotic expansion give for for the transport map $x_i \to x_f(x_i)$, its asymptote and its derivative:

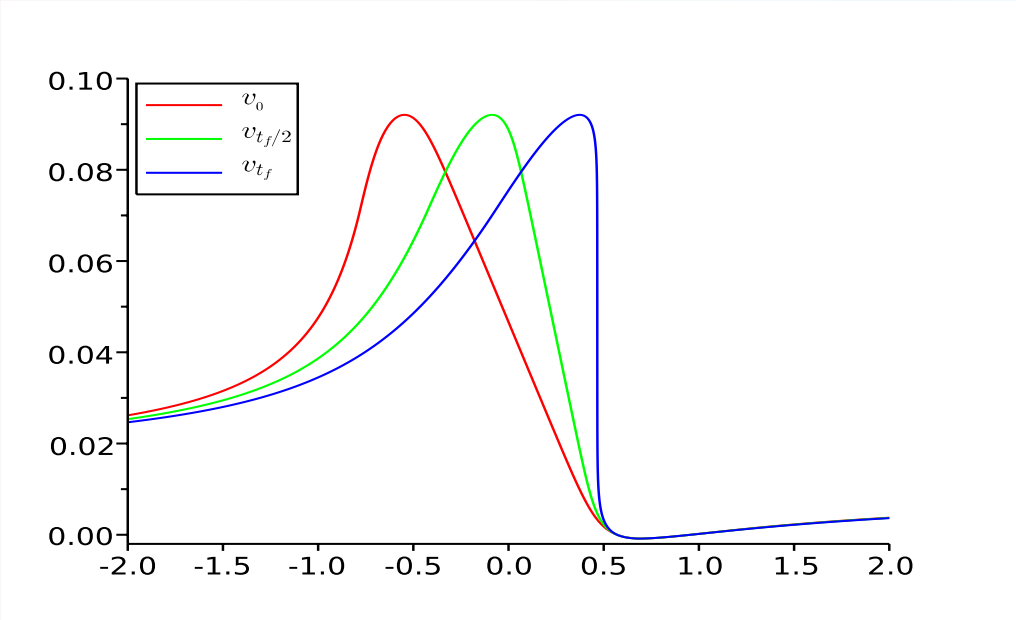


- Initial, half-time, and final **Gibbs** potentials R and control potentials U for $t_f = 10s$ (left) and $t_f = 1s$ (right) are:



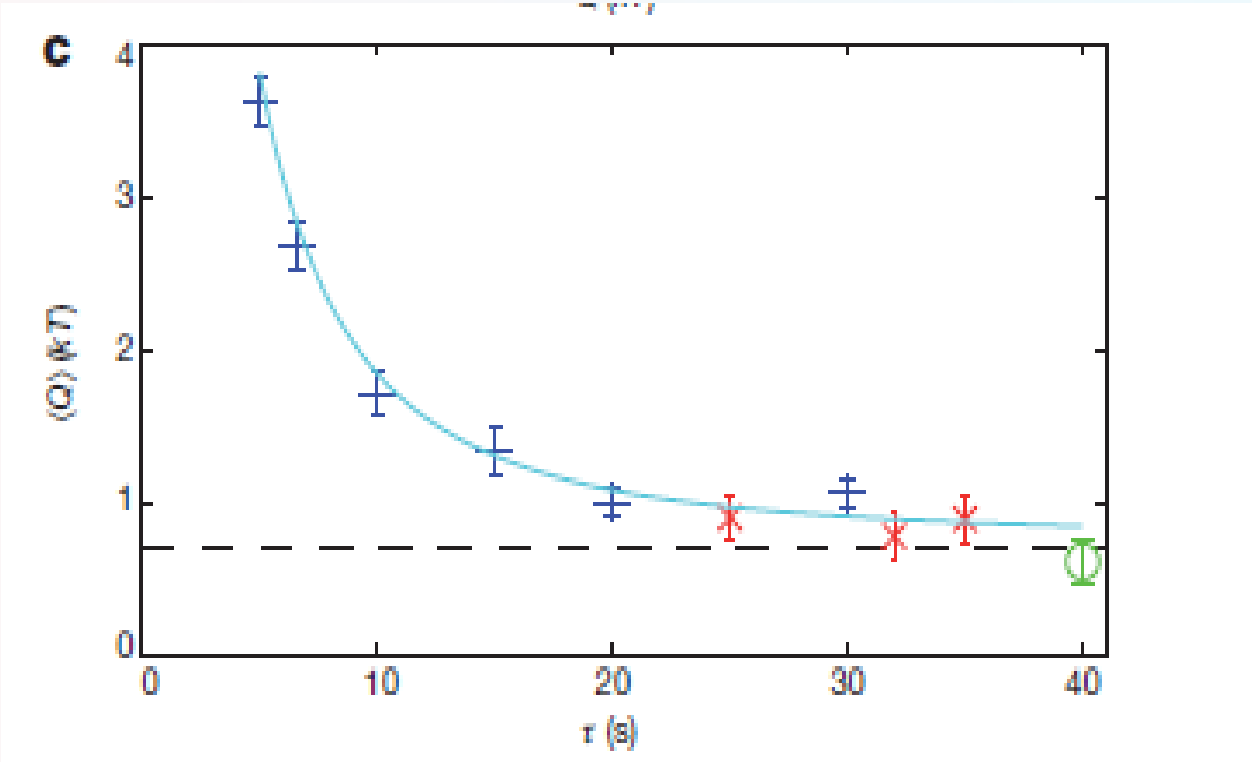
- Heat dissipation exceeds the **Landauer** bound by less than 40% for $t_f = 10s$ and almost 4 times for $t_f = 1s$

- The optimal ˙current velocities describe nascent shocks:



- The model describes an experimental situation where a $2\mu m$ colloidal particle is manipulated by laser tweezers to verify the **Landauer** bound (**Bérut-Arakelyan1-Petrosyan-Ciliberto-Dillenschneider-Lutz** Nature **483** (2012), 187-189)

- The *ad hoc* experimental protocol, that will be improved, needed twice more time to descend to the same heat release as the optimal protocol



(for $t_f = 10s$ the released heat exceeded the **Landauer** bound ~ 2.5 times rather than by 40%)

Generalizations

- The above refinement of the **2nd Law** still holds for the general overdamped **Langevin** evolution with non-conservative forces $\boldsymbol{f} \neq \boldsymbol{\nabla} U$ if

$$Q = \int_0^{t_f} f_i(t, \boldsymbol{x}(t)) \circ dx^i(t)$$

but for the optimal protocol $\boldsymbol{f} = \boldsymbol{\nabla} U$

- If the mobility matrix M depends on $\boldsymbol{x}$ similar results hold with the quadratic form $(y-x) \cdot M^{-1}(y-x)$ in the cost fuction replaced by the distance squared $d(x,y)^2$ in the **Riemannian** metric

$$g = (d\boldsymbol{x}) \cdot M(\boldsymbol{x})^{-1} (d\boldsymbol{x})$$

(optimal transport with such a cost function was used by **Lott-Villani** to prove results in **Riemannian** geometry)

- In the $N \to \infty$ **mean field limit** of the N-particle overdamped **Langevin** dynamics

$$\frac{d\boldsymbol{x}_n}{dt} \;=\; -M\left(\nabla U(t,\boldsymbol{x}_n) + \sum_{m=1}^{N} \frac{1}{N} \boldsymbol{\nabla} V(\boldsymbol{x}_n - \boldsymbol{x}_m)\right) \;+\; \boldsymbol{\eta}_n(t)$$

with i.i.d. white noises $\boldsymbol{\eta}_n$ going between factorized states $\otimes_n \rho_i$ and $\otimes_n \rho_f$ during time t_f, the **total entropy production per particle** satisfies the same lower bound as before

- The mean-field dynamics keeps the factorized form $\otimes_n \rho$ of the state with ρ evolving via the **nonlinear Fokker-Planck equation**

$$\partial_t \rho \,+\, \boldsymbol{\nabla} \cdot (\rho\, \boldsymbol{v}) \;=\; 0 \qquad \text{for} \qquad \boldsymbol{v} = M \boldsymbol{\nabla} (R - U - V * \rho)$$

- The optimal control $U(t,\boldsymbol{x})$ satisfies here the relation

$$U(t,\boldsymbol{x}) \;=\; R(t,\boldsymbol{x}) \;-\; \int V(\boldsymbol{x}-\boldsymbol{y})\, \rho(t,\boldsymbol{y})\, d\boldsymbol{y} \;-\; \Psi(t,\boldsymbol{x})$$

with $\rho,\ R,\ \Psi$ given as before by the optimal transport map

Quantum Stochastic Thermodynamics

- For the quantum **Markovian** evolution

$$\frac{d}{dt}\rho(t) \;=\; \mathcal{L}(t)\,\rho(t)$$

where $\mathcal{L}(t)$ is the time-dependent **Lindblad** super-operator

$$\mathcal{L}\,\rho \;=\; -i[K,\rho] \;+\; \sum_i \tau_i \big(L_i \rho L_i^* \;-\; \tfrac{1}{2} L_i^* L_i \rho \;-\; \tfrac{1}{2} \rho L_i^* L_i \big)$$

such that $\mathcal{L}(t)\,\rho_{th}(t) = 0$ for $\rho_{th}(t) = \frac{1}{Z(t)}\, \mathrm{e}^{-\frac{H(t)}{k_B T}}$ one has

$$S_{sys}(t) \;=\; -k_B\, \ln \rho(t)\,, \qquad \big\langle\, S_{sys}(t) \,\big\rangle \;=\; -k_B\, \mathbf{tr}\, \rho(t)\, \ln \rho(t)$$

$$\Delta S_{env} \;=\; \frac{1}{T} \int_0^{t_f} \mathcal{L}(t)^\dagger H(t)\; dt \;\equiv\; \frac{Q}{T}$$

von Neumann entropy

- The **2nd Law** takes the form

$$\boxed{\big\langle \Delta S_{tot} \big\rangle \;=\; \big\langle \Delta S_{sys} \;+\; \Delta S_{env} \big\rangle \;\geq\; 0}$$

- One may again inquire about the minimum over some reasonable subclasses of time-dependent Markovian evolutions of $\langle \Delta S_{tot} \rangle$, given ρ_i, ρ_f and t_f

- No general results available but a related problem of work minimization was studied for a model of single level **quantum dot** (a **qubit**) in **Esposito-Kawai-Lindenberg-Van den Broeck**: EPL **89** (2010)

- The **Hilbert** space of states of the dot is spanned by $|0\rangle$ (no electron) and $|1\rangle$ (one electron) and the **Lindbladian** obtained in the limit of weak coupling between the dot and the lead electrons corresponds to

$$K = e_0|0\rangle\langle 0| + e_1|1\rangle\langle 1| \qquad L_1 = |0\rangle\langle 1| \qquad L_2 = |1\rangle\langle 0|$$

$$\tau_1 = \frac{\gamma_0}{e^{-\frac{\epsilon-\mu}{k_B T}} + 1}, \qquad \tau_2 = \frac{\gamma_0}{e^{\frac{\epsilon-\mu}{k_B T}} + 1}$$

where $\epsilon(t)$ is the energy of the single level of the dot and μ is the chemical potential of lead electrons

- The thermal **Gibbs** state such that $\mathcal{L}\rho_{th} = 0$ corresponds to the **Hamiltonian**

$$H = \mu|0\rangle\langle 0| + \epsilon|1\rangle\langle 1|$$

(in general $K \neq H$ but $[K, H] = 0$)

- Similar model but with

$$\tau_1 = \frac{\gamma_0}{1 - e^{-\frac{\hbar\omega}{k_B T}}}, \qquad \tau_2 = \frac{\gamma_0}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

describes a 2-level atom in weak interaction with radiation where $\hbar\omega > 0$ is the resonant photon energy

- It is convenient to describe the 2-dimensional density matrices of a **qubit** by the **Bloch** vectors $\vec{v}$ with $|\vec{v}| \leq 1$

$$\rho = \frac{1}{2}\left(1 + \vec{v}\cdot\vec{\sigma}\right) = \frac{1}{2}\begin{pmatrix} 1+v^3 & v^1 - iv^2 \\ v^1 + iv^2 & 1-v^3 \end{pmatrix}$$

with unit vectors corresponding to pure states

- In terms of **Bloch** vectors, the dynamics takes the form

$$\begin{aligned}
\dot{v}^1 &= (e_0 - e_1)v^2 - \frac{1}{2}(\tau_1 + \tau_2)v^1 \\
\dot{v}^2 &= -(e_0 - e_1)v^1 - \frac{1}{2}(\tau_1 + \tau_2)v^2 \\
\dot{v}^3 &= -(\tau_1 + \tau_2)v^3 - \tau_1 + \tau_2
\end{aligned}$$

with

$$\begin{aligned}
\langle \Delta S_{sys} \rangle &= \Big[- \tfrac{1+|\vec{v}|}{2} \ln \big(\tfrac{1+|\vec{v}|}{2}\big) - \tfrac{1-|\vec{v}|}{2} \ln \big(\tfrac{1-|\vec{v}|}{2}\big) \Big]_{t=0}^{t=t_f} \\
\langle \Delta S_{env} \rangle &= \frac{1}{2} k_B \int_0^{t_f} \dot{v}^3 \ln \frac{\tau_2}{\tau_1} \, dt \\
&= \frac{1}{2} k_B \int_0^{t_f} \dot{v}^3 \ln \frac{1 + v^3 + \gamma_0^{-1} \dot{v}^3}{1 - v^3 \mp \gamma_0^{-1} \dot{v}^3} \, dt
\end{aligned}$$

where $\frac{\tau_2}{\tau_1}$ was calculated from the equation for $\dot{v}^3$ with the upper sign corresponding to the quantum dot and the lower one to the 2-level atom

- Minimization of $\langle \Delta S_{env} \rangle$ over controls $\epsilon(t)$ or $\hbar\omega(t)$ becomes standard mechanical problem

- **Solution** for the **quantum dot**:

$$\langle \Delta S_{env} \rangle_{min} = \frac{1}{2} k_B \left(G_{\pm}(v_f^3) - G_{\pm}(v_i^3) \right)$$

for $G_{\pm}(x) = x \ln \frac{K+1+x \pm \sqrt{K(K+1-x^2)}}{K+1-x \mp \sqrt{K(K+1-x^2)}} \pm \ln \frac{K+1+x+\sqrt{K(K+1-x^2)}}{K+1-x+\sqrt{K(K+1-x^2)}}$

$$\pm 2\sqrt{K} \arctan \frac{x}{\sqrt{K+1-x^2}} + 2 \ln(1 \mp x) .$$

with the upper sign for $v_f^3 > v_i^3$ and the lower one for $v_f^3 < v_i^3$ and $K > 0$ is obtained from the limiting values of v^3 via the relation

$$\gamma_0 t_f = F_{\pm}(v_f^3) - F_{\pm}(v_i^3)$$

for $F_{\pm}(x) = -\ln(1 \mp x) \pm \frac{1}{\sqrt{K}} \arctan \frac{x}{\sqrt{K+1-x^2}}$

$$\pm \frac{1}{2} \ln \frac{K+1-x+\sqrt{K(K+1-x^2)}}{K+1+x+\sqrt{K(K+1-x^2)}}$$

General remarks

- Dynamics of $v^{1,2}$ is independent of that of v^3, in particular,

$$|v^1|^2 + |v^2|^2 = \mathrm{e}^{-\gamma_0 t}\left(|v_i^1|^2 + |v_i^2|^2\right)$$

  hence not all ρ_i and ρ_f may be connected by interpolating dynamics in the time window $[0, t_f]$

- Even for diagonal states a minimal time to join them is required:

$$\gamma_0 t_f^{min} = \begin{cases} \ln \frac{1-v_i^3}{1-v_f^3} & \text{if} \quad v_i^3 < v_f^3 \,, \\ \ln \frac{1+v_i^3}{1+v_f^3} & \text{if} \quad v_i^3 > v_f^3 \,, \end{cases}$$

  (this also holds in the bosonic case of 2-state atom if $0 \geq v_i^3 > v_f^3$)

- For long times

$$\langle \Delta S_{env} \rangle_{min} = \left[\frac{1+v^3}{2} \ln\left(\frac{1+v^3}{2}\right) + \frac{1-v^3}{2} \ln\left(\frac{1-v^3}{2}\right) \right]_{t=0}^{t=t_f} + O(t_f^{-1})$$

and $\lim_{t_f \to \infty} \langle \Delta S_{tot} \rangle_{min} > 0$ if $\rho_{i,f}$ are not diagonal whereas $\langle \Delta S_{tot} \rangle_{min} = O(t_f^{-1})$ at long times for diagonal states

- The memory erasure going from the initial mixed or pure state

$$\rho_i = \begin{cases} \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) \\ \frac{1}{2}(|0\rangle + |1\rangle)(\langle 0| + \langle 1|) \end{cases}$$

to the final pure state $\rho_f = |0\rangle\langle 0|$ with $\langle \Delta S_{sys} \rangle = \begin{cases} -k_B \ln 2 \\ 0 \end{cases}$ dissipates at least $k_B T \ln 2$ of heat but requires infinite time

- The case of the 2-state atom is more difficult to analyze but the last point still holds

Conclusions and further problems

- For the overdamped **Langevin** evolution between two fixed statistical states, the minimal total **entropy production** is equal to $\frac{1}{t_f T}$ times the minimal quadratic cost of deterministic transport of the states
- The result implies a finite-time correction to the **Landauer** bound for the heat release during memory erasure possibly relevant for future computer design
- For the evolution between **Gibbs** states, the optimal protocol requires initial and final jumps of the potential and this is still true for the qubit
- Similar question underlying **Finite-Time Thermodynamics** may be studied for other non-equilibrium classical and quantum evolutions
- For underdamped **Langevin** processes (**Gomez-Marin-Schmiedl-Seifer** 2008) or for jump **Markov** processes (**Mejìa-Monasterio-Muratore -Ginanneschi-Peliti** 2012) they lead to **stochastic Bellman equations**

It is, of course, apparent that both the thermal noise and the requirements for energy dissipation are on a scale which is entirely negligible in present-day computer components. The dissipation as calculated, however, is an absolute minimum. Actual devices which are far from minimal in size and operate at high speeds will be likely to require a much larger energy dissipation to serve the purpose of erasing the unnecessary details of the computer's past history.

Rolf Landauer

in "*Irreversibility and Heat Generation in the Computing Process*",

IBM Journal of Res. and Dev. **5:3** (1961)

Today's silicon-based microprocessor chips rely on electric currents, or moving electrons, that generate a lot of waste heat. But microprocessors employing nanometer-sized bar magnets like tiny refrigerator magnets for memory, logic and switching operations theoretically would require no moving electrons.

Such chips would dissipate only 18 millielectron volts of energy per operation at room temperature, the minimum allowed by the second law of thermodynamics and called the Landauer limit. That's 1 million times less energy per operation than consumed by today's computers.

Robert Sanders

from public release, University of California - Berkeley,
July 1, 2011