Fluctuation relations and some applications

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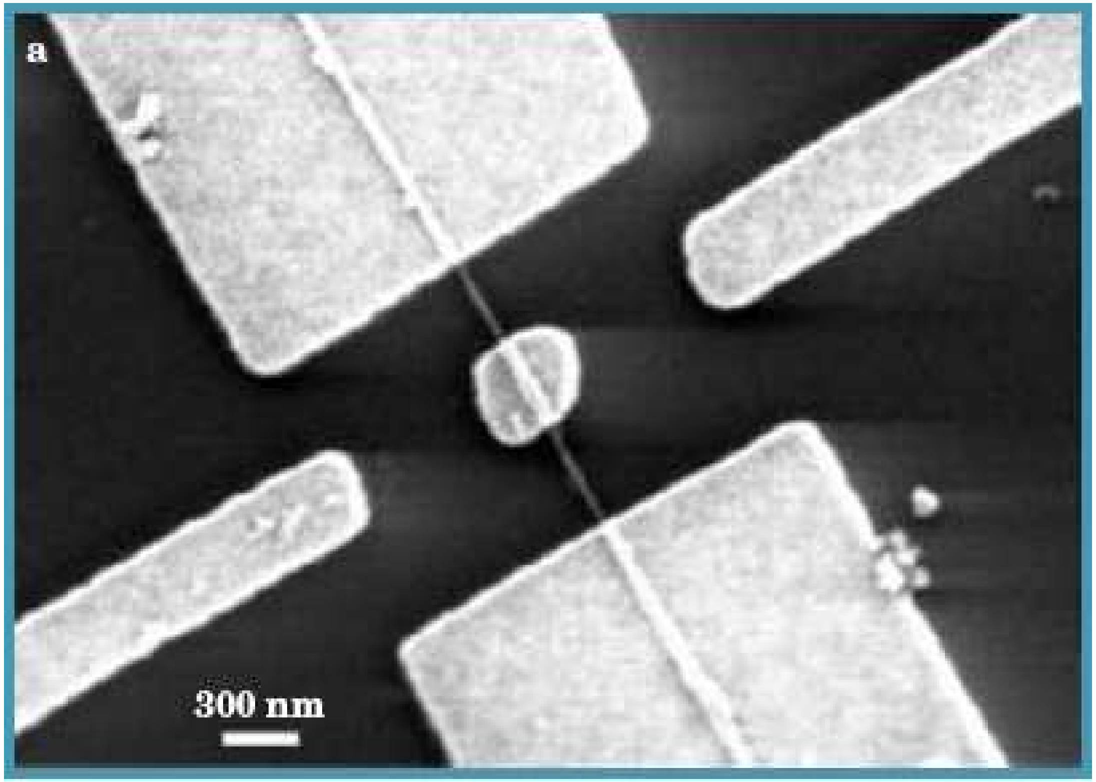
Summary

- Small systems
- Generalized second law: The Hasano-Sasa relation
- Microscopic reversibility and Loschmidt's paradox
- The "time-reversal" identities and the fluctuation theorems
- Exploiting the Jarzynski relation: The histogram method
- Exploring driven systems: The cloning technique
- Perspectives

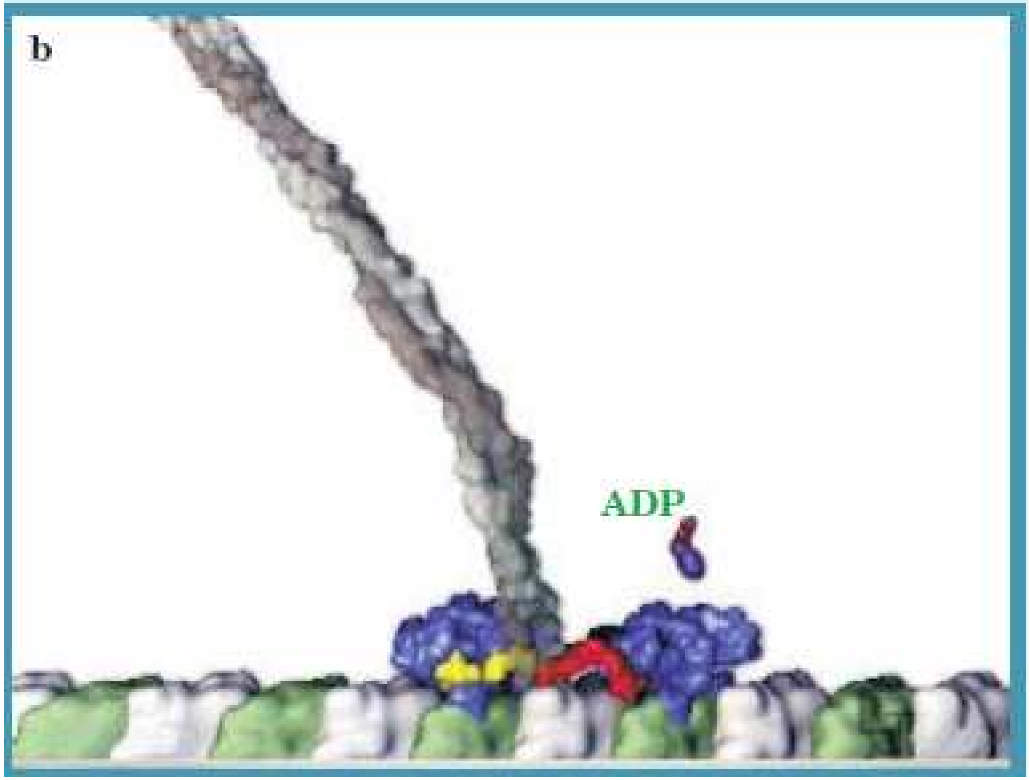
Small systems: Artificial nanomachines



A metal-plate rotor attached to a multiwalled nanotube

Fennimore et al., 2003

Small systems: Natural nanomachines



The kinesin-microtubule system: one 8-nm step every 10–15 ms

ATP $\longrightarrow$ ADP + P + $\sim 20\,T$ ($k_{\rm B} = 1$)

Typically $\Delta W \sim 12\,T$, efficiency $\sim$ 60%   Dissipated power: $\sim 20\,T$ per second

Milligan Laboratory, Scripps Research Institute

Evolution equation

$P(x,t)$: pdf of microstate x

$$\frac{\partial P}{\partial t} = \widehat{L}_{\mu(t)}\, P$$

$\widehat{L}_{\mu}$: Liouville operator depending on parameter μ
Manipulation: $t \longrightarrow \mu(t)$, $0 \leq t \leq t_{\mathrm{f}}$, $\mu(0) = 0$
Steady state: for each μ,

$$\widehat{L}_{\mu}\, P_{\mu}^{\mathrm{SS}} = 0, \qquad \forall \mu$$

The Hatano-Sasa relation

$\phi(x,\mu)$: "Steady state hamiltonian"

$$\phi(x,\mu) = -\ln P_\mu^{\mathrm{SS}}(x)$$

Define

$$A(t) = \int_0^t \mathrm{d}t' \; \dot{\mu}(t') \; \frac{\partial \phi}{\partial \mu}\bigg|_{\mu(t'),x(t')}$$

Then, if the pdf is P_0^{SS} at $t = 0$,

$$\boxed{P_{\mu(t)}^{\mathrm{SS}}(x) = \left\langle \delta(x - x(t))\, \mathrm{e}^{-A(t)} \right\rangle}$$

Average over initial condition and noise

Hatano and Sasa, 2001

Conservative forces: The Jarzynski relation

For conservative forces

$$
\begin{aligned}
\phi(x,\mu) &= \frac{E(x,\mu)-F_\mu}{T} \\
\mathrm{d}A(t) &= \frac{1}{T}\,\dot\mu(t)\;\frac{\partial(E-F)}{\partial\mu}\bigg|_{\mu(t),x(t)} \\
&= \frac{1}{T}\,\dot\mu(t)\;\frac{\partial E}{\partial\mu}\bigg|_{\mu(t),x(t)} - \frac{1}{T}\,\mathrm{d}F_{\mu(t)} = \frac{1}{T}\,(\mathrm{d}W-\mathrm{d}F)
\end{aligned}
$$

$$
\left\langle \delta(x-x(t))\,\mathrm{e}^{-W/T}\right\rangle = \mathrm{e}^{-(E(x,\mu(t))-F_0)/T} = \boxed{P^{\mathrm{eq}}_{\mu(t)}(x)\,\frac{Z_{\mu(t)}}{Z_0}}
$$

Jarzynski, 1997

Proof

Consider the joint pdf $\Phi(x, A, t)$ of x and A
Evolution equation for Φ:

$$\frac{\partial \Phi}{\partial t} = \widehat{L}_\mu \, \Phi + \dot{\mu} \, \frac{\partial \phi}{\partial \mu} \, \frac{\partial \Phi}{\partial A}$$

Define

$$\Psi(x, t) = \int \mathrm{d}A \, \mathrm{e}^{-A} \, \Phi(x, A, t)$$

Then

$$\frac{\partial \Psi}{\partial t} = \widehat{L}_\mu \, \Psi - \dot{\mu} \, \frac{\partial \phi}{\partial \mu} \, \Psi = \frac{\partial}{\partial t} \, \mathrm{e}^{-\phi(x,\mu(t))}$$

Driven Brownian particle

Langevin equation:

$$m\ddot{r}_i = -\gamma \dot{r}_i - \frac{\partial U}{\partial r_i} + f_i + \eta_i(t)$$

$$\langle \eta_i(t) \rangle = 0; \qquad \langle \eta_i(t)\eta_i(t') \rangle = 2\gamma T \delta_{ij}\delta(t-t'), \qquad \forall t, t'$$

Kramers equation ($\dot{r}_i = p_i/m$)

$$\frac{\partial P}{\partial t} = \sum_i \left\{ \left[\frac{\partial}{\partial r_i}\left(-\frac{p_i}{m}\right) P \right] + \frac{\partial}{\partial p_i}\left[\left(\gamma \frac{p_i}{m} + \frac{\partial U}{\partial r_i} - \boldsymbol{f}_i \right) P + \gamma T \frac{\partial}{\partial p_i} P \right] \right\}$$

Energy balance

$$E(x) = E(\vec{r},\vec{p}) = \sum_i \frac{p_i^2}{2m} + U(\vec{r})$$

$$\mathrm{d}E = \underbrace{\left(-\gamma\frac{\vec{p}}{m} + \vec{\eta}(t)\right)\cdot \mathrm{d}\vec{r}}_{-\mathrm{d}Q_{\mathrm{tot}}} + \underbrace{\vec{f}\cdot\mathrm{d}\vec{r} + \frac{\partial E}{\partial \mu}\,\mathrm{d}\mu}_{\mathrm{d}W_{\mathrm{ext}}}$$

$$\mathrm{d}Q_{\mathrm{tot}} = \mathrm{d}Q_{\mathrm{ex}} + \underbrace{\left(\vec{f} - \frac{\partial U}{\partial \vec{r}} + T\frac{\partial \phi}{\partial \vec{r}}\right)\cdot\mathrm{d}\vec{r} + \left(-\frac{p}{m} + T\frac{\partial\phi}{\partial\vec{p}}\right)\cdot\mathrm{d}\vec{p}}_{\mathrm{d}Q_{\mathrm{hk}}}$$

$$\mathrm{d}A = \frac{\partial\phi}{\partial\mu}\,\dot{\mu}\,\mathrm{d}t = \frac{\mathrm{d}Q_{\mathrm{ex}}}{T} + \mathrm{d}\phi$$

Generalized Second Law

$$\begin{aligned} 0 &= \ln \mathrm{Tr}\, P^{\mathrm{SS}}_{\mu(t)} \\ &= \ln \langle \exp(-A) \rangle = \ln \left\langle \exp\left(-\frac{Q_{\mathrm{ex}}}{T} - \Delta\phi \right) \right\rangle \\ &\leq -\frac{1}{T} \langle Q_{\mathrm{ex}} \rangle - \Delta \langle \phi \rangle \end{aligned}$$

$$\langle \phi \rangle = -\,\mathrm{Tr} \ln P^{\mathrm{SS}}\, P^{\mathrm{SS}} = S\left[P^{\mathrm{SS}} \right]$$

$$\boxed{T\,\Delta S \geq -\langle Q_{\mathrm{ex}} \rangle}$$

Entropy balance

Local entropy:

$$s(x,t) = -\ln P(x,t)$$

Crooks,1999; Qian, 2002

$$\mathrm{d}Q_{\mathrm{tot}} = \mathrm{d}Q_1 + \underbrace{\left(\vec{f} - \frac{\partial U}{\partial \vec{r}} + T\frac{\partial s}{\partial r}\right) \cdot \mathrm{d}\vec{r} + \left(-\frac{p}{m} + T\frac{\partial s}{\partial p}\right) \cdot \mathrm{d}\vec{p}}_{\mathrm{d}Q_2}$$

$$\boxed{\left\langle \frac{\mathrm{d}Q_1}{T} \right\rangle = \mathrm{d}s}$$

Loschmidt's paradox

Thomson (1874) and Loschmidt (1876):

> To every initial state x_0 of a mechanical system leading to a decrease in Boltzmann's H function, corresponds an initial state $\mathrm{I}\,x_0$ leading to its increase

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In small systems, transient increases of Boltzmann's H are to be expected

Microscopic reversibility I

Mechanical system described by $x = (p, r)$

Time reversal operator: $\mathrm{I}\, x = (-p, r)$

Time-reversal invariance of the hamiltonian: $E(\mathrm{I}\, x) = E(x)$

Solution of the equations of motion:

$$x(t, x_0) : \qquad (\dot{p}, \dot{r}) = \left(-\frac{\partial E}{\partial r}, \frac{\partial E}{\partial p} \right)$$

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Time reversal of the trajectories

The time-reversed trajectory $\mathrm{I}\, x(t, \mathrm{I}\, x_0)$ is also a solution:

$$\mathrm{I}\, x(t, \mathrm{I}\, x_0) = \mathrm{I}\, x(-t, x_0)$$

Microscopic reversibility II

Stochastic evolution equation for the pdf $P(x,t)$:

$$\frac{\partial P}{\partial t} = \widehat{L}_\mu \, P$$

Microscopic reversibility:

$$\mathcal{Q}\,\psi(x) = \mathrm{e}^{-E(x)/T}\,\psi(\mathrm{I}\,x) : \qquad \mathcal{Q}^{-1}\widehat{L}\mathcal{Q} = \widehat{L}^\dagger$$

For the Kramers equation with non-conservative force $\vec{f}$:

$$\mathcal{Q}^{-1}\widehat{L}\mathcal{Q} = \widehat{L}^\dagger - \frac{\vec{f}}{T}\cdot\left(\frac{\vec{p}}{m}\right)$$

Observations

- I speak of Boltzmann's H and not of the entropy: H is a dynamic observable and the entropy is not
- Typically the probability of a fluctuation is $\propto \mathrm{e}^{-\mathcal{F}/T}$
- Thus a system is “small” if free energy differences are $\mathrm{O}\left(T\right)$

The time-reversal relation

Evolution operator:

$$\mathcal{U}(t,t_0) = \mathrm{T}\exp\left(\int_{t_0}^{t} \mathrm{d}t'\ \widehat{L}_{\mu(t')}\right)$$

$$\widetilde{\mathcal{U}}(t,t_0) := \mathcal{Q}_t^{-1}\mathcal{U}(t,t_0)\mathcal{Q}_{t_0}$$

satisfies

$$\begin{aligned}\frac{\partial}{\partial t}\widetilde{\mathcal{U}}(t,t_0) &= \dot{\mathcal{Q}}_t^{-1}\mathcal{U}(t,t_0)\mathcal{Q}_{t_0} + \mathcal{Q}_t^{-1}\widehat{L}_{\mu(t)}\mathcal{Q}_t\widetilde{\mathcal{U}}(t,t_0) \\ &= \left[\frac{\partial E/T}{\partial t} + \widehat{L}^{\dagger}_{\mu(t)} - \frac{\vec{f}}{T}\cdot\frac{\vec{p}}{m}\right]\widetilde{\mathcal{U}}(t,t_0)\end{aligned}$$

Transition probabilities for short time intervals

$$\mathcal{Q}^{-1}_{t+\Delta t}\mathcal{U}(x',t+\Delta t;x,t)\,\mathcal{Q}_t$$
$$= \mathrm{e}^{((E(x',t+\Delta t)-E(x,t))/T}\mathcal{U}(\mathrm{I}\,x',t+\Delta t;\mathrm{I}\,x,t)$$
$$= \mathcal{U}(x,t+\Delta t;x',t)\ \exp\left[-\left(\frac{\vec{f}}{T}\cdot\frac{\vec{p}}{m}-\frac{\partial E(x')}{\partial t}\right)\Delta t\right]$$

$$\frac{\mathcal{U}(x',t+\Delta t;x,t)}{\mathcal{U}(\mathrm{I}\,x,t+\Delta t;\mathrm{I}\,x',t)}$$
$$= \exp\left[\left(\vec{f}\cdot\frac{\vec{p}}{m}\,\Delta t-\frac{\partial E}{\partial x}\,(x'-x)/T\right)\right]$$
$$= \exp\left(\mathrm{d}Q_2/T\right)$$

Crooks's reversal relation

A path is coarsely defined by the "gates"

$$\omega = (x_0, 0) \longrightarrow (x_1, t_1) \longrightarrow \cdots$$
$$\cdots \longrightarrow (x_{k-1}, t_{k-1}) \longrightarrow (x_k = x, t_k = t)$$

Then

$$\frac{P(\omega, \mu | x_0, 0)}{P(\widetilde{\omega}, \widetilde{\mu} | \mathrm{I}\, x, t)} = \left\langle \exp\left(\int_0^t \frac{\mathrm{d}Q_2}{T} \right) \right\rangle$$

where

$$\widetilde{\omega} = (\mathrm{I}\, x, t_0) \longrightarrow (\mathrm{I}\, x_{k-1}, \tilde{t}_{k-1}) \longrightarrow \cdots \longrightarrow (\mathrm{I}\, x_1, \tilde{t}_1) \longrightarrow (\mathrm{I}\, x_0, t)$$

$\tilde{t}_k = t - t_k$, $\widetilde{\mu}(t) = \mu(\tilde{t})$

Average over all paths $x(t)$ conditioned by the gates

Seifert's relation

Continuous limit: paths $\omega = x(t)$, $\forall t$
Arbitrary initial pdf's $p_0(x_0)$ for ω **and** $p_1(\mathrm{I}\, x)$ for $\widetilde{\omega}$:

$$R[\omega, p_0, p_1] \;:=\; \ln \frac{P(\omega, \mu | x_0, 0) p_0(x_0)}{P(\widetilde{\omega}, \tilde{\mu} | \mathrm{I}\, x, t) p_1(\mathrm{I}\, x)} \;=\; \int_0^t \frac{\mathrm{d}Q_2}{T} + \ln \frac{p_0(x_0)}{p_1(x_1)}$$

Averaging over the paths

$$\left\langle \mathrm{e}^{-R} \right\rangle \;=\; \mathrm{Tr}\, P(\omega, \mu | x_0, 0) p_0(x_0)\, \mathrm{e}^{-R} \;=\; \mathrm{Tr}\, P(\widetilde{\omega}, \tilde{\mu} | \mathrm{I}\, x, t) p_1(\mathrm{I}\, x) = 1$$

A first fluctuation theorem

1. Entropy production must sometimes be negative!
2. Take $p_0(x,0)$ arbitrary, $p_1(x) = P(x,t)$ (starting from this initial condition)

$$R = \int \frac{\mathrm{d}Q_2}{T} - \Delta s = \int \frac{\mathrm{d}Q_{\mathrm{tot}}}{T} = \Delta s_{\mathrm{tot}}$$

Thus

$$\boxed{\frac{P(\Delta s_{\mathrm{tot}})}{P(-\Delta s_{\mathrm{tot}})} = \mathrm{e}^{\Delta s_{\mathrm{tot}}}}$$

The Gallavotti-Cohen fluctuation theorem

3. In particular for $\mu(t) =$ const., $p_0(x) = p_1(x) = P^{\mathrm{SS}}_{\mu}(x)$:

$$R \simeq \frac{\dot{Q}_2}{T} t = \sigma t$$

$$\boxed{\frac{P(\sigma)}{P(-\sigma)} = \mathrm{e}^{\sigma t}}$$

Gallavotti and Cohen, 1995

Back to Jarzynski

4. Take $p_0 = \exp(-(E_{\mu(0)} - F_{\mu(0)})/T)$ and $p_1 = \exp(-(E_{\mu(t)} - F_{\mu(t)})/T)$. Then

$$\begin{aligned} R &= \Delta S_m + \left[\left(E(x,t) - F_{\mu(t)}\right) - \left(E(x,0) - F_{\mu(0)}\right)\right]/T \\ &= W_\mathrm{d}/T \end{aligned}$$

Thus

$$1 = \left\langle \mathrm{e}^{-W_\mathrm{d}/T} \right\rangle = \left\langle \mathrm{e}^{-W/T} \right\rangle \mathrm{e}^{\Delta F/T}$$

Evaluation of free-energy landscapes

$$\begin{aligned}\mathcal{F}_0(M) &= -T \ln \mathrm{Tr}\, \delta(M - M(x))\, \mathrm{e}^{-E_0(x)/T} \\ Z_0 &= \int \mathrm{d}M\ \mathrm{e}^{-\mathcal{F}_0(M)/T} = \mathrm{Tr}\, \mathrm{e}^{-E_0(x)/T}\end{aligned}$$

Manipulation: $t \longrightarrow E_{\mu(t)}(x)$, $E_{\mu(0)}(x) = E_0(x)$,

$$E_\mu(x) = E_0(x) + U_\mu(M(x))$$

The basic identity

A. Imparato and L. Peliti, 2005

$$\left\langle \delta(M - M(x)) \mathrm{e}^{-\beta W} \right\rangle_t = \int \mathrm{d}x \, \delta(M - M(x)) \frac{\mathrm{e}^{-\beta E_{\mu(t)}(x)}}{Z_0}$$
$$= \mathrm{e}^{-(\mathcal{F}_0(M) - F_0)/T} \mathrm{e}^{-U_{\mu(t)}(M)/T}$$

Generalization of Hummer and Szabo, 2001

The histogram method

Thus

$$\mathrm{e}^{U_{\mu(t)}(M)/T}\left\langle\delta(M-M(x))\mathrm{e}^{-W/T}\right\rangle_t=\mathrm{e}^{-(\mathcal{F}_0(M)-F_0)/T}$$

$\mathcal{N}$ trajectories (M_t^k, W_t^k), sampled at discrete times t_j
Discrete bins $M_\ell \leq M \leq M_\ell + \Delta M_\ell$

$$\begin{aligned}
r(M_\ell, t_j) &= Z_0\,\mathrm{e}^{U_{\mu(t_j)}(M_\ell)/T}\,\overline{\theta_\ell(M(t_j))\mathrm{e}^{-W/T}} \\
&= Z_0\,\mathrm{e}^{U_{\mu(t)}(M_\ell)/T}\,\frac{1}{\mathcal{N}}\sum_{k=1}^{\mathcal{N}}\theta_\ell(M_{t_j}^k)\,\mathrm{e}^{-W_{t_j}^k/T} \\
\Delta R(M_\ell) &= \mathrm{e}^{-(\mathcal{F}_0(M_\ell)-F_0)/T}\,\delta M_\ell=\langle r(M_\ell,t_j)\rangle\,,\quad \forall \ell, j
\end{aligned}$$

The best estimate

$$\Delta R^*(M_\ell) = \sum_j r(M_\ell, t_j) p_j$$

$$0 \le p_j \le 1, \qquad \sum_j p_j = 1$$

Best estimate:

$$p_j = \frac{\lambda}{\mathrm{Var}\, r(M_\ell, t_j)} \propto \frac{\mathrm{e}^{U_{\mu(t_j)}(M_\ell)/T}}{\overline{\mathrm{e}^{-W_{t_j}}}}$$

Braun et al., 2004

A mean-field Ising model

$$\mathcal{F}_0(M) = -\frac{J}{2N}M^2 - TS(M)$$

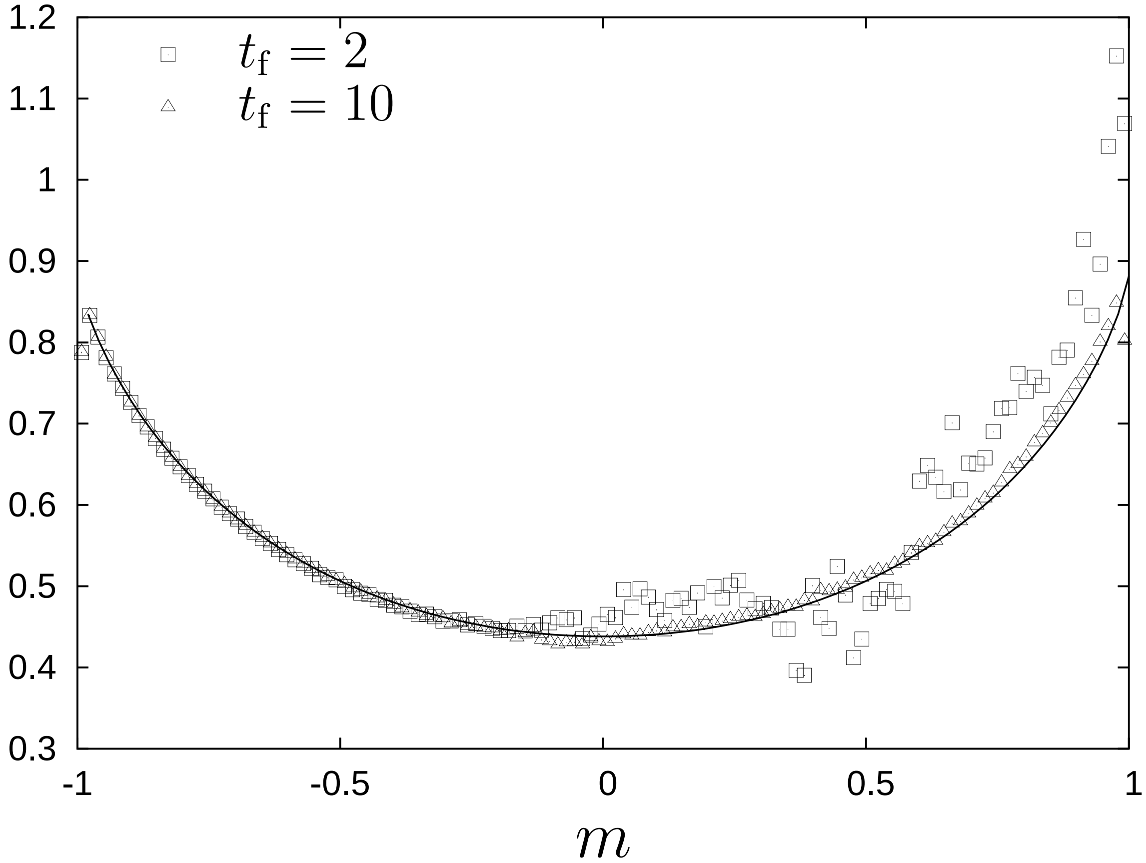
$$S(M) = -\left[\left(\frac{N+M}{2}\right)\log\left(\frac{N+M}{2}\right) + \left(\frac{N-M}{2}\right)\log\left(\frac{N-M}{2}\right)\right]$$

$$U_h(M) = -hM$$

$$m = \frac{M}{N}$$

$$f_0^*(m) = -\frac{T}{N}\ln R^*(M)$$

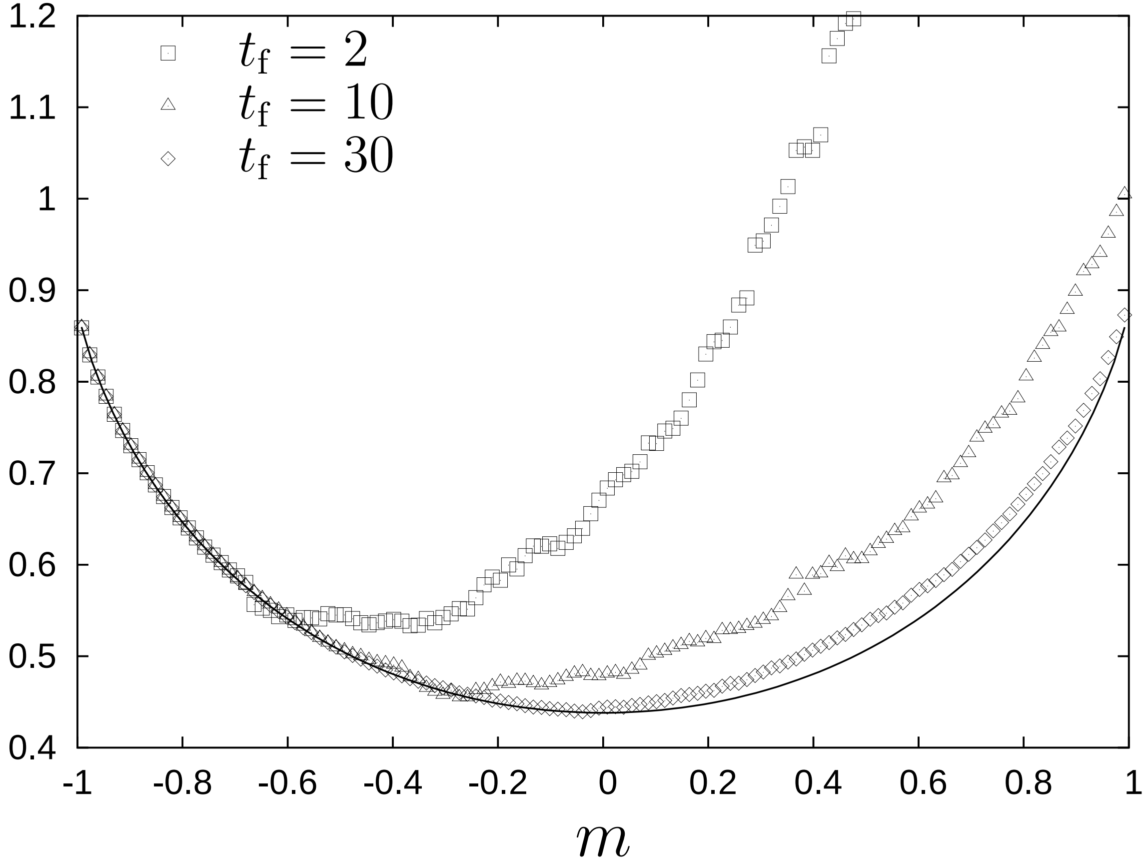
Linear protocol



$h(t) = h_0 + \frac{h_1 - h_0}{t_\mathrm{f}}\, t$

$h_1 = -h_0 = 1$, $t_\mathrm{f} = 2, 10$, $N = 10$, $\mathcal{N} = 10^4$ samples

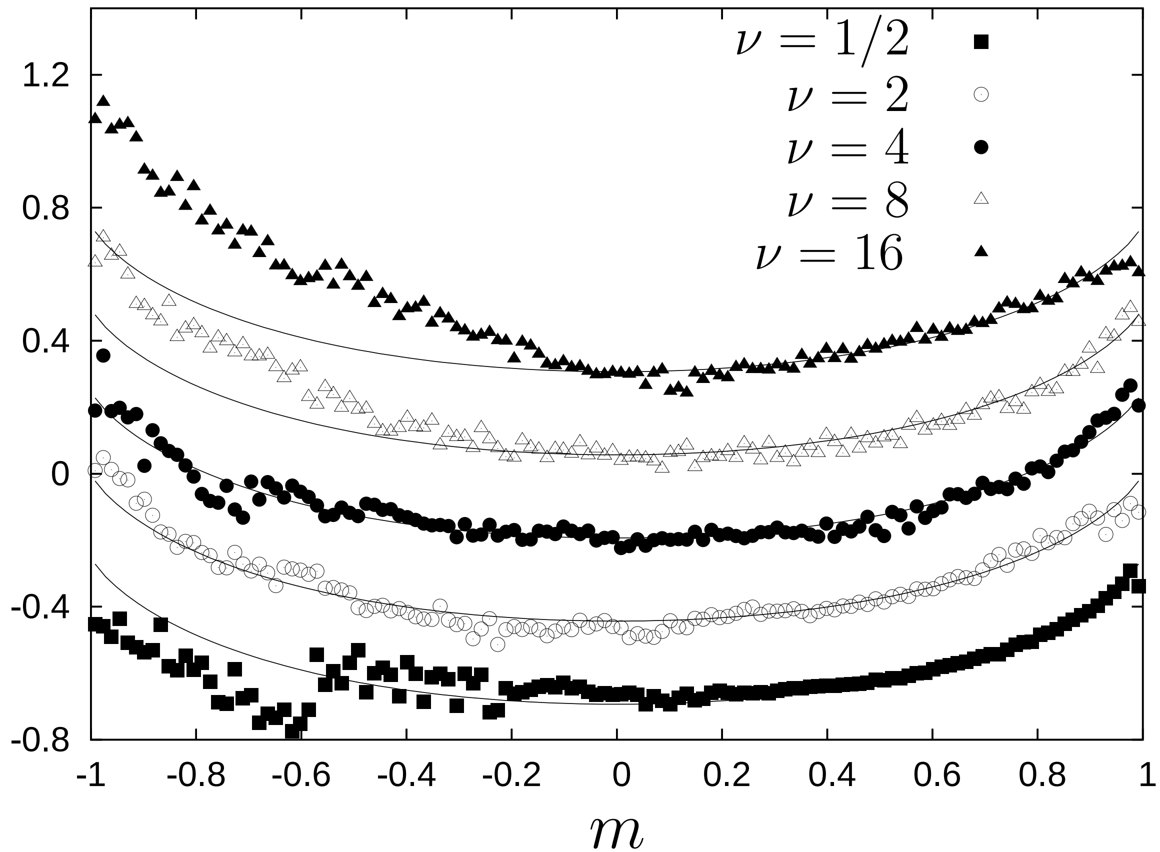
A larger system



$h(t) = h_0 + \frac{h_1 - h_0}{t_f}\, t$

$h_1 = -h_0 = 1$, $t_f = 2, 10$, $N = 100$, $\mathcal{N} = 10^4$ samples

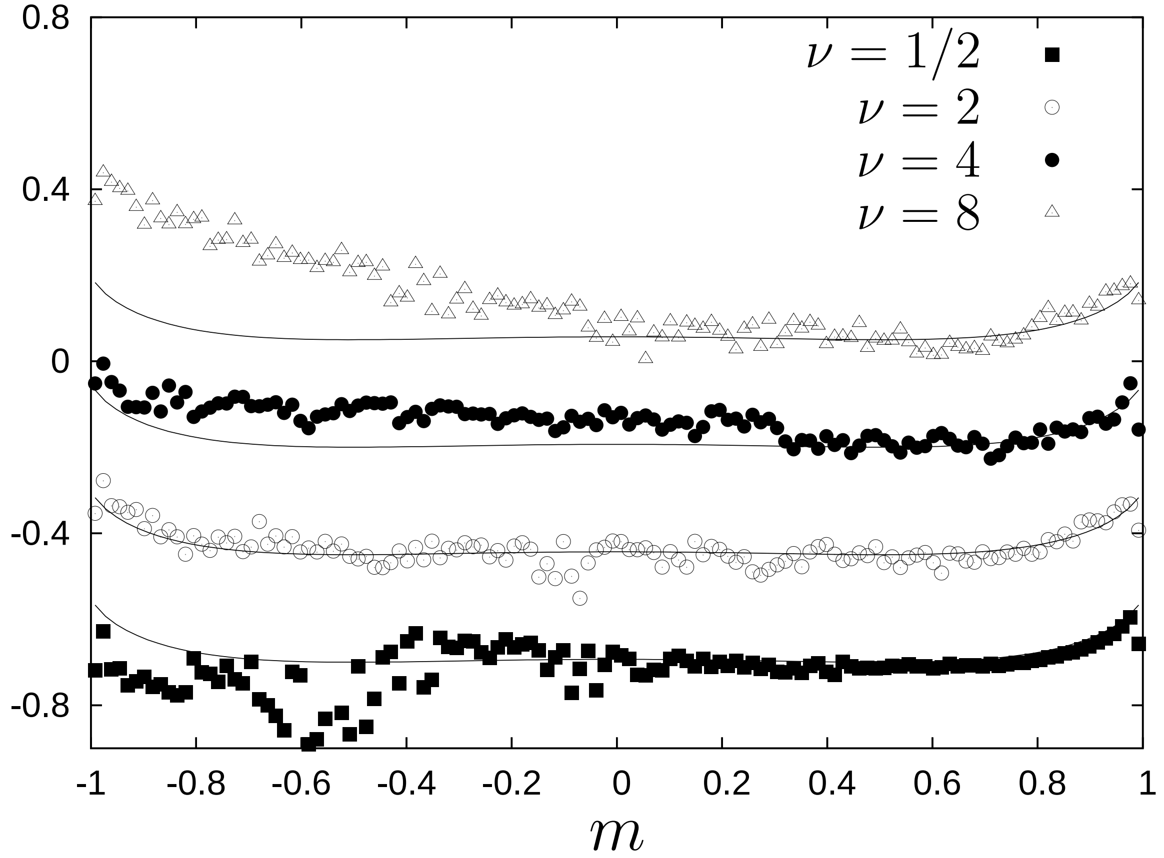
Oscillatory protocol



$h(t) = h_0 \sin(2\pi\nu t), \qquad 0 \leq t \leq t_{\rm f}$

$h_0 = 1$, $N = 10$, $J_0 = 0.5$, $t_{\rm f} = 2$, $\mathcal{N} = 10^4$ samples

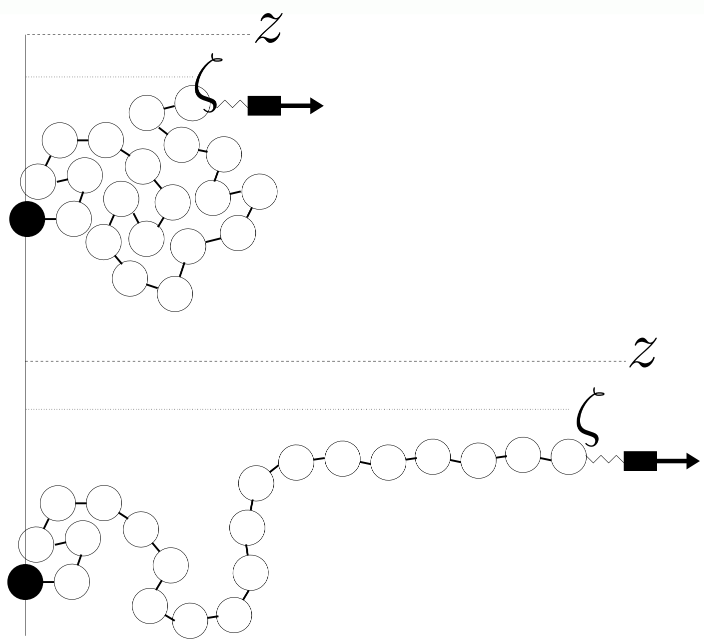
At lower temperatures



$h(t) = h_0 \sin(2\pi\nu t), \qquad 0 \leq t \leq t_{\mathrm{f}}$

$h_0 = 1$, $N = 10$, $J_0 = 1.1$, $t_{\mathrm{f}} = 2$, $\mathcal{N} = 10^4$ samples

Unzipping of a model homopolymer



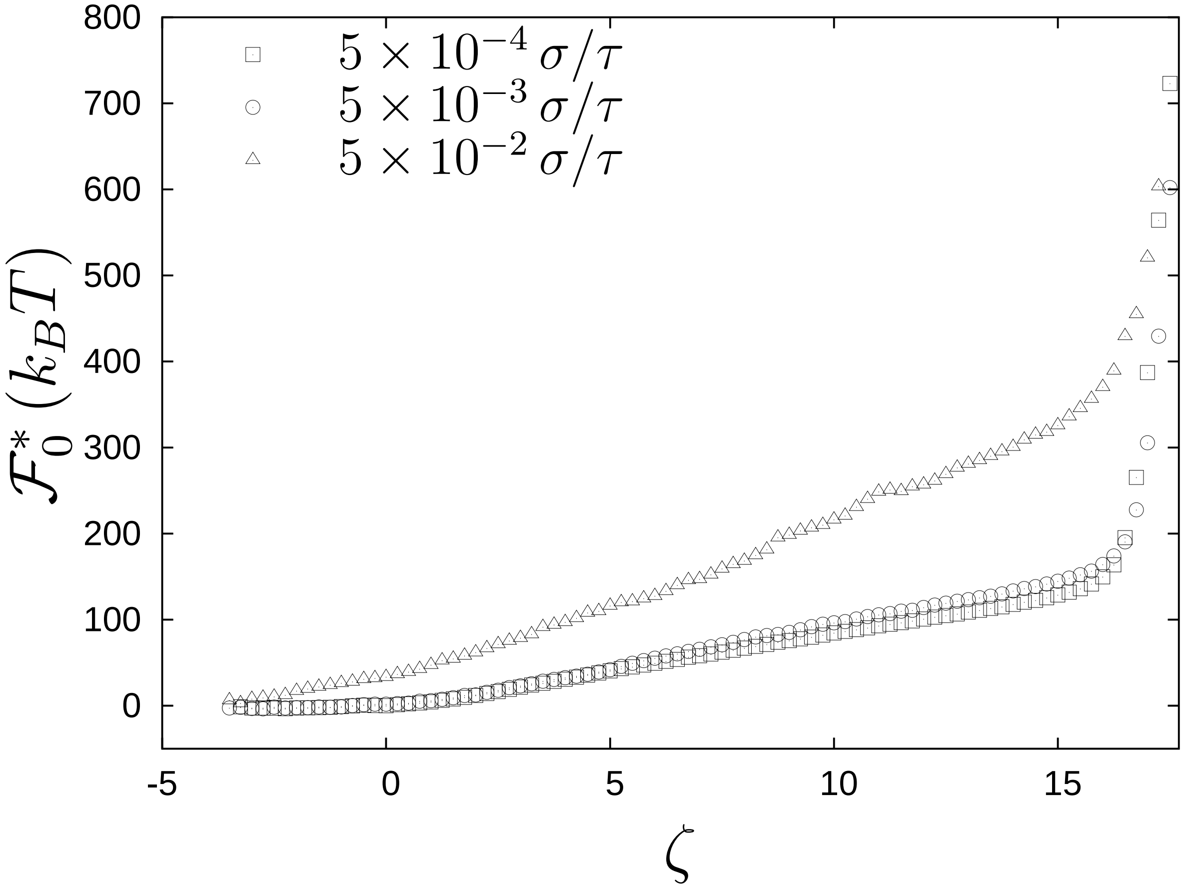
$U_{z(t)(\zeta)} = \frac{1}{2} k \left(\zeta - z(t)\right)^2$

L-J potential (ϵ, σ) + harmonic potential for successive beads

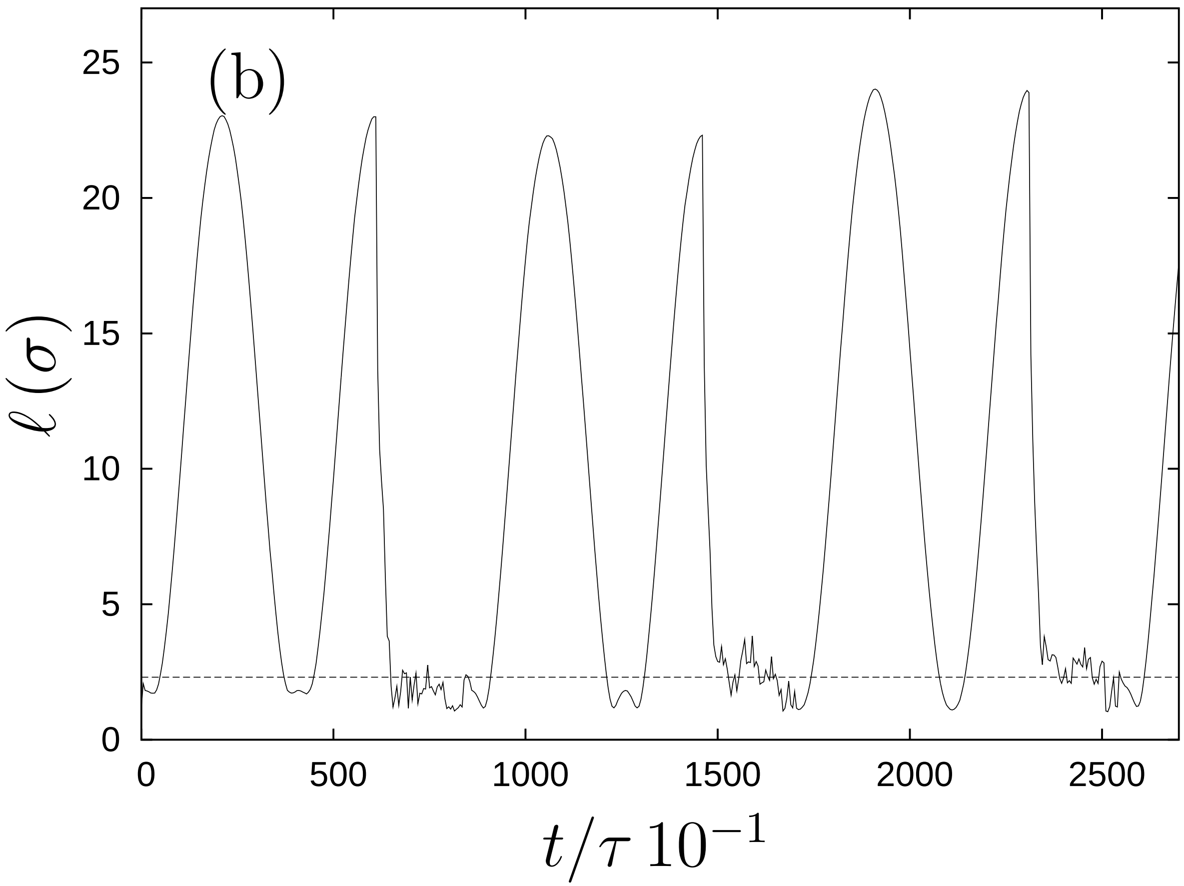
$N = 20$, $\sigma = 0.5$ nm, $\epsilon = 1$ kcal/mol, $m = 3 \cdot 10^{-25}$ kg $\tau = \sqrt{m\sigma^2/\epsilon} \simeq 3.3$ ps,

$\gamma = 15m/\tau$, $k = 5000\epsilon/\sigma^2$, $T = 300$ K

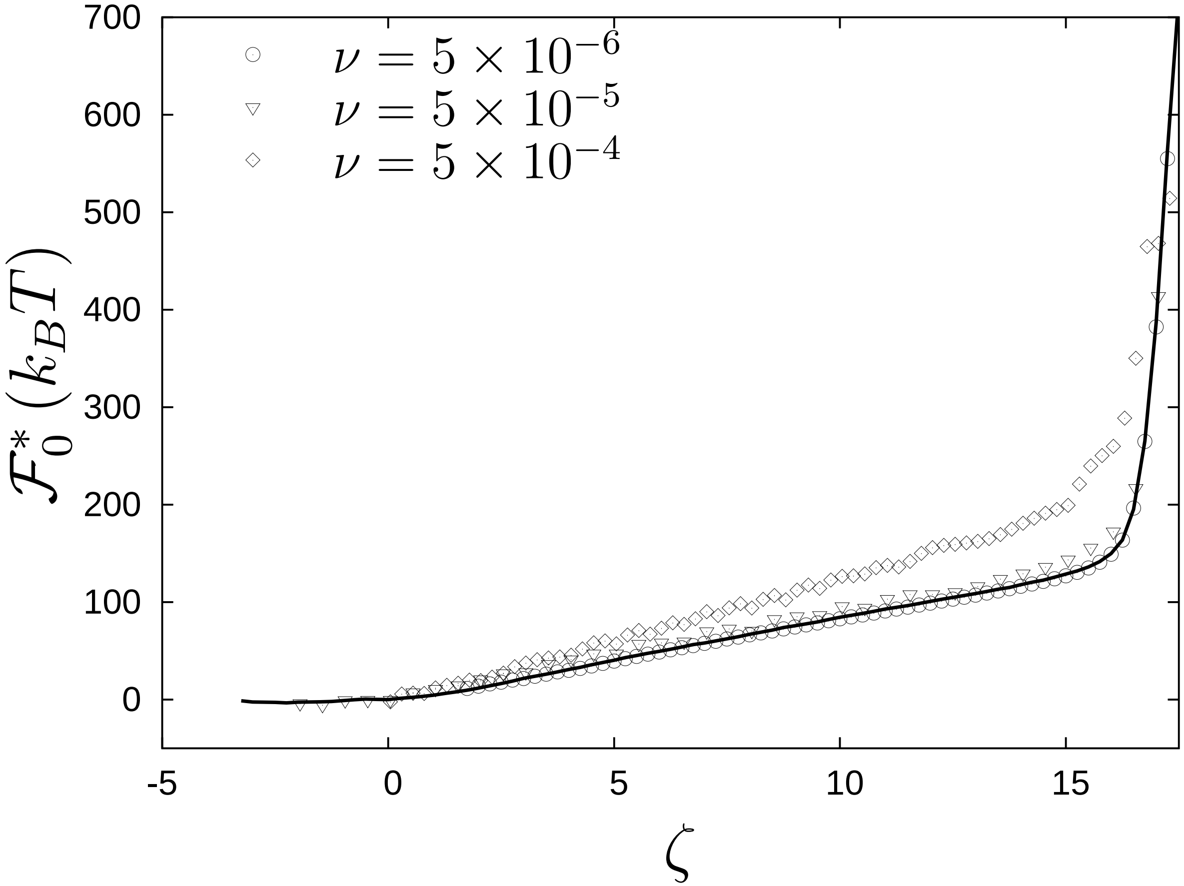
Linear protocol



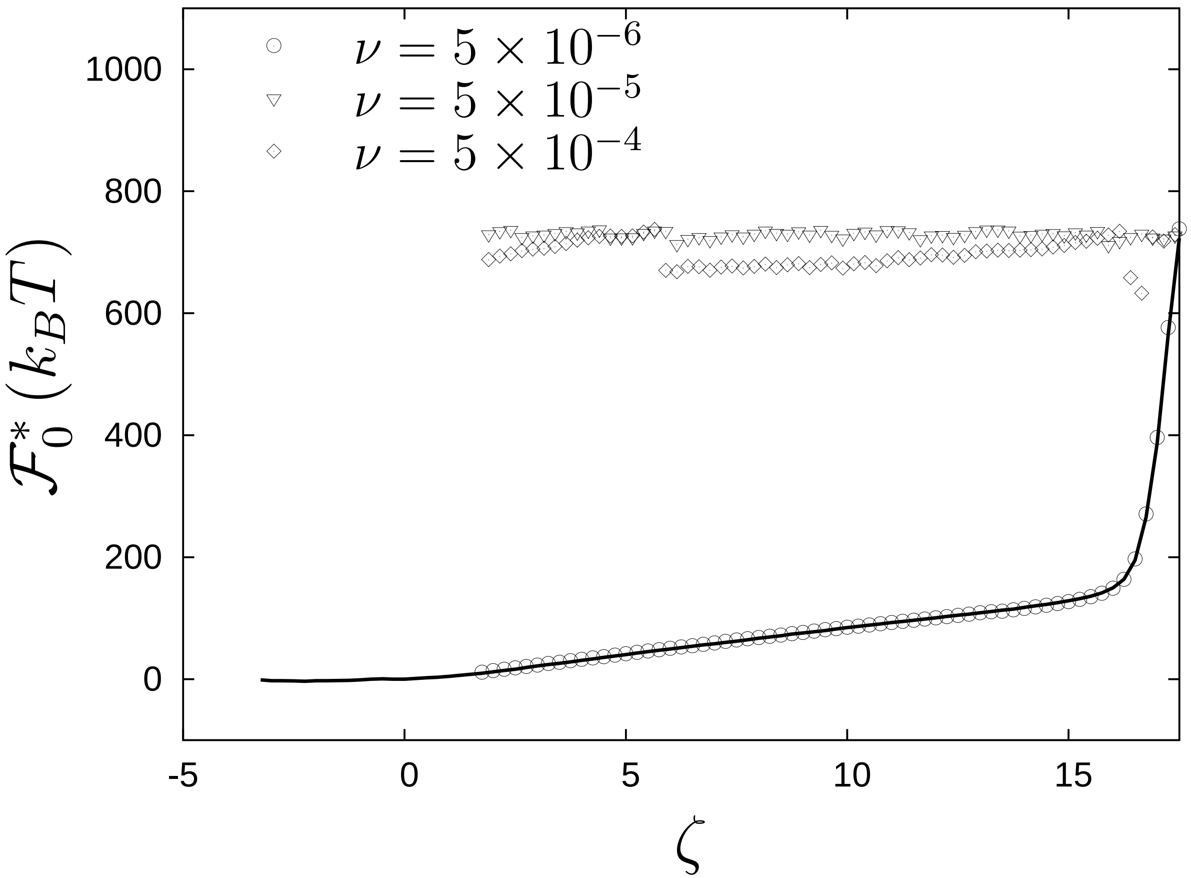
Oscillatory protocol: "Pulsed" protocol



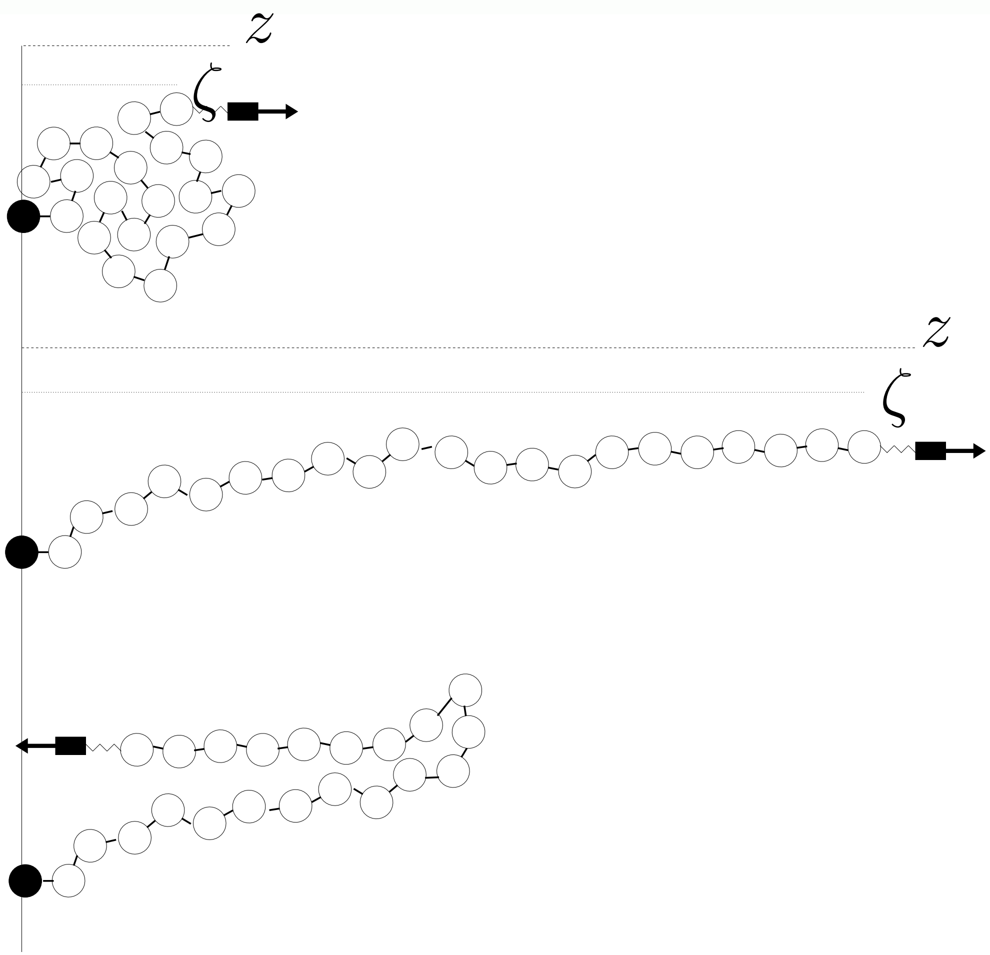
The free energy



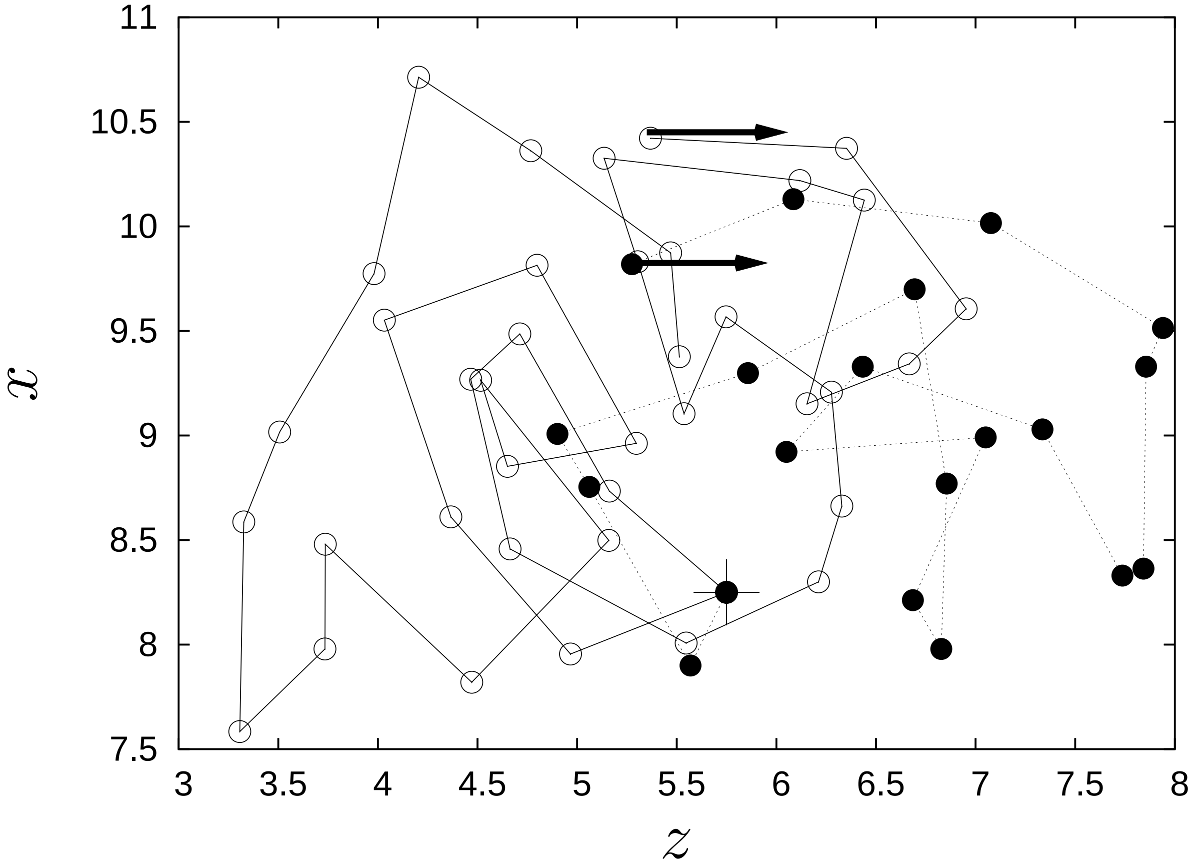
The “always attached” protocol



What is happening?



The configurations



Discussion

- The JE is effective (via the histogram method) to reconstruct free-energy landscapes for systems small enough (small energy barriers)
- Care must be taken that the monitored collective coordinate is “good”, i.e., that the distribution of the *transverse* degrees of freedom is sufficiently sampled during manipulation
- The choice of the manipulation protocol affects the reliability of the results

Exploring nonequilibrium systems

C. Giardinà, J. Kurchan, L. Peliti, 2005

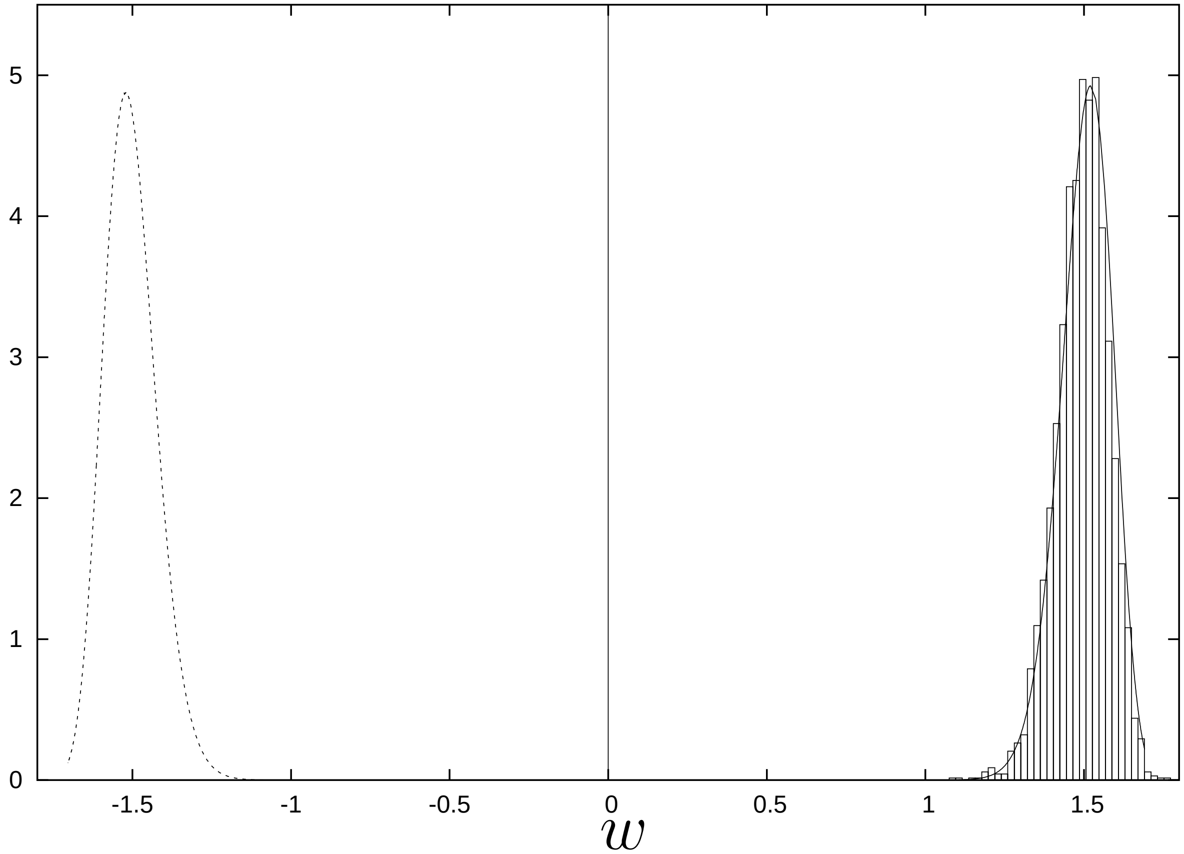
Evolution equations:

$$\frac{\partial \Psi}{\partial t} = \widehat{L}\,\Psi + A\,\Psi$$

Then Ψ is given by a weighted average:

$$\Psi(x,t) = \left\langle \delta(x - x(t)) \exp\left(\int_0^t \mathrm{d}t'\ A(t') \right) \right\rangle$$

The weight can be wild

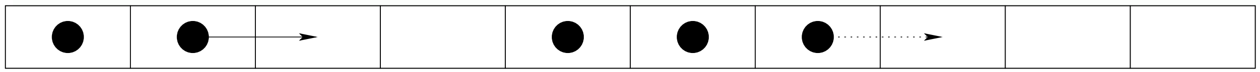


Work distribution $P(W/N)$ for the Ising model
Dashed line: Weighted work distribution $P(W/N)\mathrm{e}^{-W/T}$

Can we improve our statistics?

- Interpret $\Psi(x,t)$ as a density of walkers
- Walkers move according to the Langevin equation
- Walkers reproduce or die depending on the local value of A
- Thus Ψ samples the weighted probability, not the original one!

The Totally Asymmetric Exclusion Process (TASEP)



At any given time step t, a given particle moves to the right with probability α if the target site is empty
Configuration $\mathcal{C} = (n_i)$, $n_i \in \{0, 1\}$, $i = 1, L$, periodic b.c.
Current J:

$$J_{\mathcal{C}'\mathcal{C}} = \begin{cases} 1, & \text{if one particle jumps to the right;} \\ 0, & \text{if nothing happens.} \end{cases}$$

We wish to evaluate

$$\mathrm{e}^{\Lambda(\lambda)} = \left\langle \exp\left(\lambda \sum_t J_{\mathcal{C}_{t+1}\mathcal{C}_t} \right) \right\rangle$$

The large-deviation function

$$\mathrm{Prob}[\mathcal{C}_0, \mathcal{C}_1, \ldots, \mathcal{C}_T] = U_{\mathcal{C}_T \mathcal{C}_{T-1}} \cdots U_{\mathcal{C}_2 \mathcal{C}_1} \cdot U_{\mathcal{C}_1 \mathcal{C}_0}$$

$$\mathrm{e}^{\Lambda(\lambda)} = \sum_{\mathcal{C}_1, \ldots, \mathcal{C}_T} \tilde{U}_{\mathcal{C}_T \mathcal{C}_{T-1}} \cdots \tilde{U}_{\mathcal{C}_1 \mathcal{C}_0} = \sum_{\mathcal{C}_T} \left[\tilde{U}^T \right]_{\mathcal{C}_T \mathcal{C}_0}$$

where

$$\tilde{U}_{\mathcal{C}'\mathcal{C}} := \mathrm{e}^{\lambda J_{\mathcal{C}'\mathcal{C}}} U_{\mathcal{C}'\mathcal{C}}$$

Define

$$K_{\mathcal{C}} := \sum_{\mathcal{C}'} \tilde{U}_{\mathcal{C}'\mathcal{C}}, \qquad U'_{\mathcal{C}'\mathcal{C}} \equiv \tilde{U}_{\mathcal{C}'\mathcal{C}} K_{\mathcal{C}}^{-1}$$

$$\mathrm{e}^{\Lambda(\lambda)} = \sum_{\mathcal{C}_2, \ldots, \mathcal{C}_T} U'_{\mathcal{C}_T \mathcal{C}_{T-1}} K_{\mathcal{C}_{T-1}} \cdots U'_{\mathcal{C}_1 \mathcal{C}_0} K_{\mathcal{C}_0}$$

The simulation steps

- A cloning step:

$$P_{\mathcal{C}}(t+1/2) = K_{\mathcal{C}} P_{\mathcal{C}}(t)$$

$$G \text{ clones of } \mathcal{C} : G = \begin{cases} [K_{\mathcal{C}}]+1, & \text{with probability } K_{\mathcal{C}} - [\\ [K_{\mathcal{C}}], & \text{otherwise} \end{cases}$$

The simulation steps

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- A shift step:

$$P_{\mathcal{C}'}(t+1) = \sum_{\mathcal{C}} U'_{\mathcal{C}'\mathcal{C}} P_{\mathcal{C}}(t+1/2)$$

The simulation steps

- A cloning step:

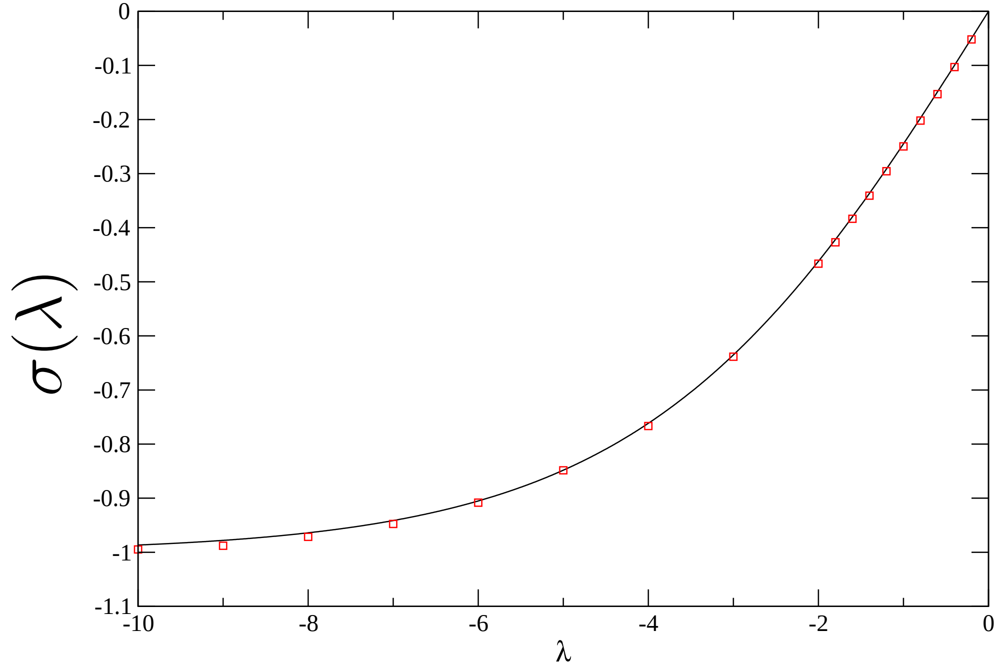
$$P_{\mathcal{C}}(t+1/2) = K_{\mathcal{C}} P_{\mathcal{C}}(t)$$

G clones of $\mathcal{C}$: $G = \begin{cases} [K_{\mathcal{C}}]+1, & \text{with probability } K_{\mathcal{C}} - [K \\ [K_{\mathcal{C}}], & \text{otherwise} \end{cases}$

- A shift step:

$$P_{\mathcal{C}'}(t+1) = \sum_{\mathcal{C}} U'_{\mathcal{C}'\mathcal{C}} P_{\mathcal{C}}(t+1/2)$$

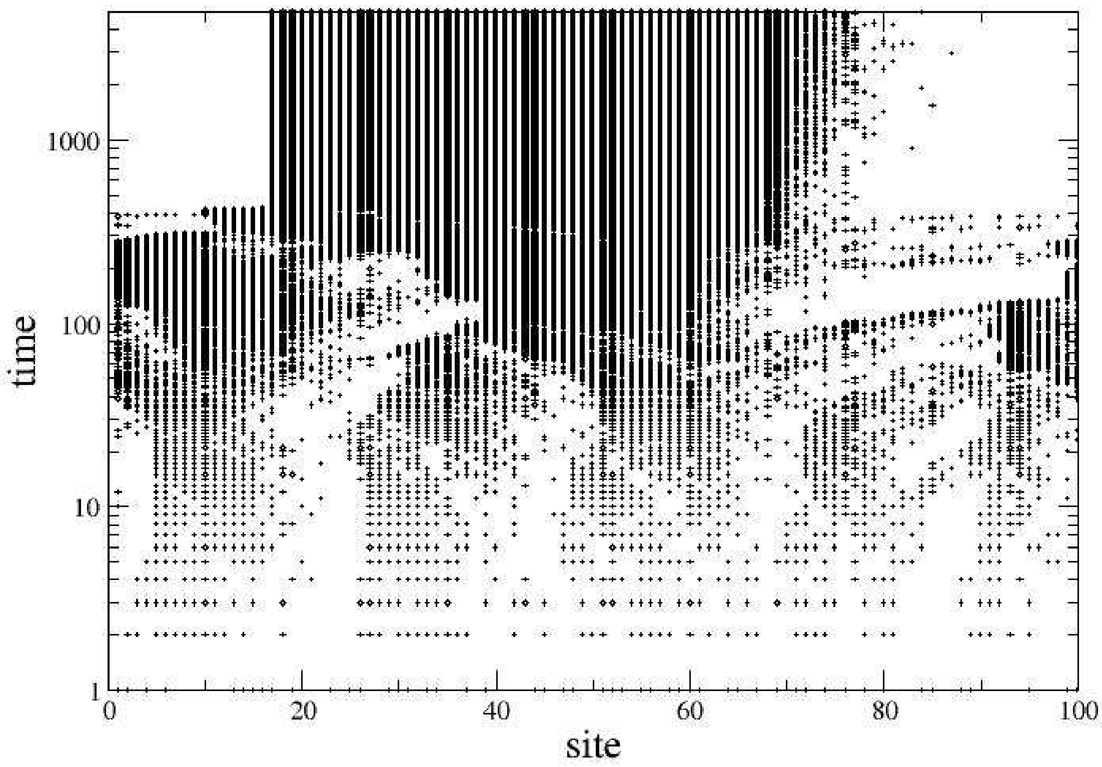
- Overall cloning step with an adjustable rate $M_t = N/(N+G)$ (the same for all configurations)



For long times

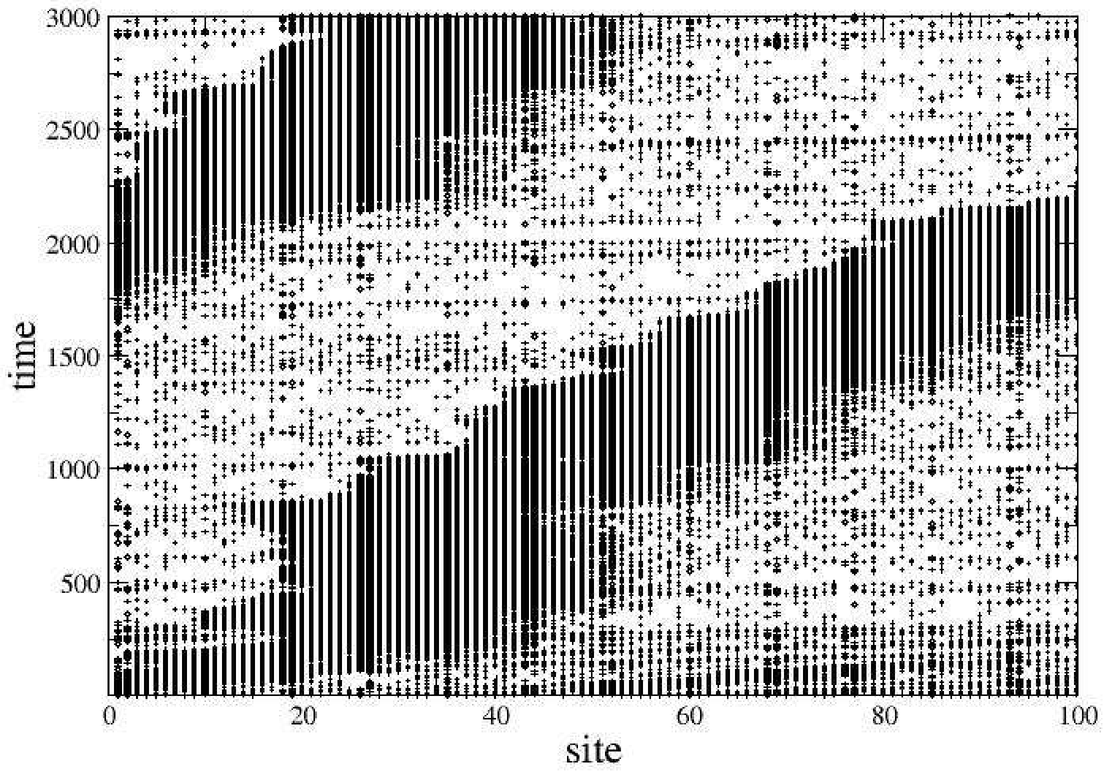
$$-\lim_{t\to\infty}\frac{1}{t}\ln[M_T\cdots M_2\cdot M_1]=\lim_{t\to\infty}\frac{\Lambda(\lambda)}{t}=\sigma(\lambda)$$

The configurations



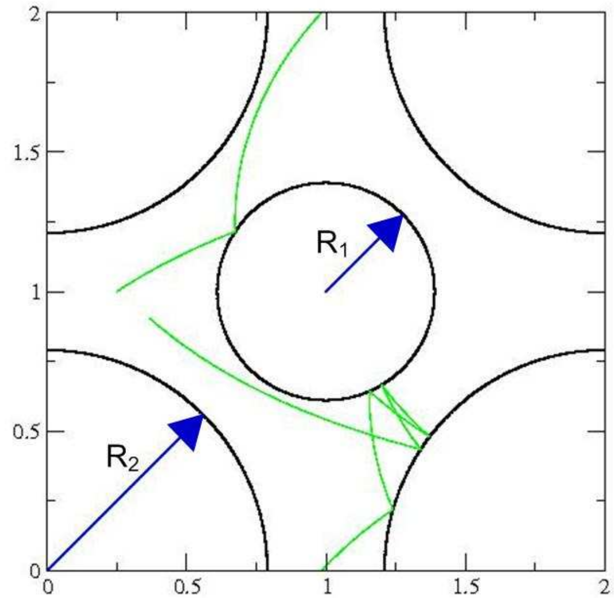
Space-time diagram for a ring of $N = 100$ sites, $\lambda = -50$ and density 0.5
Note the logarithmic scale on the y-axis

Moving shock waves



Space-time diagram for a ring of $N = 100$ sites, $\lambda = -30$ and density 0.3

The Lorentz gas

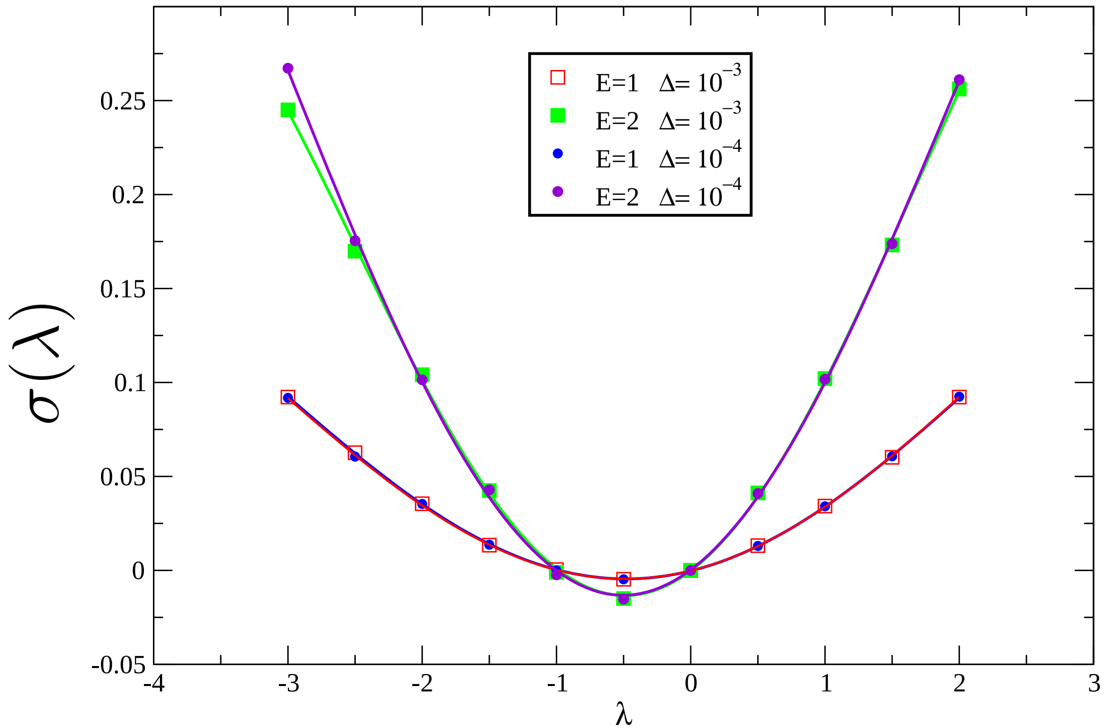


$$\ddot{x}_i = -E_i + \gamma(t)\dot{x}_i, \qquad i = 1, 2$$

$$\gamma(t) = \sum_i E_i \dot{x}_i$$

$$\Lambda(\lambda) = \ln \left\langle \exp\left(\int_0^t \mathrm{d}t' \; \gamma(t') \right) \right\rangle$$

The Gallavotti-Cohen relation



Data for $\vec{E} = (E, 0)$, $E = 1, 2$ and noise intensity $\Delta = 10^{-3}, 10^{-4}$

Discussion

- Efficient sampling technique (minutes on PC)
- So far restricted to steady states
- Beyond steady states: sampling of the initial condition (TBD)

Perspectives

- “Local” fluctuation relations
- Experimental checks: Electrical circuits (Ciliberto et al.)
- Energetics of molecular engines

Thanks

My collaborators:

Thanks

My collaborators:

- For the exploration of general identities and free-energy landscapes: **Alberto Imparato**
- For the cloning simulation technique: **Cristian Giardinà and Jorge Kurchan**