Asymptotics of work distributions in driven Langevin systems

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Motivation

fluctuating nano-machines
stochastic thermodynamics

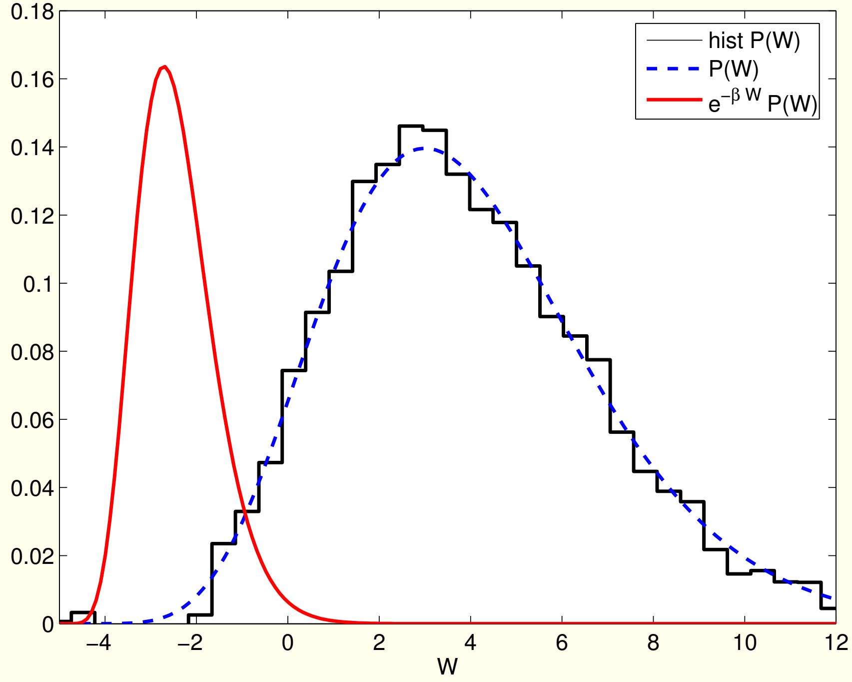
$\longleftrightarrow$

large deviation properties
tails of distributions

Here:

asymptotics of $P(W)$
improving estimates for ΔF from

$$e^{-\beta \Delta F} = \langle e^{-\beta W} \rangle$$



Aim: Combine analytical information on the tail of $P(W)$ with the histogram.

Basic equations

Langevin dynamics

$$\dot{x} = -V'(x, t) + \sqrt{\frac{2}{\beta}}\,\xi(t) \quad , \quad P(x_0) = \frac{e^{-\beta V_0(x_0)}}{Z_0} \quad , \quad W[x(\cdot)] = \int_0^{t_1} dt\, \dot{V}(x(t), t)$$

Transformation of probability

$$P(W) = \int \frac{dx_0}{Z_0}\, e^{-\beta V_0(x_0)} \int dx_1 \int\limits_{x(0)=x_0}^{x(t_1)=x_1} \mathcal{D}x(\cdot)\, p[x(\cdot)|x_0, x_1]\; \delta(W - W[x(\cdot)])$$

$$= \int \frac{dx_0}{Z_0} \int dx_1 \int \frac{dq}{4\pi/\beta} \int\limits_{x(0)=x_0}^{x(t_1)=x_1} \mathcal{D}x(\cdot)\; e^{-\beta S[x(\cdot), q]}$$

Stochastic action

$$S[x(\cdot), q] = V_0(x_0) + \frac{1}{2} \int\limits_0^{t_1} dt\; [\frac{1}{2}(\dot{x} + V')^2 + iq\dot{V}] - \frac{i}{2} qW \qquad [\ldots] = \tilde{L}(\dot{x}, x, t, q)$$

Method of optimal fluctuation

Contraction principle: The probability of an unlikely event is dominated by the probability of its most probable cause.

Here: Tails of $P(W)$ are dominated by $\bar{x}(\cdot)$ maximizing $p[x(\cdot)]$ under the constraint $W[\bar{x}(\cdot)] = W$.

Formally: $\beta \to \infty$ and saddle-point calculation of integrals.

$$P(W) = \frac{e^{-\beta S[\bar{x}(\cdot),\bar{q}]}}{Z_0 \sqrt{R\, Q(t_1)/\beta}} \left(1 + \mathcal{O}(1/\beta)\right)$$

Includes contributions from the optimal trajectory and its neighbourhood.

Specific features of the present case

Euler-Lagrange equation:

$$\frac{d}{dt}\frac{\partial \tilde{L}}{\partial \dot{x}} - \frac{\partial \tilde{L}}{\partial x} = 0, \qquad \left.\frac{\partial \tilde{L}}{\partial \dot{x}}\right|_{t=0} - V_0'(x_0) = 0 \;, \qquad \left.\frac{\partial \tilde{L}}{\partial \dot{x}}\right|_{t=t_1} = 0$$

One optimal trajectory $\bar{x}(t;W)$ for each value of W

$\bar{x}(t;W)$ quantifies balance between "unlikeliness" in x_0 and $\xi(t)$

Fluctuation determinant $Q(t_1)$:

$$\ddot{Q} + 2\bar{V}''\dot{Q} + [(2 - i\bar{q})\dot{\bar{V}}'' + (\dot{\bar{x}} - \bar{V}')\bar{V}''']Q = 0$$

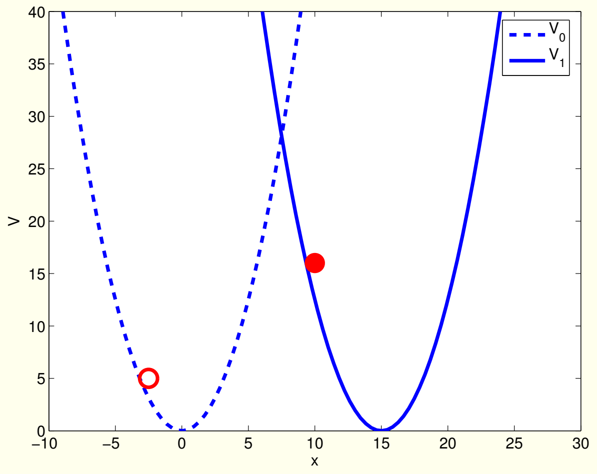
boundary conditions: $Q(t=0) = 1 \;,\; \dot{Q}(t=0) = 0$

Constraint:

Omit fluctuations violating the constraint

$$R = \int_0^{t_1} dt \int_0^{t_1} dt' \, \dot{V}'(\bar{x}(t),t) \left[\frac{\delta^2 \bar{S}}{\delta x(t)\delta x(t')}\right]^{-1} \dot{V}'(\bar{x}(t'),t')$$

First example: The sliding parabola



$$V(x,t) = \frac{(x-t)^2}{2}$$

Exact solution:

$$P(W) = \sqrt{\frac{\beta}{2\pi\, 2(t_1 - 1 + e^{-t_1})}}\; e^{-\beta \frac{(W-(t_1-1+e^{-t_1}))^2}{4(t_1-1+e^{-t_1})}}$$

Asymptotic estimate:

$$\bar{x} = \frac{1}{2}(2t + e^{-t} - e^{t-t_1}) - \frac{W(2 - e^{-t} - e^{t-t_1})}{2(t_1 + e^{-t_1} - 1)}$$

$$\bar{S} = \frac{(W - (t_1 + e^{-t_1} - 1))^2}{4(t_1 + e^{-t_1} - 1)}$$

$$0 = \ddot{Q} + 2\dot{Q}, \quad Q(0) = 1,\ \dot{Q}(0) = 0$$

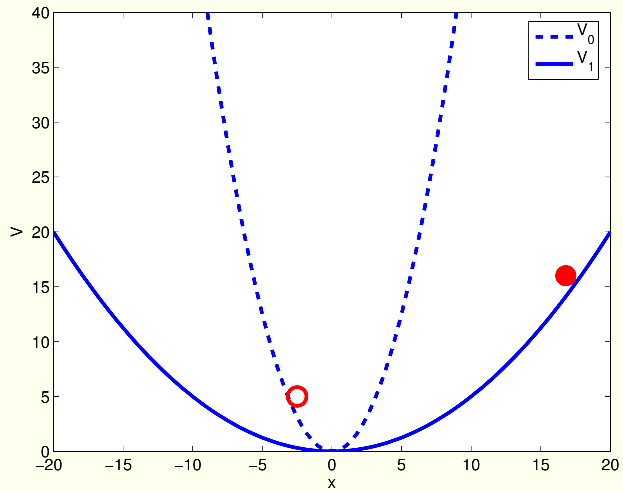
$$Q(t_1) = 1$$

$$\delta^2 \bar{S} = -\frac{1}{2}\,\delta''(t-t') + \frac{1}{2}\,\delta(t-t')$$

$$\delta^2 \bar{S}^{-1} = -2\theta(t-t')\sinh(t-t') \;+\; e^{t-t'},\ \dot{V}' \equiv -1$$

$$R = 2(t_1 - 1 + e^{-t_1})$$

Second example: The breathing parabola

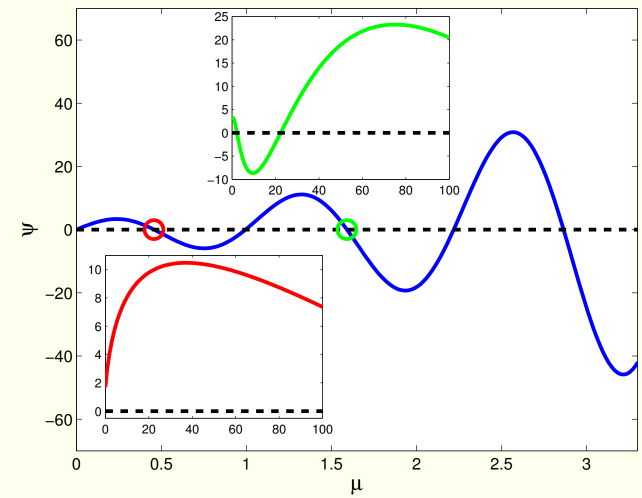


$$V(x,t) = \frac{k(t)}{2}x^2$$

$$P(W) = ???$$

$\mu = \sqrt{iq - 9/4} \longrightarrow$ ELE is a Sturm-Liouville problem

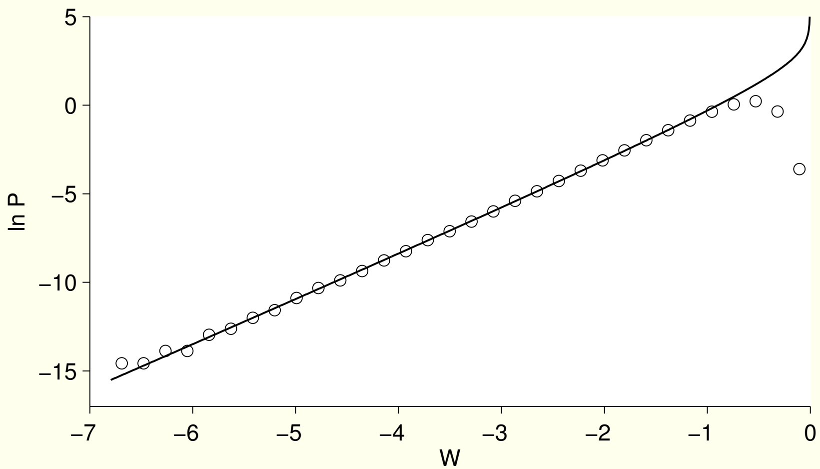
infinitly many minima of $S[x(\cdot)]$



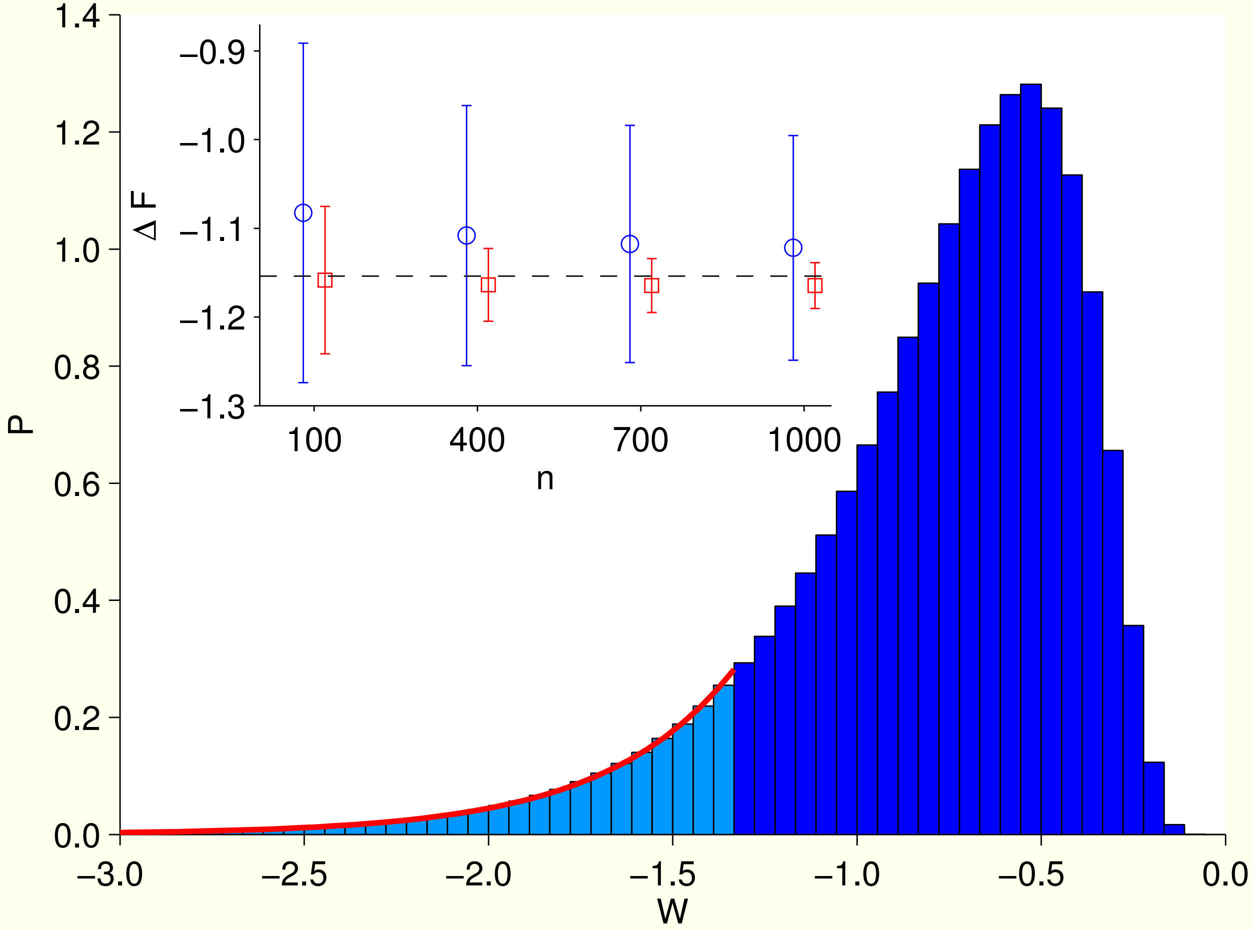
$$k(t) = \frac{1}{1+t}$$

$$\bar{x} = \pm\sqrt{-W}g(t)$$

$$P(W) \sim \frac{e^{\beta\, h(\mu_0) W}}{\sqrt{-W}}$$



Improving the ΔF estimate



Third example: The Blickle experiment

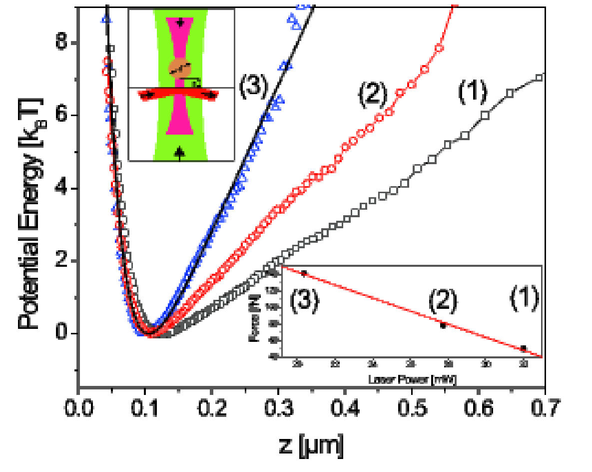
(Phys. Rev. Lett. **96**, 070603 (2006))

$$V(x,t) = Ae^{-\kappa(x-a)} + B(t)(x-a)$$

$$D(x) = \frac{D_0}{1+R/x}$$

$$\dot{x} = -D(x)V'(x,t) + D'(x) + \sqrt{2D(x)}\,\xi(t)$$

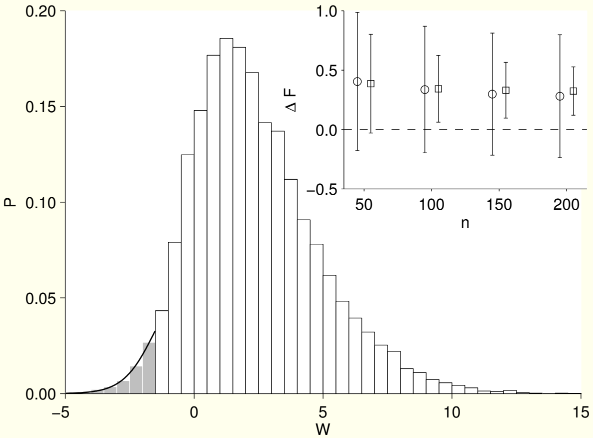
16500 experimental values of W



$$L(x,\dot{x},t) = \frac{1}{4D(x)}\Big(\dot{x} + D(x)V'(x,t) - D'(x)\Big)^2$$

$$0 = \ddot{x} - \frac{D'}{2D}\dot{x}^2 + (1-iq)D\dot{V}' + \ldots.$$

Determine $\bar{S}$ numerically, no prefactor yet.



Summary

- Analytical expressions for the asymptotics of work distributions in driven Langevin systems.
- Method of optimal fluctuation corresponding to contraction principle of large deviation theory.
- May improve ΔF estimates from the Jarzynski equation if histogram and asymptotics overlap.