Biased dynamics for Brownian particles

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We consider a Brownian particle in a potential $U(x)$

$$\dot{x} = -\Gamma U'(x) + \eta;\ \langle \eta(t)\eta(t')\rangle = 2\Gamma k_B T \delta(t-t'). \tag{1}$$

The heat exchanged with the environment is

$$Q(t) = \int \mathrm{d}x\, U'(x) = \int_0^t \mathrm{d}s\, \dot{x}(s) U'(x(s)). \tag{2}$$

We want to evaluate the PDF of Q, $\phi(Q,t)$, or its generating function $\Psi(\lambda,t)$. The latter function can be defined as

$$\Psi(\lambda,t) = \int \mathrm{d}x_0 p(x_0) \int \mathcal{D}\omega_t\, P[\omega_t] \mathrm{e}^{\lambda Q[\omega_t]}, \tag{3}$$

and its derivative reads

$$\frac{\partial \Psi}{\partial \lambda} = \int \mathrm{d}x_0 p(x_0) \int \mathcal{D}\omega_t\, Q[\omega_t] P[\omega_t] \mathrm{e}^{\lambda Q[\omega_t]} = \Psi(\lambda,t) \langle Q \rangle_\lambda, \tag{4}$$

where

$$\langle X \rangle_\lambda = \frac{1}{\Psi(\lambda,t)} \int \mathrm{d}x_0 p(x_0) \int \mathcal{D}\omega_t\, X[\omega_t] P[\omega_t] \mathrm{e}^{\lambda Q[\omega_t]}. \tag{5}$$

Let us consider a small time step τ, and a transition $x_t \to x'_{t+1}$, the probability for this transition to happen is

$$P(x'|x) = \delta(x' - (x + \tau\dot{x}))\mathcal{P}(\eta_t) = \delta(x' - (x+\tau\dot{x}))\mathrm{e}^{-\eta_t^2 \tau\alpha}\mathcal{N}, \tag{6}$$

where $\alpha = 1/(4\Gamma k_B T)$, and $\mathcal{N} = \sqrt{\tau\alpha/\pi}$ is the normalization constant for $\mathcal{P}(\eta_t)$. The probability (6) is normalized when one integrates over x' and η. Let $Q_{x',x} = \tau U'(x)\dot{x} = \tau U'(x)(-\Gamma U'(x) + \eta_t)$ be the heat associated with the transition, let us consider

$$\begin{aligned}
\mathrm{e}^{\lambda Q_{x',x}} P(x'|x) &= \delta(x' - (x+\tau\dot{x})) \exp\left\{[-(\alpha\eta^2 - \lambda U'\eta) - \lambda\Gamma U'^2]\tau\right\}\mathcal{N} && (7)\\
&= \delta(x' - (x + \tau(-\Gamma U'(x) + \eta)) \exp\left\{\left[-\alpha\left(\eta - \frac{\lambda U'}{2\alpha}\right)^2 + \frac{(\lambda U')^2}{4\alpha} - \lambda\Gamma U'^2\right]\tau\right\}\mathcal{N} && (8)\\
&= \delta(x' - (x + \tau\left[(-\Gamma + \frac{\lambda}{2\alpha})U'(x) + \tilde{\eta})\right] \mathrm{e}^{-\alpha\tilde{\eta}^2\tau}\mathcal{N} \exp\left[\frac{(\lambda U')^2}{4\alpha} - \lambda\Gamma U'^2\right]\tau && (9)
\end{aligned}$$

The first part of this equation, is a transition probability (is correctly normalized), and corresponds to a Brownian motion with a kinetic constant that depends on λ

$$\dot{x} = (-\Gamma + \frac{\lambda}{2\alpha})U'(x) + \tilde{\eta}, \tag{10}$$

where $\tilde{\eta}$ is again a Gaussian noise with variance $2\Gamma k_B T$. Thus we can run simulations, and over these simulations we have to calculate the average of the term $\exp\left[\frac{(\lambda U')^2}{4\alpha} - \lambda\Gamma U'^2\right]\tau$, appearing in eq. (9), that, differently from $Q_{x',x}$, does not depend explicitly on the noise.

Thus we have

$$\langle Q \rangle_\lambda = \frac{\int \mathrm{d}x_0 p(x_0) \int \mathcal{D}\tilde{\omega}_{\lambda,t}\, Q(\tilde{\omega}_{\lambda,t}) P(\tilde{\omega}_{\lambda,t}) \exp\left[\int \mathrm{d}t\, U'^2 \Gamma\lambda(\lambda k_B T - 1)\right]}{\int \mathrm{d}x_0 p(x_0) \int \mathcal{D}\tilde{\omega}_t\, P(\tilde{\omega}_{\lambda,t}) \exp\left[\int \mathrm{d}t\, U'^2 \Gamma\lambda(\lambda k_B T - 1)\right]}, \tag{11}$$

where $\tilde{\omega}_{\lambda,t}$ are trajectories generated by the dynamics (10). Note that in we obtain the term $\lambda(\lambda k_B T - 1)$, signaling the usual Gallavotti-Cohen symmetry for $\lambda = 0$, β. Important remark: the initial conditions, and thus the distribution

$p(x_0)$, are not affected by the substitution $\eta \to \tilde{\eta}$, and thus one has to start the simulations by equilibrating the particle with the "unperturbed" dynamics. This is important, because the term $-\Gamma + \lambda/(2\alpha)$ in eq. (10) becomes positive for $\lambda > 2\Gamma\alpha$, corresponding to a negative kinetic coefficient.

We consider now the simple potential

$$U(x) = \frac{k}{2}x^2, \tag{12}$$

simulate the process (10), and calculate the two averages, appearing at the numerator and at the denominator of the rhs of eq. (11). For this potential, the generating function in the long time limit reads $\Psi(\lambda, t \to \infty) = 1/\sqrt{1 - (\lambda/\beta)^2}$, and thus $\langle Q \rangle_\lambda = \partial_\lambda \Psi/\Psi = \tilde{\lambda}/(1 - \tilde{\lambda}^2)$, where $\tilde{\lambda} = \lambda/\beta$.

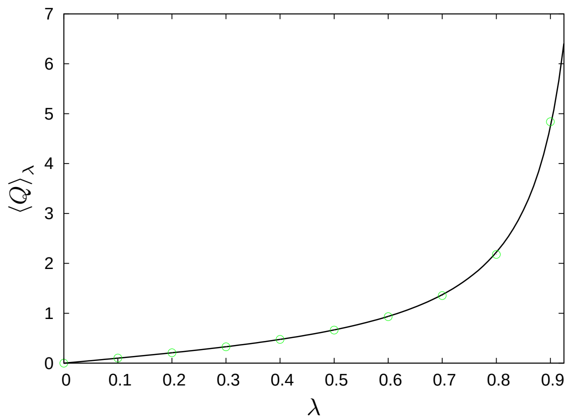

FIG. 1: Points: $\langle Q \rangle_\lambda$ as given by eq. (11) for the potential (12). The averages are taken by simulating the process defined in eq. (10), with 10^6 trajectories, and $\Gamma = k_B T = k = 1$. The full line correspond to the expected function $\tilde{\lambda}/(1 - \tilde{\lambda}^2)$

The same procedure can be repeated with the moving potential

$$U(x,t) = \frac{k}{2}(x - vt)^2, \tag{13}$$

where v is the velocity of the potential equilibrium position. The cumulant generating function reads

$$\lim_{t\to\infty} \frac{1}{t} \log[\Psi(\lambda, t \to \infty)] = \mu(\lambda) = \frac{v^2}{\Gamma}\lambda(\lambda T - 1), \tag{14}$$

and thus

$$\langle Q \rangle_\lambda = t\partial_\lambda \mu(\lambda) = \frac{v^2 t}{\Gamma}(2\lambda T - 1). \tag{15}$$

The results are reported in fig. 2.

The same formalism can be generalized to a particle with inertia (Kramers equation instead of the Smoluchowski equation, and suitable definition for Q), or even if one considers N interacting particles coupled to a number of heat baths at different temperature.

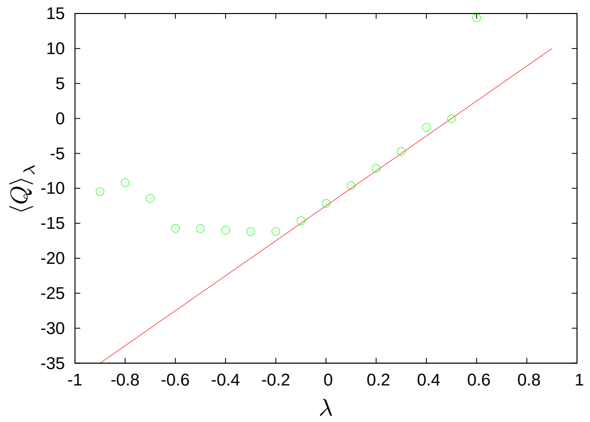

FIG. 2: Points: $\langle Q \rangle_\lambda$ as given by eq. (11) for the potential (13). The averages are taken by simulating the process defined in eq. (10), with 10^6 trajectories, $\Gamma = k_B T = k = 1$, $v = 0.5$, and $t = 50$. The full line correspond to the expected function (15).