Stochastic thermodynamics for SDEs

AI

1 Stochastic Heat and Work

The dynamics of a 1D system is governed by the Hamiltonian

$$H(x,p) = \frac{p^2}{2m} + U(x). \tag{1}$$

Denoting a time derivative by a dot the Langevin equations of motion for the particle are given by

$$\dot{x} = \frac{p}{m}, \tag{2}$$

$$\dot{p} = -U'(x) - \gamma \frac{p}{m} + \eta(t), \tag{3}$$

with white noise correlation

$$\langle \eta(t)\eta(t') \rangle = 2\gamma k_B T \delta(t-t'). \tag{4}$$

The total force on the particle is composed of a deterministic force, a friction force, and a fluctuating force, the last two arising from the bath at temperature T. Let us calculate the time derivative of the Hamiltonian

$$\frac{dH}{dt} = \dot{x}\, \partial_x H + \dot{p}\, \partial_p H = \frac{p(t)}{m} \left(-\gamma p(t)/m + \eta(t)\right). \tag{5}$$

where we have used eqs.(2)–(3) to obtain the last equality, and the rightmost expression is the rate of work performed by the heat reservoir on the system, i.e., the heat flux.

Thus we write the expression for the trajectory-dependent stochastic heat

$$Q(t) = \int_0^t dt' \frac{p(t')}{m} \left(-\gamma p(t')/m + \eta(t')\right) = \int_0^t dt' \dot{x}(t') \left(\dot{p}(t') + U'(x(t'))\right). \tag{6}$$

We now consider the case where the Hamiltonian depends explicitly on time

$$H(x,p,\lambda(t)) = \frac{p^2}{2m} + U(x,\lambda(t)). \tag{7}$$

We calculate again the total time derivative of the Hamiltonian

$$\frac{dH}{dt} = \dot{x}\,\partial_x H + \dot{p}\,\partial_p H + \partial_t H = \frac{p(t)}{m}\left(-\gamma p(t)/m + \eta(t)\right) + \dot{\lambda}\partial_\lambda H, \tag{8}$$

and thus identify the trajectory-dependent heat and work

$$\begin{aligned} Q(t) &= \int_0^t dt'\,\frac{p(t')}{m}\left(-\gamma p(t')/m + \eta(t')\right) && (9) \\ &= \int_0^t dt'\,\dot{x}(t')\left(\dot{p}(t') + U'(x(t'),\lambda(t'))\right), && (10) \\ W(t) &= \int_0^t dt'\,\dot{\lambda}(t')\partial_\lambda H(x(t'),p(t'),\lambda)|_{\lambda=\lambda(t')}, && (11) \end{aligned}$$

respectively, and

$$\Delta H(t) = Q(t) + W(t). \tag{12}$$

In the overdamped case, the stochastic equation reads

$$\dot{x}(t) = -\Gamma\partial_x U(x(t),\lambda(t)) + \tilde{\eta}(t), \qquad \langle\tilde{\eta}\tilde{\eta}'\rangle = 2\Gamma T\delta(t-t'), \tag{13}$$

with $\Gamma = 1/\gamma$. The change in the system energy reads

$$\frac{dU}{dt} = \dot{x}\,\partial_x U + \dot{\lambda}(t)\partial_\lambda U, \tag{14}$$

and the work done by the stochastic forces, i.e, the heat is given by

$$Q(t) = \int_0^t dt'\,\dot{x}(t')\left(\dot{x}(t') + \tilde{\eta}(t')\right)/\Gamma = \int_0^t dt'\,\dot{x}(t')\partial_x U(x(t'),\lambda(t')), \tag{15}$$

while the work done by the external agent is given by

$$W(t) = \int_0^t dt'\,\dot{\lambda}(t')\partial_\lambda U(x(t'),\lambda(t')), \tag{16}$$

with

$$\Delta U(t) = Q(t) + W(t). \tag{17}$$

2 A simple model for stochastic heat transport

We consider a classical harmonic oscillator in contact with two heat baths at temperatures T_i, $i = 1, 2$.

The Langevin equation reads

$$m\ddot{x}(t) = -m\omega_s^2 x(t) - \bar{\gamma}\dot{x}(t) + \eta_1(t) + \eta_2(t), \qquad \langle \eta_i(t)\eta_j(t')\rangle = 2\gamma_i \delta_{i,j} T_i \delta(t-t'), \tag{18}$$

with $\bar{\gamma} = \gamma_1 + \gamma_2$. The (long time limit) solution in Fourier space reads

$$x(\omega) = -\frac{\eta_1(\omega) + \eta_2(\omega)}{m(\omega^2 - \omega_s^2) + \mathbb{i}\bar{\gamma}\omega}, \tag{19}$$

with

$$\langle \eta_i(\omega)\eta_j(\omega')\rangle = 4\pi\gamma_i \delta_{i,j} T_i \delta(\omega + \omega'). \tag{20}$$

The stochastic heat current flowing into the system from bath 1 reads

$$\frac{\mathrm{d}Q_1(t)}{\mathrm{d}t} = \dot{x}(t)(-\gamma_1 \dot{x}(t) + \eta_1(t)). \tag{21}$$

We want to calculate the average heat current

$$\left\langle \frac{\mathrm{d}Q_1(t)}{\mathrm{d}t} \right\rangle = \langle \dot{x}(t)(-\gamma_1 \dot{x}(t) + \eta_1(t))\rangle \tag{22}$$

We first calculate

$$\begin{aligned} \langle \dot{x}(t)\dot{x}(t)\rangle &= \left\langle \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathbb{i}\omega t} \mathbb{i}\omega x(\omega) \int \frac{\mathrm{d}\omega'}{2\pi} \mathrm{e}^{-\mathbb{i}\omega' t} \mathbb{i}\omega' x(\omega') \right\rangle \\ &= 2(\gamma_1 T_1 + \gamma_2 T_2) \int \frac{\mathrm{d}\omega}{2\pi} \frac{\omega^2}{m^2(\omega^2 - \omega_s^2)^2 + (\bar{\gamma}\omega)^2}, \end{aligned} \tag{23}$$

where we have used the fluctuation-dissipation relation (20). The integrand in the last expression has two simple poles in the upper half-plane

$$z_\pm = \frac{\mathbb{i}\bar{\gamma} \pm \mathbb{i}\sqrt{\bar{\gamma}^2 - 4m^2\omega_s^2}}{2m}, \tag{24}$$

and thus we can write

$$\langle \dot{x}(t)\dot{x}(t)\rangle = 2(\gamma_1 T_1 + \gamma_2 T_2) 2\pi\mathbb{i} \left[Res(z_+) + Res(z_-)\right] = \frac{\gamma_1 T_1 + \gamma_2 T_2}{m\bar{\gamma}}. \tag{25}$$

Similarly one finds

$$\langle \dot{x}(t)\eta_1(t)\rangle = \frac{\gamma_1 T_1}{m}, \tag{26}$$

and thus

$$\left\langle \dot{Q}_1(t) \right\rangle = -\left\langle \dot{Q}_2(t) \right\rangle = \frac{(T_1 - T_2)\gamma_1\gamma_2}{m(\gamma_1+\gamma_2)}. \tag{27}$$

3 Onsager–Machlup formalism

Let $\mathbf{z}$ be a trajectory in the system phase space $t \mapsto (x(t), p(t))$ (keep in mind that $\mathbf{z}$ is a trajectory and not a single point (x, p)). Similarly $\mathbf{x}$ is a trajectory in the overdamped case.

We want to evaluate the probability of observing a given trajectory, and possibly the probability of its time reverse, given that the dynamics is governed by eqs. (2)–(3).

To introduce the discussion in a simple way, let's start with a particle in the overdamped regime, described by

$$\dot{x}(t) = \Gamma F(x) + \tilde{\eta}(t), \qquad \langle \tilde{\eta}\tilde{\eta}'\rangle = 2\Gamma T\delta(t-t'). \tag{28}$$

Let us calculate the probability $P(x', t+\delta t|x, t)$, given that the probability of the Gaussian noise in the time interval δt reads

$$\mathscr{P}(\tilde{\eta}_t) = \mathrm{e}^{-\delta t \frac{\eta_t^2}{4\Gamma k_B T}}\sqrt{\frac{\delta t}{4\pi\Gamma k_B T}}. \tag{29}$$

We first introduce the time discretization

$$x(t_{k+1}) = x(t_k) + \delta t(F(x(t_k)) + \eta(t_k)), \qquad k = 0, 1, \ldots, N_t. \tag{30}$$

We have

$$\begin{aligned}
&P(x', t+\delta t|x, t) = \int \mathrm{d}\tilde{\eta}_t\, \mathscr{P}(\tilde{\eta}_t)\delta(x' - x - \delta t(\Gamma F(x) + \tilde{\eta}_t)) \\
&= \sqrt{\frac{\delta t}{4\pi\Gamma k_B T}} \int \frac{\mathrm{d}\lambda}{2\pi} \int \mathrm{d}\tilde{\eta}_t\, \exp\left[-\frac{\delta t \eta_t^2}{4\Gamma k_B T} + \mathbb{i}\lambda(x' - x - \delta t(\Gamma F(x) + \tilde{\eta}_t)\right] \\
&= \int \frac{\mathrm{d}\lambda}{2\pi} \exp\left[-\lambda^2 \Gamma k_B T \delta t + \mathbb{i}\lambda(x' - x - \Gamma F(x)\delta t)\right] \\
&= \exp\left[-\frac{(x' - x - \Gamma F(x)\delta t)^2}{4\Gamma k_B T \delta t}\right] / \sqrt{\delta t 4\pi \Gamma k_B T}
\end{aligned} \tag{31}$$

and thus

$$P(\mathbf{x}|x_0, \boldsymbol{\lambda}) = \mathrm{e}^{-\mathcal{S}(\mathbf{x},\lambda(t))}, \tag{32}$$

where the action is defined by

$$\mathcal{S}(\mathbf{x}, \boldsymbol{\lambda}) = \frac{1}{4\Gamma k_B T} \int_{t_0}^{t} dt' \left[\dot{x}(t') - \Gamma F(x(t'), \lambda(t'))\right]^2 \tag{33}$$

with

$$\int \mathcal{D}\,\mathbf{x}\; P(\mathbf{x}|x_0, \boldsymbol{\lambda}) = 1 \tag{34}$$

and the trajectory measure is defined by

$$\mathcal{D}\,\mathbf{x} = \lim_{\delta t \to 0} \prod_{k=1}^{N_t} \frac{dx_k}{\sqrt{4\pi\Gamma T \delta t}}. \tag{35}$$

The expression on the rhs of eq. (32) is called the Onsager–Machlup functional. For the time–reversed path we have

$$P(\hat{\mathbf{x}}|\hat{x}_0, \hat{\boldsymbol{\lambda}}) = \exp\left\{ -\int_{t_0}^{t} dt' \frac{1}{4\Gamma k_B T} \left[\dot{x}(t') + \Gamma F(x(t'), \lambda(t'))\right]^2 \right\}, \tag{36}$$

and one obtains the Crooks relation

$$\frac{P(\mathbf{x}|x_0, \boldsymbol{\lambda})}{P(\hat{\mathbf{x}}|\hat{x}_0, \hat{\boldsymbol{\lambda}})} = \exp\left[-\frac{1}{k_B T} \int_{t_0}^{t} dt' \dot{x}(t') F(x(t'), \lambda(t')) \right] = \mathrm{e}^{-\beta Q(\mathbf{x})}, \tag{37}$$

where the heat flowing into the system is defined in eq. (15). Introducing the final and the initial probability distribution, $p(x_f, t_f)$ and $p(x_0, t_0)$, and the system stochastic entropy $S^s(x,t) = -k_B \log p(x,t)$, we finally obtain the fluctuation relation

$$P(\mathbf{x}, \boldsymbol{\lambda}) \mathrm{e}^{-(\Delta S^B(\mathbf{x}) + \Delta S^s)/k_B} = P(\hat{\mathbf{x}}, \hat{\boldsymbol{\lambda}}), \tag{38}$$

with $\Delta S^B = -Q(\mathbf{x})/k_B$.

Similarly in the underdamped case, eqs. (2)–(3) we have

$$\begin{aligned} P(\mathbf{z}|z_0, \boldsymbol{\lambda}) &= \exp\left\{ -\frac{1}{4\gamma k_B T} \int_{t_0}^{t} dt' \left[m\ddot{x}(t') + \gamma \dot{x}(t') - F(x(t'), \lambda(t'))\right]^2 \right\} \\ P(\hat{\mathbf{z}}|\hat{z}_0, \hat{\boldsymbol{\lambda}}) &= \exp\left\{ -\frac{1}{4\gamma k_B T} \int_{t_0}^{t} dt' \left[m\ddot{x}(t') - \gamma \dot{x}(t') - F(x(t'), \lambda(t'))\right]^2 \right\} \end{aligned}$$

and the following Crooks relation

$$\frac{P(\mathbf{z}|z_0,\boldsymbol{\lambda})}{P(\hat{\mathbf{z}}|\hat{z}_0,\hat{\boldsymbol{\lambda}})} = \exp\left[-\beta\int_{t_0}^{t} dt'\dot{x}(t')(m\ddot{x}(t') - F(x(t'),\lambda(t')))\right] = \mathrm{e}^{-\beta Q(\mathbf{z})}, \quad (39)$$

where the heat flowing into the system is defined in eq. (10). Not surprisingly, also in the underdamped case the action is quadratic in the deviation from the "classical" solution

$$\mathcal{S}(\mathbf{z},\boldsymbol{\lambda}) = \frac{1}{4\Gamma k_B T}\int_{t_0}^{t} dt' \left[m\ddot{x}(t') + \gamma\dot{x}(t') - F(x(t'),\lambda(t'))\right]^2 \quad (40)$$

Finally, introducing the system stochastic entropy as given by $S^s(z,t) = -k_B \log p(z,t)$, the following fluctuation relation holds

$$P(\mathbf{z},\boldsymbol{\lambda})\mathrm{e}^{-(\Delta S^B(\mathbf{z})+\Delta S^s)/k_B} = P(\hat{\mathbf{z}},\hat{\boldsymbol{\lambda}}). \quad (41)$$