Project III : Breathing harmonic oscillator

Consider the overdamped motion of a simple harmonic oscillator governed by

$$\gamma dx(t) = -k(t)x(t)dt + \sqrt{2\gamma k_B T}dW(t) \ . \tag{5.4}$$

The spring constant $k(t)$ is varied as a function of time.

$$k(t) = \begin{cases} k_0 & \text{for } t < 0 \\ k_0 + (k_1 - k_0)t/\tau & \text{for } 0 \le t < \tau \\ k_f & \text{for } t > \tau \end{cases} \tag{5.5}$$

The internal energy of the oscillator is given by $E(x, k(t)) = \frac{1}{2}k(t)x^2$. During the time interval $0 \le t \le \tau$, the work done on the harmonic oscillator is given by $W = \int_0^\tau dt \left(\frac{dk}{dt}\right)\left(\frac{\partial E(x,k)}{\partial k}\right) = \left(\frac{k_1 - k_0}{2\tau}\right)\int_0^\tau x(t)^2 dt$. Set $\gamma = k_B = T = 1$, $k_0 = 1$, $k_1 = 2$.

[1] Obtain the partition function $Z(k)$ and the free energy $F(k)$ for the equilibrium harmonic oscillator as a function of the spring constant k.

[2] Initially, the harmonic oscillator is in the thermal equilibrium state with the distribution function $P(x) = \frac{1}{Z(k_0)}e^{-\beta k_0 x^2/2}$. Perform the numerical simulations to obtain the probability distribution function of the work $P_F(W)$ during the time interval $0 \le t \le \tau$.

[3] Perform the similar simulations to obtain the distribution $P_R(W)$ in the reverse process.

[4] Test the fluctuation theorems $\langle e^{-\beta W}\rangle_F = e^{-\beta\Delta F}$ and $P_F(W)/P_R(-W) = e^{\beta(W-\Delta F)}$ with $\Delta F = F(k_1) - F(k_0)$.