Nonequilibrium Statistical Physics

MMathPhys Noneq Stat Phys Course: Problem Sheet 2

Week 4, Hilary 2020

Qu 1. A Master equation for $\mathcal{P}_n(t)$ can be converted into a differential equation for the probability generating function $F(z,t)$, defined as

$$F(z,t) = \sum_n z^n \mathcal{P}_n(t) \quad ,$$

which satisfies the condition $F(1,t) = 1$.

Solve the Poisson process

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}_n(t) = -g\left(\mathcal{P}_n - \mathcal{P}_{n-1}\right)$$

using this method, subject to the initial condition of $n = 0$ at $t = 0$.

Solve the birth-death process

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}_n(t) = \mu(n+1)\mathcal{P}_{n+1} + \lambda(n-1)\mathcal{P}_{n-1} - (\mu+\lambda)n\mathcal{P}_n$$

using this method, subject to the initial condition of $n = 1$ at $t = 0$.

Qu 2. Use the path-integral formulation of stochastic dynamics for a particle in a harmonic potential $U(\mathbf{r}) = \frac{1}{2}k\mathbf{r}^2$ to show that

$$\mathcal{P}(\mathbf{x},t|\mathbf{x}_0,t_0) = \left(\frac{\beta k}{2\pi\left[1-e^{-2k(t-t_0)/\zeta}\right]}\right)^{3/2} \exp\left\{-\frac{\beta k}{2}\,\frac{\left[\mathbf{x}-\mathbf{x}_0\,e^{-k(t-t_0)/\zeta}\right]^2}{\left[1-e^{-2k(t-t_0)/\zeta}\right]}\right\} \quad .$$

You are expected to derive the prefactor using path-integration of the fluctuations. Discuss how this calculation reflects on the choice of $\Theta(0)$ used in the derivation.

Justify the form of the result by examining the limits of $k \to 0$, $t \to t_0$, and $t_0 \to -\infty$.

Qu 3. The path integral calculation in Question 2 does not require that the potential be stable (i.e. $k > 0$). Therefore, our result provides a quick route to calculating crossover time for transition across a barrier in the form of an inverted harmonic potential with $k = -\nu\zeta$, where $\nu > 0$. Considering the 1D case for simplicity, calculate the flux $J(x,t|x_0,0)$ associated with the suitably generalized probability distribution

$$\mathcal{P}(x,t|x_0,0) = \left(\frac{\nu}{2\pi D\left[e^{2\nu t}-1\right]}\right)^{1/2} \exp\left\{-\frac{\nu}{2D}\,\frac{\left[x - x_0\,e^{\nu t}\right]^2}{\left[e^{2\nu t}-1\right]}\right\} \quad .$$

Use the flux to construct the probability distribution for the transit time, corresponding to transition from $x_0 = -\Delta x$ to $x = \Delta x$ as

$$P(t) \equiv \frac{J(\Delta x, t| -\Delta x, 0)}{\int_0^\infty \mathrm{d}t\, J(\Delta x, t| -\Delta x, 0)} \quad .$$

Note that the transition corresponds to crossing the barrier $\beta\Delta E = \nu\Delta x^2/(2D)$. Show that

$$P(t) = \frac{\nu}{\sqrt{2\pi}}\,\frac{\sqrt{\beta\Delta E}}{\left[1-\mathrm{erf}\left(\sqrt{\beta\Delta E}\right)\right]}\,\frac{\exp\left\{-\beta\Delta E\coth(\nu t/2)\right\}}{\sinh(\nu t/2)\sqrt{\sinh\nu t}} \quad .$$

Write down an expression for the mean transition time $\mathcal{T}_\times$, and (by using the asymptotic forms of the special functions in the integral as justified) show that in the limit of $\beta\Delta E \gg 1$ we obtain

$$\mathcal{T}_\times \simeq \frac{1}{\nu}\left[\ln\left(2\beta\Delta E\right) + \gamma\right] \quad .$$

How can we justify this in comparison with the Kramers escape time that features an exponential dependence on the barrier height?

Qu 4. Use the operator representation of the path integral formalism to show that the conditional probability for orientation has the following closed form expression:

$$\mathcal{P}(\hat{\mathbf{n}}, t|\hat{\mathbf{n}}_0, 0) = \sum_{\ell,m} e^{-D_r \ell(\ell+1)t}\, Y^*_{\ell,m}(\hat{\mathbf{n}}) Y_{\ell,m}(\hat{\mathbf{n}}_0) \quad .$$