A15282W1

Honour School of Mathematical and Theoretical Physics Part C
Master of Science in Mathematical and Theoretical Physics

NONEQUILIBRIUM STATISTICAL PHYSICS

Trinity Term 2017

WEDNESDAY, 31ST MAY 2017, 2:30pm to 4:00pm

You should submit answers to 2 of the 3 questions.

You must start a new booklet for each question which you attempt. Indicate on the front sheet the numbers of the questions attempted. A booklet with the front sheet completed must be handed in even if no question has been attempted.

The numbers in the margin indicate the weight that the Examiners anticipate assigning to each part of the question.

Do not turn this page until you are told that you may do so

1. Consider a generic one-step process

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}_n(t) = r_{n+1}\,\mathcal{P}_{n+1}(t) + q_{n-1}\,\mathcal{P}_{n-1}(t) - (q_n + r_n)\,\mathcal{P}_n(t) \quad , \tag{1}$$

where $\mathcal{P}_n(t)$ is the probability of finding the system in state n at time t.

(a) [3 marks] Discuss the physical meaning of the various terms in (1). Show that (1) implies the conservation of probability.

(b) [3 marks] Discuss how 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

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

What condition on F guarantees conservation of probability?

(c) [6 marks] Solve the Poisson process

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

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

(d) [3 marks] Consider a population of some species A that can undergo the following two processes:

$$A \overset{\lambda}{\to} A + A \quad , \qquad A \overset{\lambda}{\to} 0 \quad ,$$

i.e., each A can give birth to another A with rate λ, or, it can die with the same rate. Show that this birth-death process is described by the following Master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}_n(t) = \lambda(n+1)\mathcal{P}_{n+1} + \lambda(n-1)\mathcal{P}_{n-1} - 2\lambda n\mathcal{P}_n \quad .$$

(e) [8 marks] Solve the above birth-death process using the method of generating function discussed above, subject to the initial condition of $n = 1$ at $t = 0$.

(f) [2 marks] Find the solution when the growth rate $\lambda(t)$ is time dependent.

2. A stochastic Brownian dynamics is described by the Langevin equations

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{v}\left(\mathbf{r}(t)\right) + \mathbf{u}(t) \quad , \tag{2}$$

where the components of $\mathbf{u}(t)$ are Gaussian white noise variables with correlations

$$\langle u_i(t) \rangle = 0 \quad , \quad \langle u_i(t) u_j(t') \rangle = 2D\, \delta_{ij} \delta(t - t') \quad ,$$

and $\mathbf{v}(\mathbf{r})$ represents an arbitrary drift velocity.

(a) [3 marks] Discuss how the Markov property of (2) can be used in constructing a path-integral representation for the conditional probability $\mathcal{P}(\mathbf{x}, t|\mathbf{x}_0, t_0)$ of finding the system at position $\mathbf{x}$ at time t, knowing that it has started from position $\mathbf{x}_0$ at time t_0.

(b) [3 marks] Show that a key building block in the constructed path-integral will be

$$\mathcal{P}(\mathbf{y}, t' + \Delta t|\mathbf{y}', t') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{y}')+W} \quad ,$$

where

$$W = \ln \left\langle e^{-ik_i \Delta r_i} \right\rangle \simeq -ik_i \langle \Delta r_i \rangle - \frac{1}{2} k_i k_j \left[\langle \Delta r_i \Delta r_j \rangle - \langle \Delta r_i \rangle \langle \Delta r_j \rangle \right] \quad ,$$

and Δr_i represents the time integral of (2) over a finite time interval Δt.

(c) [2 marks] Show that

$$\langle \Delta r_i \rangle \simeq v_i(\mathbf{r}(t'))\Delta t + O(\Delta t^{3/2}) \quad .$$

(d) [7 marks] Show that

$$\langle \Delta r_i \Delta r_j \rangle - \langle \Delta r_i \rangle \langle \Delta r_j \rangle = \mathcal{M}_{ij}(2D\Delta t) + O(\Delta t^{5/2}) \quad ,$$

where

$$\mathcal{M}_{ij} = \delta_{ij} + \Theta(0)\, \Delta t\, (\partial_j v_i + \partial_i v_j) \quad ,$$

involves the Heaviside function at the origin $\Theta(0)$, which is ambiguous.

(e) [7 marks] Using the above results, show that

$$\mathcal{P}(\mathbf{y}, t' + \Delta t|\mathbf{y}', t') = \frac{1}{(4\pi D\Delta t)^{3/2}} \times \exp\left\{ -\frac{\Delta t}{4D} \left[\frac{(\mathbf{y} - \mathbf{y}')}{\Delta t} - \mathbf{v}(\mathbf{y}') \right]^2 - \Delta t\, \Theta(0) \left[\boldsymbol{\nabla} \cdot \mathbf{v}(\mathbf{y}') \right] + O(\Delta t^{3/2}) \right\} \quad .$$

(f) [3 marks] Finally, take the continuum limit to show

$$\mathcal{P}(\mathbf{x}, t|\mathbf{x}_0, t_0) = \mathcal{N} \int_{\mathbf{r}(t_0)=\mathbf{x}_0}^{\mathbf{r}(t)=\mathbf{x}} \mathcal{D}\mathbf{r}(\tau)\, e^{-\mathcal{S}} \quad ,$$

where $\mathcal{S}$ is an action. Find $\mathcal{S}$.

3. (a) [8 marks] Explain how we can build a formulation to calculate the mean first passage time $\mathcal{T}(\mathbf{x})$ (the mean escape time from a region, starting at an initial point $\mathbf{x}$). Show that for diffusion in a potential $U(\mathbf{x})$ the mean first passage time satisfies the following equation

$$-\beta \boldsymbol{\nabla} U(\mathbf{x}) \cdot \boldsymbol{\nabla} \mathcal{T}(\mathbf{x}) + \boldsymbol{\nabla}^2 \mathcal{T}(\mathbf{x}) = -\frac{1}{D} \quad . \tag{3}$$

(b) [4 marks] Show that (3) can be integrated in 1D to obtain

$$e^{-\beta U(x)} \frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x} - e^{-\beta U(x_0)} \left. \frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x} \right|_{x_0} = -\frac{1}{D} \int_{x_0}^{x} \mathrm{d}x' \, e^{-\beta U(x')} \quad .$$

(c) [6 marks] For a symmetric potential profile $[U(-x) = U(x)]$ that has a metastable state (local minimum) at the origin that is surrounded by two symmetric barriers (separating it from the two symmetric global minima at $\pm\infty$), derive an expression for the mean first passage time for a particle that is initially at the origin.

(d) [7 marks] Assume that the main features of the potential landscape, i.e. the minimum and the two maxima, are sharp and use the Kramers approximation to simplify the expression for the escape time.