UNIVERSITY OF CAMBRIDGE

MATHEMATICAL TRIPOS Part III

Thursday, 9 June, 2022 9:00 am to 11:00 am

PAPER 356

STOCHASTIC PROCESSES IN THEORETICAL PHYSICS AND BIOLOGY

Before you begin please read these instructions carefully

Candidates have TWO HOURS to complete the written examination.

Attempt no more than **TWO** questions.
There are **THREE** questions in total.
The questions carry equal weight.

STATIONERY REQUIREMENTS
Cover sheet
Treasury tag
Script paper
Rough paper

SPECIAL REQUIREMENTS
None

You may not start to read the questions printed on the subsequent pages until instructed to do so by the Invigilator.

1 Consider a discrete-state continuous-time Markov process with rates w_{mn} and occupation probability $P(n,t)$. The entropy for this system is defined to be

$$S(t) = \sum_n P(n,t) \log P(n,t).$$

(a) Derive an expression for the entropy production in this system.

Consider a system with two states, labelled by the index $n = 1, 2$. The dynamics is modelled as a Markov process with rates $w_{12} = \alpha$ and $w_{21} = \beta$.

(b) Write down the evolution equation for the state probability $P(n,t)$.

(c) Show that the solution for the initial condition $P(1,0) = p$, $P(2,0) = 1-p$ is

$$P(1,t) = \frac{1}{\alpha+\beta}\left[\beta + re^{-(\alpha+\beta)t}\right]$$
$$P(2,t) = \frac{1}{\alpha+\beta}\left[\alpha - re^{-(\alpha+\beta)t}\right]$$

where $r = \alpha p - \beta(1-p)$.

(d) Compute the relaxational and steady state entropy production for this system.

(e) Hence, or otherwise, show that this system is always in detailed balance as $t \to \infty$.

Now consider a system with three states, labelled by the index $n = 1, 2, 3$ with rates $w_{12} = \alpha, w_{21} = \beta$, $w_{23} = \alpha, w_{32} = \beta$, $w_{31} = \alpha, w_{13} = \beta$.

(f) Write down the evolution equation for the state probability $P(n,t)$. Show that the solution for initial condition $P(1,0) = 1$, $P(2,0) = 0$, $P(3,0) = 0$ is

$$P(1,t) = \frac{1}{3}\left[1 + 2e^{-3\phi t}\cos\left(\sqrt{3}\psi t\right)\right]$$
$$P(2,t) = \frac{1}{3}\left[1 - 2e^{-3\phi t}\cos\left(\sqrt{3}\psi t - \frac{\pi}{3}\right)\right]$$
$$P(3,t) = \frac{1}{3}\left[1 - 2e^{-3\phi t}\cos\left(\sqrt{3}\psi t + \frac{\pi}{3}\right)\right]$$

where $\phi = (\alpha+\beta)/2$ and $\psi = (\alpha-\beta)/2$.

(g) Show that the entropy production for this system is

$$\dot{S} = (\alpha-\beta)\log\frac{\alpha}{\beta} + \sum_i \left[\alpha P(i,t) - \beta P(j,t)\right]\log\frac{P(i,t)}{P(j,t)}$$

where $j = i + 1[\text{mod } 3]$ and that the entropy flowing out of the system is

$$S_{neq} = (\alpha-\beta)\log\frac{\alpha}{\beta}.$$

(h) Hence, or otherwise, identify the condition for this system to be out of detailed balance.

2 Consider a particle with unit mass at position $X_t \in \mathbb{R}$ with velocity $V_t \in \mathbb{R}$ at time t evolving according to the stochastic differential equation (SDE)

$$\mathrm{d}V_t = -\left[U'(X_t) + \gamma V_t\right]\mathrm{d}t + \sqrt{2\gamma k_B T}\,\mathrm{d}W_t, \qquad \mathrm{d}X_t = V_t \mathrm{d}t, \tag{1}$$

where k_B is the Boltzmann constant and T the temperature.

a) Explain the physical system this may describe and the significance of the positive constant γ. Write the Fokker–Planck equation satisfied by the probability density $f(x, v, t)$ of the stochastic process (X_t, V_t). Provide a heuristic argument at the level of the SDE to eliminate V_t in the limit $\gamma \gg 1$ and obtain an equation for X_t alone. Hence argue that, in this limit, the probability density $p(x, t) = \int_{\mathbb{R}} f(x, v, t)\mathrm{d}v$ satisfies

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial p}{\partial x} + \phi'(x)p\right]. \tag{2}$$

where $D = k_B T/\gamma$ and $\phi(x) = U(x)/\gamma$.

b) Consider the potential $\phi(x) = \sin(x) - F_0 x$ with $F_0 \geqslant 0$. Show that if $0 \leqslant F_0 < 1$, $\phi(x)$ has one local minimum and one local maximum in each period, at $m_k = m + 2\pi k$ and $M_k = M + 2\pi k$, $k \in \mathbb{Z}$, respectively. Sketch $\phi(x)$.

Now consider the function

$$\hat{p}(x, t) = \sum_{k=-\infty}^{\infty} p(x + 2\pi k, t), \qquad x \in \Omega = (M_0, M_1). \tag{3}$$

Show that $\hat{p}$ is a probability density in Ω that satisfies (2) with periodic boundary conditions. Show that the stationary solution is

$$\hat{p}_s(x) = \frac{J_0 u(x)}{D(1 - e^{-2\pi F_0/D})} \quad \text{with } u(x) = e^{-\phi(x)/D}\int_x^{x+2\pi} e^{\phi(y)/D}\mathrm{d}y,$$

where J_0 is a constant. What does J_0 physically represent and how is it determined?

c) The mean velocity of the overdamped process $v = \mathbb{E}(\mathrm{d}X_t)/\mathrm{d}t$ satisfies

$$v(t) = \int_{-\infty}^{\infty} J(x, t)\mathrm{d}x,$$

where J is the probability flux, $J(x, t) = -D\frac{\partial p}{\partial x} - \phi'(x)p$. Determine the steady-state mean velocity v_s and deduce from it the net direction of motion for $F_0 > 0$.

[QUESTION CONTINUES ON THE NEXT PAGE]

d) For $F_0 \in (0,1)$ and $k_B T \ll 1$, show that

$$v_s \approx 2\pi(k_+ - k_-),$$

where k_+ and k_- are the escape rates from m_0 to M_1 and M_0 respectively, given by

$$k_+ = \frac{\sqrt{|\phi''(m_0)\phi''(M_1)|}}{2\pi} e^{-\Delta\phi_+/D}, \qquad k_- = \frac{\sqrt{|\phi''(m_0)\phi''(M_0)|}}{2\pi} e^{-\Delta\phi_-/D},$$

and $\Delta\phi_+ = \phi(M_1) - \phi(m_0)$, $\Delta\phi_- = \phi(M_0) - \phi(m_0)$ are the potential barriers.

Use $k_\pm$ to reduce the continuous process X_t to a continuous-time random walk on the local minima of $\phi(x)$, $\{m_k\}_{k\in\mathbb{Z}}$, providing the transition rates $W(k|l)$ to jump from m_l to m_k for $k, l \in \mathbb{Z}$. What is the distribution of the residence time in each state?

e) Consider now the same process in a bounded domain, so that the reduced model contains a finite number of wells $w_0, w_1, \ldots, w_K$ with absorbing boundaries at each end. Write the pseudocode for an exact algorithm to simulate the random walk for one particle.

Suppose now that we have N independent particles performing the same random walk. Discuss how the implementation of the algorithm may change between the cases $N \ll K$ and $N \gg K$.

Hint: you may use without proof the Laplace's formula that states, given $\Phi(x,y) : \Omega \to \mathbb{R}$ of the form $\Phi(x,y) = \phi_1(x) + \phi_2(y)$ with the global maximum at $(x,y) = (m, M) \in \Omega$,

$$\int_\Omega e^{\lambda\Phi(x,y)} \mathrm{d}x\mathrm{d}y \sim \frac{e^{\lambda\Phi(m,M)}}{\lambda} \frac{2\pi}{\sqrt{|\partial_x^2\Phi(m,M)\partial_y^2\Phi(m,M)|}}, \qquad \text{for } \lambda \gg 1.$$

3 A simple model for bacterial chemotaxis in one dimension consists of a particle (the bacterium) at position $X_t \in \mathbb{R}$ and velocity $V_t \in \{-s, s\}$ at time t, with

$$\mathrm{d}X_t = V_t \mathrm{d}t, \tag{1}$$

and V_t evolves according to a Poisson process: the particle at x changes its velocity from s to $-s$ at rate $\lambda^+(x)$, and from $-s$ to s at rate $\lambda^-(x)$. The turning rates are given by

$$\lambda^{\pm}(x) = \lambda_0 \mp bc'(x),$$

where $c(x)$ describes the concentration of a chemoattractant substance (which is fixed in time). Assume that $|c'(x)| < \lambda_0/b$ for all $x \in \mathbb{R}$.

a) Is the stochastic process (X_t, V_t) discrete or continuous? Is (X_t, V_t) a Markovian process? What about X_t alone?

b) Let $p^{\pm}(x,t)\mathrm{d}x = \mathbb{P}(X_t \in [x, x+\mathrm{d}x), V_t = \pm s)$ be the probability that, at time t, the bacterium is at position x, moving with velocity $\pm s$. Write the system of equations satisfied by $p^+(x,t)$ and $p^-(x,t)$. By considering the total probability density $p(x,t) = p^+(x,t) + p^-(x,t)$ and the flux $j(x,t) = s[p^+(x,t) - p^-(x,t)]$, obtain a closed equation for $p(x,t)$.

c) Consider the large λ_0 limit, and find appropriate scalings for s and b such that the total probability density $p(x,t)$ evolves according to

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial p}{\partial x} - \chi p c' \right), \tag{2}$$

Give the expressions of D and χ in terms of the parameters s, λ_0, b, and the conditions on $c(x)$ for (2) to have a stationary solution in $\mathbb{R}$. What stochastic differential equation does X_t satisfy in this limit?

d) Consider a population of N bacteria at positions X_t^i, for $i = 1, \ldots, N$, evolving accoding to

$$\mathrm{d}X_t^i = \chi c'(X_t^i)\mathrm{d}t - \frac{1}{N}\sum_{j=1, j\neq i}^{N} u'(X_t^i - X_t^j)\mathrm{d}t + \sqrt{2D}\mathrm{d}W_t^i, \tag{3}$$

where W_t^i are N independent Wiener processes and $u(x)$ is a symmetric function, $u(-x) = u(x)$, and monotonically decreasing for $x > 0$. What is the physical interpretation of u?

Consider the one-particle probability density $p(x_1,t)$, defined as $p(x_1,t)\mathrm{d}x = \mathbb{P}(X_t^1 \in [x_1, x_1 + \mathrm{d}x))$. Write down the evolution equation for $p(x_1,t)$ in terms of the two-particle probability density $P_2(x_1, x_2, t)$, defined as

$$P_2(x_1, x_2, t)\mathrm{d}x_1\mathrm{d}x_2 = \mathbb{P}(X_t^1 \in [x_1, x_1 + \mathrm{d}x_1), X_t^2 \in [x_2, x_2 + \mathrm{d}x_2)).$$

Derive a closed equation for $p(x_1,t)$ using the mean-field approximation as $N \to \infty$.

END OF PAPER