A15282W1

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

NONEQUILIBRIUM STATISTICAL PHYSICS

Trinity Term 2016

WEDNESDAY, 01 JUNE 2016, 14.30 to 16.00

You should submit answers to two of the three 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 microswimmer moving in two dimensions, whose motion is described by the Langevin equations

$$\mathbf{v}(t) = \frac{d\mathbf{r}}{dt} = v\,\mathbf{n}(t) + \mathbf{u}(t) \quad , \quad \frac{d\theta}{dt} = \omega + \beta(t) \quad , \tag{1}$$

where $\mathbf{r}(t) = (x(t), y(t))$, $\mathbf{n}(t) = (\cos\theta(t), \sin\theta(t))$ and $\mathbf{u}(t)$, $\beta(t)$ are Gaussian white noise variables with correlations

$$\langle u_i(t)\rangle = 0 \quad , \quad \langle u_i(t)u_j(t')\rangle = 2\,D\,\delta_{ij}\,\delta(t-t') \ , \quad i,j = 1,2 \ ,$$

$$\langle \beta(t)\rangle \ = 0 \quad , \quad \langle \beta(t)\beta(t')\rangle \ = 2\,D_r\,\delta(t-t') \ .$$

(a) [5 marks] Discuss the physical meaning of the various terms in (1). Do (1) describe a Markov process? Justify your answer.

(b) [10 marks] Show that

$$\langle [\theta(t) - \theta(0)]^2 \rangle = \omega^2 t^2 + 2D_r t \ ,$$

and

$$\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle = 4D\delta(t) + v^2\cos(\omega t)e^{-D_r t} \ .$$

Provide details of your workings.

(c) [5 marks] Show that the mean-square displacement is given by

$$\begin{aligned}\langle [\mathbf{r}(t) - \mathbf{r}(0)]^2 \rangle = & \, 4Dt + \frac{2v^2 D_r t}{D_r^2 + \omega^2} + \frac{2v^2(\omega^2 - D_r^2)}{(D_r^2 + \omega^2)^2} \\ & + \frac{2v^2\, \mathrm{e}^{-D_r t}}{(D_r^2 + \omega^2)^2}\left[(D_r^2 - \omega^2)\cos\omega t - 2\omega D_r \sin\omega t\right] .\end{aligned}$$

(d) [5 marks] Discuss the limiting behaviours of $\langle [\mathbf{r}(t) - \mathbf{r}(0)]^2 \rangle$ for short and long times. What happens in between?

What is the Fokker-Planck equation for the probability distribution of the swimmer's position at very late times?

2. Consider the stochastic dynamics of two particles under the influence of hydrodynamic interactions, whose trajectories are denoted as $R_i^\alpha(t)$, where $\alpha = 1, 2$ (particle label) and $i = 1, 2, 3$ (coordinate index). The particles interact with a potential $U(|\mathbf{R}^2 - \mathbf{R}^1|)$, and are otherwise free. Due to the hydrodynamic interactions, some components of the mobility tensor $\mu_{ij}^{\alpha\beta}$, which we will represent as $\boldsymbol{\mu}^{\alpha\beta}$, could be functions of $\mathbf{R}^2 - \mathbf{R}^1$. Both particles are spherical, and have radii of a_1 and a_2.

   (a) [2 marks] In the asymptotic regime where the particles are far from one another, write down expressions for the components of the mobility tensor, and identify those that depend on $\mathbf{R}^2 - \mathbf{R}^1$.

   (b) [4 marks] Write down the Langevin equations for the system, defining any new quantities that you need to introduce.

   (c) [6 marks] Explain briefly how the Langevin equations can be used to derive the following Fokker-Planck equation:

$$\begin{aligned}\partial_t \mathcal{P}(\mathbf{R}^1, \mathbf{R}^2, t) = {} & \boldsymbol{\nabla}_1 \cdot \left[\boldsymbol{\mu}^{11} \cdot (k_\mathrm{B}T\, \boldsymbol{\nabla}_1 \mathcal{P} + \boldsymbol{\nabla}_1 U\, \mathcal{P}) + \boldsymbol{\mu}^{12} \cdot (k_\mathrm{B}T\, \boldsymbol{\nabla}_2 \mathcal{P} + \boldsymbol{\nabla}_2 U\, \mathcal{P})\right] \\ & + \boldsymbol{\nabla}_2 \cdot \left[\boldsymbol{\mu}^{21} \cdot (k_\mathrm{B}T\, \boldsymbol{\nabla}_1 \mathcal{P} + \boldsymbol{\nabla}_1 U\, \mathcal{P}) + \boldsymbol{\mu}^{22} \cdot (k_\mathrm{B}T\, \boldsymbol{\nabla}_2 \mathcal{P} + \boldsymbol{\nabla}_2 U\, \mathcal{P})\right], \quad (2)\end{aligned}$$

   where $\boldsymbol{\nabla}_\alpha$ denotes gradient with respect to $\mathbf{R}^\alpha$. Justify any choices you make in modifying the equations.

   (d) [7 marks] Using a transformation to the centre of mass coordinates $\mathbf{R} = \frac{1}{2}\left(\mathbf{R}^2 + \mathbf{R}^1\right)$ and the relative coordinates $\mathbf{r} = \mathbf{R}^2 - \mathbf{R}^1$, show that the Fokker-Planck equation can be written as

$$\begin{aligned}\partial_t \mathcal{P}(\mathbf{R}, \mathbf{r}, t) = {} & k_\mathrm{B}T\, \boldsymbol{\nabla}_\mathbf{R} \cdot [\mathbf{M} \cdot \boldsymbol{\nabla}_\mathbf{R} \mathcal{P}] + k_\mathrm{B}T \left(\mu^{22} - \mu^{11}\right) \boldsymbol{\nabla}_\mathbf{R} \cdot (\boldsymbol{\nabla}_\mathbf{r} \mathcal{P}) \\ & + \frac{1}{2}\left(\mu^{22} - \mu^{11}\right)(\boldsymbol{\nabla}_\mathbf{r} U) \cdot (\boldsymbol{\nabla}_\mathbf{R} \mathcal{P}) + \boldsymbol{\nabla}_\mathbf{r} \cdot [\mathbf{m} \cdot (k_\mathrm{B}T\, \boldsymbol{\nabla}_\mathbf{r} \mathcal{P} + \boldsymbol{\nabla}_\mathbf{r} U\, \mathcal{P})], \quad (3)\end{aligned}$$

   where $\mathbf{M} = \frac{1}{4}\left(\boldsymbol{\mu}^{11} + \boldsymbol{\mu}^{22} + 2\boldsymbol{\mu}^{12}\right)$ and $\mathbf{m} = \boldsymbol{\mu}^{11} + \boldsymbol{\mu}^{22} - 2\boldsymbol{\mu}^{12}$.

   (e) [6 marks] By calculating $\partial_t \langle \mathbf{R} \cdot \mathbf{R} \rangle$ directly from the Fokker-Planck equation or otherwise, show that the diffusion coefficient of the centre of mass of the pair of particles is given by

$$D_\mathrm{CM} = \frac{k_\mathrm{B}T}{12} \int \mathrm{d}^3\mathbf{r}\; \mathrm{tr}\left(\boldsymbol{\mu}^{11} + \boldsymbol{\mu}^{22} + 2\boldsymbol{\mu}^{12}\right) \frac{1}{Z}\, e^{-U(\mathbf{r})/k_\mathrm{B}T},$$

   at equilibrium, where $Z = \int \mathrm{d}^3\mathbf{r}\; e^{-U(\mathbf{r})/k_\mathrm{B}T}$ is the canonical partition function describing the internal degrees of freedom of the compound system. Justify the form of this result.

3. (a) [6 marks] Using path-integration, find the expression for the conditional probability $\mathcal{P}(\mathbf{r}, t|\mathbf{r}_0, t_0)$ of finding a freely diffusing particle in $d = 3$ at position $\mathbf{r}$ at time t, knowing that it has started from position $\mathbf{r}_0$ at time t_0. Write down the corresponding forms of the same quantity in arbitrary dimension d.

(b) [3 marks] Write down the path-integral representation for the conditional probability, for a particle that undergoes stochastic dynamics in a potential $V(\mathbf{r})$, using Stratonovich convention ($\Theta(0) = 1/2$).

(c) [12 marks] For a harmonic potential $V(\mathbf{r}) = \frac{1}{2}k\mathbf{r}^2$, show that

$$\mathcal{P}(\mathbf{r}, t|\mathbf{r}_0, t_0) = \left(\frac{\beta k}{2\pi\left[1 - e^{-2k(t-t_0)/\zeta}\right]}\right)^{3/2} \exp\left\{-\frac{\beta k}{2}\frac{\left[\mathbf{r} - \mathbf{r}_0\, e^{-k(t-t_0)/\zeta}\right]^2}{\left[1 - e^{-2k(t-t_0)/\zeta}\right]}\right\} \quad . \qquad (4)$$

where $\beta = 1/(k_\mathrm{B}T)$ is the inverse temperature and ζ is the friction coefficient.

(d) [1 mark] Can k be negative? If so, what type of question can one address by setting k to negative values?

(e) [3 marks] Justify the form of (4) by examining different limiting behaviours that related the result to an expected or known form.