Nonequilibrium Statistical Physics

MMathPhys Noneq Stat Phys Course: Problem Sheet 1

Week 2, Hilary 2020

Qu 1. Consider a microswimmer moving in 2D described by its position $\mathbf{r}(t) = (x(t), y(t))$ and orientation $\hat{\mathbf{n}}(t) = (\cos\theta(t), \sin\theta(t))$, with velocity $\mathbf{v} = v\,\hat{\mathbf{n}}$ along its director (constant speed).

The Langevin equations describing translation and rotation of the swimmer are:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = v\,\hat{\mathbf{n}}(t) + \mathbf{u}(t) \quad , \quad \frac{\mathrm{d}\theta}{\mathrm{d}t} = \beta(t) \quad ,$$

where $\mathbf{u}(t)$ and $\beta(t)$ are Gaussian white noises whose correlations are given by

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

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

Show that the orientational memory is lost exponentially with time:

$$\langle \hat{\mathbf{n}}(t)\cdot\hat{\mathbf{n}}(0)\rangle = e^{-D_r t}$$

Use the orientational auto-correlation to show that the translational Mean-Squared Displacement is given as

$$\Delta L(t)^2 = 4D\,t + \frac{2v^2}{D_r}\left[t + \frac{1}{D_r}\left(e^{-D_r t} - 1\right)\right] .$$

Discuss the limiting behaviours for short and long times.

Qu 2. Let $y = \pm 1$. Show that

$$\mathcal{P}(y,t \mid y',t') = \frac{1}{2}\left\{1 + e^{-2\gamma(t-t')}\right\}\delta_{y,y'} + \frac{1}{2}\left\{1 - e^{-2\gamma(t-t')}\right\}\delta_{y,-y'}$$

obeys the Chapman-Kolmogorov equation.

Show that

$$\mathcal{P}(y,t) = \frac{1}{2}(\delta_{y,1} + \delta_{y,-1})$$

is a stationary solution. Write $P(y,t \mid y',t')$ as a 2×2 matrix and formulate the Chapman-Kolmogarov equation as a property of that matrix.

Qu 3. This question is about a continuous random walk, also known as a Wiener process.
Show that for $-\infty < y < \infty$ and $t_2 > t_1$ the Chapman-Kolmogorov equation is satisfied for

$$\mathcal{P}(y_2,t_2 \mid y_1,t_1) = \frac{1}{\sqrt{4\pi D(t_2-t_1)}}\exp\left\{-\frac{(y_2-y_1)^2}{4D(t_2-t_1)}\right\} .$$

Choose $P(y_1,0) = \delta(y_1)$. Show that for $t > 0$

$$P(y,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left\{-\frac{y^2}{4Dt}\right\} .$$

Show that $P(y,t)$ obeys the diffusion equation $\partial_t P = D\,\partial_y^2 P$.

Qu 4. A particle suspended in a fluid undergoes Brownian motion in one dimension with position $x(t)$ and velocity $v(t)$. This motion is modelled by the Langevin equation

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + \eta(t),$$

where $\eta(t)$ is a Gaussian random variable characterized completely by the averages $\langle\eta(t)\rangle = 0$ and $\langle\eta(t_1)\eta(t_2)\rangle = \Gamma\delta(t_1 - t_2)$. Discuss the physical origin of each of the terms in the Langevin equation.

What is meant by the term *Markov process*? Illustrate your answer by discussing which of the following are Markov processes: (a) $v(t)$ alone; (b) $x(t)$ alone; (c) $v(t)$ and $x(t)$ together.

Show that for $t > 0$

$$x(t) = \frac{v(0)}{\gamma}\,(1 - \mathrm{e}^{-\gamma t}) + \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\; \mathrm{e}^{-\gamma(t_1 - t_2)}\,\eta(t_2)$$

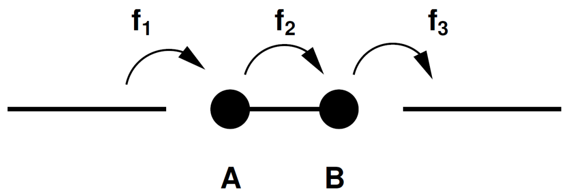
is a solution of the Langevin equation with initial condition $x(0) = 0$. Calculate the average $\langle x(t)\,v(t)\rangle$ and discuss its limiting behaviour at short and long times.

Qu 5. The time evolution of a stochastic system is represented by a master equation of the form

$$\frac{\mathrm{d}p_n(t)}{\mathrm{d}t} = \sum_m W_{nm} p_m(t)\,.$$

Explain briefly the meaning of this equation and discuss the assumptions on which it is based. What general conditions should the matrix elements W_{nm} satisfy?

A molecule lies between two atomic-scale contacts and conducts charge between them. A simple model of this situation is illustrated below. The model has three states: the molecule may be uncharged, or may carry a single charge at either site A or site B but not both. Charges hop between these sites, and between the sites and the contacts, at the rates indicated in the figure. (For example, a charge at site A has probability f_2 per unit time of hopping to site B.)



Write down a master equation for this model. For the stationary state of the system, calculate the occupation probabilities of the three states, and show that the average number of charges flowing through the molecule per unit time is

$$\frac{f_1 f_2 f_3}{f_1 f_2 + f_1 f_3 + f_2 f_3}\,.$$

Consider the case $f_1 = f_2 = f_3 \equiv f$. The molecule is uncharged at time $t = 0$. Show that the probability $p(t)$ for it to be uncharged at a later time t is

$$p(t) = \frac{1}{3} + \frac{2}{3}\exp\left(-\frac{3}{2}ft\right)\cos\left(\frac{\sqrt{3}}{2}ft\right)\,.$$