Stochastic Processes in Natural Sciences

Christmas Problems 2023

Problem 1: From the Rayleigh description to the Brownian picture

The Rayleigh particle is the same particle as the Brownian particle, but studied on a finer time scale. In this problem, we will see how changing the time scale of observation to longer makes it more appropriate to use the Brownian description.

- For a Rayleigh particle, we argued that its velocity can be treated as a random variable and therefore the corresponding Fokker-Planck equation is:

$$\frac{\partial P(v,t)}{\partial t} = \gamma \left\{ \frac{\partial}{\partial v}(vP) + \frac{k_B T}{M} \frac{\partial^2 P}{\partial v^2} \right\} \tag{1}$$

- We have shown the solution to the FP equation above to define the Ornstein-Uhlenbeck process – what is the distribution function of the transition probability?

- On a coarser time scale, when the times of interest are much larger than the velocity relaxation time scale γ^{-1}, the description by velocity becomes irrelevant. Instead, the position is treated as a random variable, and the FP equations takes the form

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P}{\partial x^2}$$

- We need to show that upon coarse-graining, we recover the Brownian description from the Rayleigh picture. To do so, consider the position of the particle

$$\Delta x(t) = \int_{t_0}^{t} \mathrm{d}t' v(t'), \tag{2}$$

  with $x(t=0)=0$.

- First, show that $x(t)$ is Gaussian. The fact that x is Gaussian means that to characterise it we only need the mean and the autocorrelation function.

- Find $\langle x(t) \rangle$.

- Find the expression for the autocorrelation function $\langle\langle x(t_2)x(t_1)\rangle\rangle$ using the position defined as above. See that in general the process X for arbitrary times is not Markovian. Now show that on a coarse time scale, when $t_1, t_2 - t_1 \gg \gamma^{-1}$, the autocorrelation function becomes

$$\langle\langle x(t_2)x(t_1)\rangle\rangle = \frac{2k_B T}{M\gamma} \min(t_1, t_2).$$

  Conclude that X is a zero-mean Gaussian process with the autocorrelation as above, therefore it is a Wiener process, and satisfies the FP equation

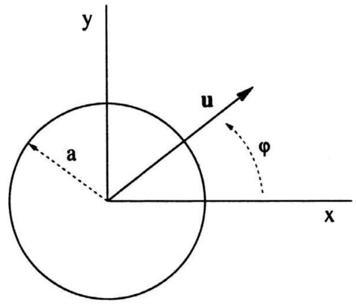
$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P}{\partial x^2}. \tag{3}$$

  Thus deduce the fluctuation-dissipation relationship

$$D = \frac{k_B T}{M\gamma}.$$

From this example we can see that the Wiener process may be treated as a long-time integral of the Ornstein-Uhlenbeck process.

Problem 2: Debye's rigid rotator



Consider a spherical particle of radius a with a picked out direction, say a net dipole moment $\boldsymbol{m}$ which we can write as $\boldsymbol{m} = m\boldsymbol{u}$, with $\boldsymbol{u}$ being a unit vector. Suppose now the particle is constrained to rotate only about a fixed axis, and that it is immersed in a fluid. Choosing the rotation plane spanned by the axes x and y, we cen describe the rotations by a single angle φ, as drawn above.

Collisions with the fluid will generate a fluctuating torque on the sphere. At the same time, if we try to rotate the sphere by an external, there will be a systematic drag resistance from the fluid, i.e. the torque $M_r = -\zeta_r\dot{\varphi}$. The corresponding Smoluchowski (Fokker-Planck) equation for the probability density $P(\varphi, t)$ of finding the vector $\boldsymbol{u}$ to be at an angle φ at time t,

$$\frac{\partial P(\varphi, t)}{\partial t} = D_r \frac{\partial^2 P(\varphi, t)}{\partial \varphi^2},$$

with the rotational diffusion coefficient $D_r = k_B T/\zeta_r$.

- **Solve** the Smoluchowski equation with the initial condition $P(\varphi, 0) = \delta(\varphi - \varphi_0)$. **Find and interpret** the approximate form solution for very long times $t \to \infty$. For short times this distribution becomes Gaussian around φ_0 (no need to show this).
  Hint: use the separation of variables and the representation of Dirac delta as a a Fourier series

$$\delta(\varphi - \varphi_0) = \frac{1}{2\pi} + \frac{1}{\pi}\sum_{m=1}^{\infty} \cos m(\varphi - \varphi_0).$$

- Now assume that there is an external torque due to an electric field $\boldsymbol{E}$ in the x direction. This means that there will be an external potential energy $V(\phi) = -\boldsymbol{m} \cdot \boldsymbol{E} = -mE\cos\varphi$ and a corresponding torque $M = -\frac{\partial V}{\partial \varphi}$. **Show** that the Smoluchowski equation in this case becomes

$$\frac{\partial P}{\partial t} = D_r \frac{\partial}{\partial \varphi}\left(\frac{\partial P}{\partial \varphi} + \xi P \sin\varphi\right),$$

  with the dimensionless field $\xi = mE/k_B T$.

- In 1913, Debye considered a model dipole in a weak and steadily oscillating field $\xi(t) = \xi_0 e^{-i\omega t}$, with $\xi_0 \ll 1$. In this weak field limit, we can solve the first order, linear response problem by expanding the distribution function in the small parameter ξ_0,

$$P = P_0 + \xi_0 P_1 + \ldots,$$

  with the zero-field uniform distribution $P_0 = (2\pi)^{-1}$. **Find** the resulting equation for P_1. **Check** that

$$P_1(\varphi, t) = \frac{\cos\varphi}{2\pi(1 - i\omega\tau)} e^{-i\omega t},$$

  is a particular solution of this equation, where a characteristic time scale $\tau = 1/D_r$ appears. In fact, this is the solution that satisfies periodicity conditions in φ (no need to show this). In further calculations, Debye used this relationship to find the polarisation of the medium $\mathcal{P} \propto \langle\cos\varphi\rangle$ and the frequency dependent index of refraction.