

Problem Set 11 – Microhydrodynamics & fluctuations

Problem 1: Drift and diffusion under a constant force

Consider a one-dimensional overdamped Brownian particle subject to a constant force F . Its probability density satisfies

$$\frac{\partial P}{\partial t} = -\mu F \frac{\partial P}{\partial x} + D \frac{\partial^2 P}{\partial x^2}, \quad D = \mu k_B T,$$

with initial condition $P(x, 0) = \delta(x)$.

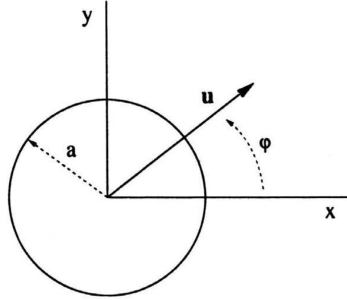
- (a) Show that the solution can be written as a drifting Gaussian

$$P(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - \mu Ft)^2}{4Dt}\right].$$

- (b) Compute $\langle x(t) \rangle$ and $\langle [x(t) - \langle x(t) \rangle]^2 \rangle$.
- (c) Compare the result with pure diffusion and explain which part comes from deterministic drift and which part comes from thermal fluctuations.
- (d) Show that the mean-square displacement relative to the origin, $\langle x(t)^2 \rangle$, contains both a term proportional to t and a term proportional to t^2 . Interpret these two contributions physically.

Problem 2: Debye's rigid rotator

Consider a spherical particle of radius a with a picked out direction, say a net dipole moment \mathbf{m} which we can write as $\mathbf{m} = m\mathbf{u}$, with \mathbf{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 can describe the rotations by a single angle φ , as drawn below.



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 equation for the probability density $P(\varphi, t)$ of finding the vector \mathbf{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 $D_r = k_B T / \zeta_r$.

- (a) Solve the Smoluchowski equation with the initial condition $P(\varphi, 0) = \delta(\varphi - \varphi_0)$. Find and interpret the approximate form of the solution for very long times $t \rightarrow \infty$. 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 Fourier series $\delta(\varphi - \varphi_0) = (2\pi)^{-1} + \pi^{-1} \sum_{m=1}^{\infty} \cos m(\varphi - \varphi_0)$.

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

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

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

- (c) 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 ,

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

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

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

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 $\mathcal{P} \propto \langle \cos \phi \rangle$ and the frequency-dependent index of refraction.

Problem 3: Brownian motion in a harmonic trap

Consider a one-dimensional Brownian particle in the harmonic potential

$$V(x) = \frac{k}{2} x^2.$$

Assume the particle diffusion coefficient to be $D = \mu k_B T$.

- Write the relevant Smoluchowski equation.
- Show that the equilibrium distribution $P_{\text{eq}}(x)$ is Gaussian and determine its variance.
- Interpret the result in terms of equipartition.
- Estimate the characteristic relaxation time of the deterministic motion in the trap.

Problem 4: The Smoluchowski operator

Consider the one-dimensional Smoluchowski equation for a particle in a potential $V(x)$,

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left[\mu V'(x) P + D \frac{\partial P}{\partial x} \right], \quad D = \mu k_B T.$$

- (a) Write the equation in the form

$$\frac{\partial P}{\partial t} = \mathcal{D}P,$$

and identify the Smoluchowski operator \mathcal{D} .

- (b) Show that $\mathcal{D}P_{\text{eq}} = 0$ for the Boltzmann distribution

$$P_{\text{eq}}(x) \propto e^{-V(x)/k_B T}.$$

- (c) Show that \mathcal{D} can be written as

$$\mathcal{D} = D \frac{\partial}{\partial x} \left(e^{-\beta V} \frac{\partial}{\partial x} e^{\beta V} \cdot \right).$$

- (d) Explain briefly why the condition $\mathcal{D}P_{\text{eq}} = 0$ means that the equilibrium distribution is a zero mode of the Smoluchowski operator.