Complementary Statistical Physics

Series 1: Brownian motion and random walk

1. Consider a spherical Brownian particle of mass m and radius r in a fluid of viscosity η at temperature T. The appropriate Langevin equation is:

$$\dot{\vec{v}}(t) = -\gamma \vec{v}(t) + \vec{\xi}(t) \quad , \tag{1}$$

where $\gamma = 6\pi r\eta/m$ and $\vec{\xi}$ represents the rapidly fluctuating interaction with the fluid: $\langle \vec{\xi}(t) \rangle = 0$ and $\langle \xi_i(t)\xi_j(t') \rangle = \Gamma/m \delta_{ij}\delta(t-t')$ for any coordinate i and j, where $\langle \dots \rangle$ is the ensemble avarage.

   1.1. Show that, in the limit $\vec{\xi}(t) = 0$, the solution of Eq. (1) is $\vec{v}(t) = \vec{v}(0)e^{-\gamma t}$.

   1.2. Derive the formal solution for the velocity $\vec{v}(t)$.

      1.2.1. Determine $\langle \vec{v}(t) \rangle$, supposing that the initial velocity is the same for all the ensemble of particles.

      1.2.2. Determine $\langle v^2(t) \rangle$. Using the theorem for the equipartition of the energy show that $\Gamma = 2\gamma k_B T$, where d is the spatial dimension of the system.

   1.3. Derive now the formal solution for the position $\vec{x}(t)$.

      1.3.1. Determine $\langle \vec{x}(t) \rangle$, assuming that the initial position and velocity is the same for the ensemble of particles.

      1.3.2. Determine $\langle x^2(t) \rangle$. Show that for long times $\langle x^2(t) \rangle \sim 2d \left[\frac{k_B T}{m\gamma}\right] t$.

2. For the system of the previous problem, the discretized version of the equation for the velocities is:

$$\vec{v}(t) - \vec{v}(0)e^{-\gamma t} = \sum_{j=1}^{t/\Delta t} \vec{\zeta}_j \quad , \qquad \vec{\zeta}_j = e^{-\gamma t} \int_{(j-1)\Delta t}^{j\Delta t} \vec{\xi}(t') e^{\gamma t'} dt' \quad . \tag{2}$$

   2.1. Using the central limit theorem, show that for each direction $i, j \in \{x, y, z\}$, $\langle (v_i(t) - v_i(0)e^{-\gamma t})(v_j(t) - v_j(0)e^{-\gamma t}) \rangle = \frac{k_B T}{m} \left[1 - e^{-2\gamma t}\right] \delta_{ij}$.

   2.2. If $P(\vec{v}, t|\vec{v}(0))$ is the density probablity for the velocity and using $P(\vec{v}, t|\vec{v}(0)) = P(v_x, t|v_x(0))P(v_y, t|v_y(0))P(v_z, t|v_z(0))$, show that:

$$P(\vec{v}, t|\vec{v}(0)) = \left[\frac{m}{2\pi k_B T\left(1 - e^{-2\gamma t}\right)}\right]^{\frac{3}{2}} \exp\left[-\frac{m\left(\vec{v} - \vec{v}(0)e^{-\gamma t}\right)^2}{2k_B T\left(1 - e^{-2\gamma t}\right)}\right] \quad . \tag{3}$$

3. In a discrete random walk in one dimension, at each step, a particle hops to the right with probability p and to the left with probability $q = 1 - p$. Let $P_N(x)$ be the probability of the particle being at position x after N steps.

   3.1. Write the master equation for the probability $P_N(x)$.

3.2. For the initial condition $P_0(x) = \delta_{x,0}$, show that the generating function for the Fourier transform,

$$P(k, z) = \sum_{N \geq 0} z^N \sum_{x=-\infty}^{\infty} e^{ikx} P_N(x) \quad , \tag{4}$$

is given by $P(k, z) = [1 - zu(k)]^{-1}$, where $u(k) = pe^{ik} + qe^{-ik}$ is the Fourier transform of the probability for single step.

3.3. Determine the distribution of probablity of the random walk.

4. Consider the continuum limit of a random walk in one dimension, which at each step, hops to the right with probability p and to the left with probability $q = 1 - p$.

4.1. For the symmetric case ($p = q = 1/2$), derive the diffusion equation ($D = 1/2$) expanding in Taylor series up to first order in time and second order in space.

4.2. Generalize the result for the asymmetric case and show that in the continuum limit:

$$\frac{\partial P(x,t)}{\partial t} + v \frac{\partial P(x,t)}{\partial x} = D \frac{\partial^2 P(x,t)}{\partial x^2} \quad . \tag{5}$$

Determine the diffusion coefficient D and the velocity v in terms of the microscopic parameters parâmetros p and q.

4.3. For the initial condition $P(x, 0) = \delta(x)$, show the solution Eq. (5) é:

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-(x-vt)^2/4Dt} \quad . \tag{6}$$