RANDOM WALKS AND LANGEVIN EQUATION

If we watch the motion of a pollen particle in a drop of liquid under the microscope then we will best describe it as random motion with a discontinuous trajectory. Such a random motion is called Brownian motion named after the biologist R. Brown who was the first to report this phenomena. Although the work of Brown has attracted a lot of attention but theoretical study of Brownian motion began with the efforts of A. Einstein to confirm the atomic nature of matter. Einstein's efforts have lead to a relationship between the macroscopic diffusion constant D and the microscopic properties of matter.

Langevin Equation

Let us consider a spherical particle of mass m and radius R immersed in a fluid whose atoms are much smaller than the particle. The density fluctuations in the fluid around the particle causes the particle to perform agitated motion whose relaxation time is much longer than the relaxation time for the motion of the atoms in the fluid. Due to the vast difference between the two time scales for the agitated particle motion and the motion of the atoms in the fluid we can focus on the Bronian particle alone and ignore the state of the fluid. Now, consider that the particle moving in one dimension and that the effect of the fluid on the particle motion can be accounted for by a friction force that is proportional to the particle's velocity and a random force $\xi(t)$. From Newton's second law we write the governing equations for the particle's position $x(t)$ and velocity $v(t)$ which are usually called the *Langevin Equations*:

$$\frac{dv(t)}{dt} = -\frac{\gamma}{m}v(t) + \frac{1}{m}\xi(t) \tag{1}$$

$$\frac{dx(t)}{dt} = v(t) \tag{2}$$

the friction coefficient is defined as $\gamma = 6\pi\eta R$ where η is the shear viscosity of the fluid.

We will assume that the background noise $\xi(t)$ is gaussian and has zero mean $< \xi(t) >_\xi$. We mean by gaussian noise is that its realization probability distribution is a gaussian function and that its mean with respect to this distribution function is zero. To further simplify the problem we assume the noise to be white hence

$$< \xi(t)\xi(t') >_\xi = g\delta(t-t') \tag{3}$$

This means that the noise is instantaneously self correlated, the realization of noise at time instant t' is not correlated with its realization at another time instant t. Due to the fact that the noise is gaussian (even function of ξ) and has zero mean, one concludes that correlation functions that contain odd power of ξ must vanish. To solve eqs.(1) and (2) we use the transformation $v(t) = u(t)e^{-\gamma t/m}$ which give us the following solution

$$v(t) = v_0 e^{-\gamma t/m} + \frac{1}{m}\int_0^t \xi(s)e^{-\gamma(t-s)/m}ds \tag{4}$$

$$x(t) = x_0 + \frac{mv_0}{\gamma}(1-e^{-\gamma t/m}) + \frac{1}{\gamma}\int_0^t \xi(s)(1-e^{-\gamma(t-s)/m})ds \tag{5}$$

where $v(t=0) = v_0$ and $x(t=0) = x_0$. Note that because $< \xi(t) >_\xi = 0$ then

$$< v(t) >_\xi = v_0 e^{-\gamma t/m} \tag{6}$$

$$< x(t) >_\xi = x_0 + \frac{mv_0}{\gamma}(1-e^{-\gamma t/m}) \tag{7}$$

Noise effects do not appear in $< v(t) >_\xi$ and $< x(t) - x_0 >_\xi$ but as I will show below that the velocity and position correlation functions do include noise effects. To prove this we need to calculate $< v(t)v(t') >_\xi$ and the variance $< (x(t)-x_0)^2 >_\xi$ and show that they contain terms proportional to g.

First let us consider $< v(t)v(t') >_\xi$:

$$< v(t)v(t') >_\xi = \langle\left(v_0 e^{-\gamma t/m} + \frac{1}{m}\int_0^t \xi(s)e^{-\gamma(t-s)/m}ds\right)\times \left(v_0 e^{-\gamma t'/m} + \frac{1}{m}\int_0^{t'} \xi(s)e^{-\gamma(t'-s)/m}ds\right)\rangle_\xi \tag{8}$$

however, because the noise is gaussian and has zero mean then the cross product vanishes after averaging over noise realizations hence

$$< v(t)v(t') >_\xi = (v_0^2 - \frac{g}{2m\gamma})e^{-\gamma(t+t')/m} + \frac{g}{2m\gamma}e^{\gamma(t-t')/m} \tag{9}$$

when the particle is in equilibrium with the fluid its velocity correlation function must be stationary i.e $< v(t)v(t') >_\xi \equiv C_{vv}(t-t')$. This is satisfied when $v_0 = \sqrt{g/2m\gamma}$. The variance $< (x(t) - x_0)^2 >_\xi$ can be calculated in a similar manner yielding

$$\begin{aligned} < (x(t) - x_0)^2 >_\xi &= \frac{m^2}{\gamma^2}\left(v_0^2 - \frac{g}{2m\gamma}\right)(1 - e^{-\gamma t/m})^2 \\ &+ \frac{g}{\gamma^2}\left[t - \frac{m}{\gamma}(1 - e^{-\gamma t/m})\right] \end{aligned} \tag{10}$$

Note that after a long time $t \gg \tau_0 = \frac{m}{\gamma}$ the variance becomes linearly dependant on time i.e. $< (x(t) - x_0)^2 >_\xi \propto t$. This suggest defining the *diffusion coefficient* D in terms of g and γ as $D = g/2\gamma^2$. If we assume that the Brownian particle is in equilibrium with the fluid then we can apply the equipartition theorem which states that the average kinetic energy per degree of freedom for an object in equilibrium with its surrounding is $\frac{k_BT}{2}$ i.e. $\frac{m}{2} < v_0^2 >_T = \frac{k_BT}{2}$ where $< X >_T$ is the thermal average of X. From the above discussion we get $g = 2\gamma k_BT$ hence the diffusion constant is $D = k_BT/\gamma$.

Power Spectrum

Let us consider that we have a stochastic variable whose time series $\psi(t, T)$ is experimentally recorded over a finite time interval $-\frac{T}{2} \leq t \leq \frac{T}{2}$. A quantity that contain a great deal information about the stochastic process is the *Power Spectrum*

$$S_{\psi\psi}(\omega) = \lim_{T\to\infty} \frac{1}{T}\tilde{\psi}^*(\omega, T)\tilde{\psi}(\omega, T) \tag{11}$$

where $\tilde{\psi}(\omega, T)$ is the Fourier transform of $\psi(t, T)$ defined as

$$\tilde{\psi}(\omega, T) = \int_{-\infty}^{\infty} \psi(t, T)e^{\imath\omega t}dt \tag{12}$$

Note that because $\psi(t, T)$ must be real then $\tilde{\psi}(\omega, T)$ must satisfy $\tilde{\psi}^*(\omega, T) = \tilde{\psi}(-\omega, T)$. Clearly, one can easily calculate $\psi(t, T)$ if $\tilde{\psi}(t, T)$ is known

$$\psi(t, T) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{\psi}(\omega, T)e^{-\imath\omega t}d\omega \tag{13}$$

using (12) in (11) yields

$$S_{\psi\psi}(\omega) = \lim_{T\to\infty} \frac{1}{T}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \psi(t_1, T)\psi(t_2, T)e^{-\imath\omega(t_1-t_2)} \tag{14}$$

It is useful to define the time correlation function for ψ as

$$C_{\psi\psi}(\tau) = \frac{1}{T}\int_{-\infty}^{\infty} \psi(t+\tau, T)\psi(t, T)dt \tag{15}$$

Therefore, the power spectrum is

$$S_{\psi\psi}(\omega) = \int_{-\infty}^{\infty} C_{\psi\psi}(\tau)e^{-\imath\omega\tau}d\tau \tag{16}$$

Linear Response Theory

The theory that deal with the response of a system in equilibrium to weak perturbations is known as *Linear Response Theory*. In this section we will focus on a system of a simple harmonic oscillator of mass m and spring constant k immersed in a viscous fluid whose shear viscosity is η. The forces acting on mass m is the inertial force, a restoring force a frictional force proportional to the particle velocity and random kicks $\xi(t)$ generated by fluid density fluctuations. We have investigated the solution of such system earlier when we discussed Langevin equations (except that $\omega_0 \neq 0$ here). Let us now assume that in addition to all these forces exerted on the particle a small external time-dependant force $F(t)$ is applied to the system. Our goal now is to study the response of the system to the external force. We begin by writing down the equation of motion for the mass m is then

$$m\frac{d^2x_F(t)}{dt^2} + \gamma\frac{dx_F(t)}{dt} + m\omega_0^2 x_F(t) = F(t) + \xi(t) \tag{17}$$

We are interested only in the response of the system to the external force hence if we average eq.(18) over noise assuming that ξ is gaussian with zero mean we get

$$m\frac{d^2 < x_F(t) >_\xi}{dt^2} + \gamma\frac{d < x_F(t) >_\xi}{dt} + m\omega_0^2 < x_F(t) >_\xi = F(t) \tag{18}$$

This is a linear second order inhomogeneous differential equation with constant coefficients m, γ and $m\omega_0^2$ whose general solution is written as

$$< x_F(t) >_\xi = x_0(t) + \int_{-\infty}^{\infty} \chi(t-t')F(t')dt' \tag{19}$$

where $x_0(t)$ is the solution for eq.(18) when $F(t) = 0$. The function $\chi(t-t')$ is called the response function and is a measure of the system response to a driving force. The response function must be causal that is it is defined only for $t \geq t'$ and vanishes otherwise. Note that the response of the system to the external force is linear function of $F(t)$ which is the reason for the name linear response theory. We substitute (19) in (18) we find:

$$m\frac{d^2\chi(t-t')}{dt^2} + \gamma\frac{d\chi(t-t')}{dt} + m\omega_0^2\chi(t-t') = \delta(t-t') \tag{20}$$

To solve (20) we define the *Susceptibility* $\tilde{\chi}(\omega)$ as the Fourier transform of $\chi(t-t')$

$$\chi(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{\chi}(\omega)e^{-\imath\omega(t-t')}d\omega \tag{21}$$

substituting (21) in (20) we find

$$\int_{-\infty}^{\infty} \left[-m(\omega^2-\omega_0^2) - \imath\omega\gamma\right]\tilde{\chi}(\omega)e^{-\imath\omega(t-t')}d\omega = 2\pi\delta(t-t') \tag{22}$$

Multiply both sides of (22) by $e^{\imath\omega'(t-t')}$ and integrate over time we get

$$\tilde{\chi}(\omega) = \frac{1}{m(\omega_0^2-\omega^2) - \imath\gamma\omega} \tag{23}$$

Note that the susceptibility has both real part $\tilde{\chi}'(\omega)$ and imaginary part $\tilde{\chi}''(\omega)$

$$\tilde{\chi}'(\omega) = \frac{m(\omega_0^2-\omega^2)}{m^2(\omega_0^2-\omega^2)^2+\gamma^2\omega^2} \tag{24}$$

$$\tilde{\chi}''(\omega) = \frac{\gamma\omega}{m^2(\omega_0^2-\omega^2)^2+\gamma^2\omega^2} \tag{25}$$

The Fourier transform of $\chi(\omega)$ yields

$$\chi(t-t') = \frac{\sin\left(\sqrt{\omega_0^2-\frac{\gamma^2}{4m^2}}(t-t')\right)e^{-\frac{\gamma(t-t')}{2m}}}{m\sqrt{\omega_0^2-\frac{\gamma^2}{4m^2}}}\theta(t-t') \tag{26}$$

the step function $\theta(t-t')$ appear in (26) to insure the causality of $\chi(t-t')$. There are three different interesting regimes depending on the ratio $\kappa = 2m\omega_0/\gamma$ such that if $\kappa > 1$ the oscillator is called *underdamped* while it is called *overdamped* if $\kappa < 1$. Another case that is of great interest is when $\kappa = 1$ in which the system is called *critically damped.*

The susceptibility $\tilde{\chi}(\omega)$ is related to spectral density function of the equilibrium fluctuations. Let us define $\delta x(t) =< x_F(t) >_\xi - x_0(t)$. If one calculates the correlation function $C_{\delta x \delta x}(t - t') =< \delta x(t)\delta x(t') >$ and then its Fourier transform $S_{\delta x \delta x}(\omega)$ then it is easy to show that

$$S_{\delta x \delta x}(\omega) = \frac{2k_B T}{\omega} Im(\tilde{\chi}(\omega)) \tag{27}$$

This result is known as the *Fluctuation-Dissipation* theorem. This theorem is very important as it allows us to understand the equilibrium fluctuations of the system by observing the system response to weak perturbations and its behavior as it relaxes to the equilibrium state.