- HH0050 -

Fokker-Plank Equation

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In the previous lecture, we stated that the probability distribution $P(x,t)$ for a stochastic process satisfies the master equation,

$$P(x, t+\Delta t) = \int_{-\infty}^{\infty} d\Delta x \, f(\Delta x) P(x', t), \tag{1}$$

where $\Delta x = x - x'$ and $f(\Delta x)$ is the probability density for the particle to move from x' to x within the time interval Δt. Expanding the variable $x' = x - \Delta x$ in Taylor series, the above integral equation turns into the diffusion equation. However, in the presence of non-uniform force field $F(x)$, the probability density $f = f(\Delta x, x')$ also depend on the starting point x'. We shall discuss how to derive the appropriate equation when the uniformity of the system is gone. It is interesting to note that the master equation is similar to the propagation of wave function in quantum mechanics,

$$\psi(x, t') = \int_{-\infty}^{\infty} dx' \, G(x, t; x', t') \psi(x', t), \tag{2}$$

where $G(x,t;x',t')$ is the single-particle propagator. The wave function appears in the "master equation", not the probability distribution.

• Smoluchowski equation

To include the dependence on the starting point x', the master equation now take the form,

$$P(x, t+\Delta t) = \int_{-\infty}^{\infty} d\Delta x \, f(\Delta x, x') P(x', t), \tag{3}$$

where $x' = x - \Delta x$. Expand the whole integrand $f(\Delta x, x')P(x')$ in Taylor series around x,

$$\begin{aligned} P(x, t+\Delta t) = \int_{-\infty}^{\infty} d\Delta x \Big\{ & f(\Delta x, x) P(x,t) + \frac{\partial}{\partial x}\Big[f(\Delta x, x)P(x)\Big](-\Delta x) \\ & + \frac{1}{2}\frac{\partial^2}{\partial x^2}\Big[f(\Delta x, x)P(x)\Big](-\Delta x)^2 + ... \Big\}, \end{aligned} \tag{4}$$

In the following, we truncate the series at the second order and drop all higher-order terms. The first term just gives $P(x,t)$ because $f(\Delta x, x)$ is a probability density (integration to unity). Treating Δx and x as independent variables,the remaining terms can be simplified by exchanging the order of integration and differentiation,

$$P(x,t+\Delta t) - P(x,t) = -\frac{\partial}{\partial x}\Big[\Big(\int_{-\infty}^{\infty} d\Delta x\, f(\Delta x, x)\Delta x\Big)P(x)\Big] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\Big[\Big(\int_{-\infty}^{\infty} d\Delta x\, f(\Delta x, x)(\Delta x)^2\Big)P(x)\Big]. \quad (5)$$

Introduce the average displacement $\langle \Delta x \rangle$ and its variance $\langle (\Delta x)^2 \rangle$ for the stochastic process,

$$\langle \Delta x \rangle = \int_{-\infty}^{\infty} d\Delta x\, f(\Delta x, x)\Delta x = \mu_p E(x)\Delta t + \mathcal{O}[(\Delta t)^2], \quad (6)$$

$$\langle (\Delta x)^2 \rangle = \int_{-\infty}^{\infty} d\Delta x\, f(\Delta x, x)(\Delta x)^2 = 2D(x)\Delta t + \mathcal{O}[(\Delta t)^2], \quad (7)$$

where $E(x) = F(x)/q$ is the local electric field, μ_p is the mobility of the charged particle and $D(x)$ is the local diffusion constant. Taking the time interval Δt to be infinitesimal, the integral equation Eq. (5) is cast into the differential form,

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\Big[\mu_p E(x) P\Big] + \frac{\partial^2}{\partial x^2}\Big[D(x)P\Big] \quad (8)$$

The partial differential equation is known as the Smoluchowski equation.

The above equation has several interesting properties: (1) the existence of probability current (2) Boltzmann distribution as a steady-state solution. Introduce the probability current containing two parts,

$$J(x,t) = \mu_p E(x) P(x,t) - \frac{\partial}{\partial x}\Big[D(x)P(x,t)\Big]. \quad (9)$$

The drift term is driven by the external electric field and the gradient term arises from the spatial variations. It is easy to show that the Smoluchowski equation can be written in the form of continuity equation,

$$\frac{\partial P}{\partial t} + \frac{\partial J}{\partial x} = 0. \quad (10)$$

What is conserved in the continuity equation? Simple, the total probability.

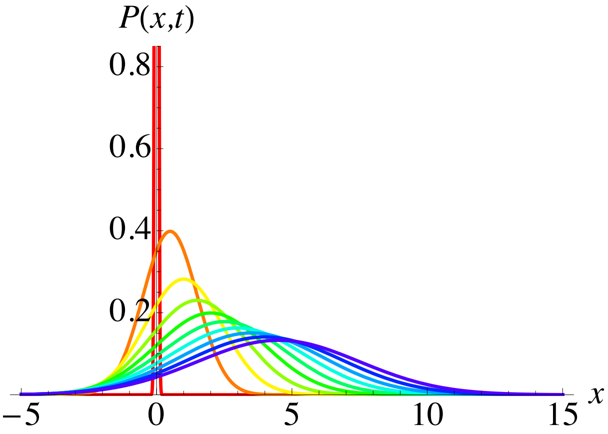

Figure 1: Drifted diffusion – time evolution of the probability distribution function $P(x,t)$ with constant $E(x)$ and $D(x)$ in the Smoluchowski equation. The initial probability distribution is $P(x,0) = \delta(x)$ (red curve), moving to the right at constant drift velocity (red to blue curves).

Suppose the local diffusion constant $D(x) = D$ is uniform and the electric field is $E(x) = -dV/dx$. Substituting the Bolzmann distribution,

$$P(x) = P_0 \, e^{-qV(x)/\tau}, \tag{11}$$

into the definition for the probability current,

$$J(x) = \left[\mu_p - Dq/\tau\right] E(x) P(x) = 0, \tag{12}$$

where we have employed the Einstein relation $D = \mu_p \tau / q$. In consequence, the Smoluchowski equation is trivially satisfied and the Bolzmann distribution serves as its steady-state solution.

If both $E(x)$ and $D(x)$ are constant, the solution is relatively simple,

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left[-\frac{(x-u_d t)^2}{4Dt}\right], \tag{13}$$

where the drift velocity $u_d = \mu_p E$. The time evolution of the probability distribution is shown in Fig. 1.

• Fokker-Plank equation

We now turn to a seemingly different problem: How thermalization is achieved? Suppose we carefully align all particles in an ideal gas to have the same momentum at $t = 0$. Due to inter-molecular collisions, at later time $t \gg \tau_c$, the system will reach the Maxwell distribution in thermal equilibrium. We can follow the same logic and write down the dynamical equation for the momentum distribution $P(p,t)$. As will become clear later, thermalization can be viewed as "confined diffusion in the momentum space".

We start with the master equation in the integral form,

$$P(p,t+\Delta t) = \int_{-\infty}^{\infty} d\Delta p\, f(\Delta p, p')P(p',t), \tag{14}$$

where $\Delta p = p - p'$ is the momentum transfer and $P(p,t)$ is probability density for momentum distribution. Again, expanding the variable $p' = p - \Delta p$ in Taylor series and truncating higher-order terms, the dynamics of the momentum distribution $P(p,t)$ is captured by the following partial differential equation,

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial p}\Big[A(p)P\Big] + \frac{1}{2}\frac{\partial^2}{\partial p^2}\Big[B(p)P\Big], \tag{15}$$

known as the Fokker-Plank equation. The mean $A(p)$ and variance $B(p)$ within the time interval Δt are defined as

$$A(p) \equiv \lim_{\Delta t\to 0} \frac{\langle \Delta p\rangle}{\Delta t}, \tag{16}$$

$$B(p) \equiv \lim_{\Delta t\to 0} \frac{\langle (\Delta p)^2\rangle}{\Delta t}. \tag{17}$$

In principle, $A(p)$ and $B(p)$ can be computed from the inter-molecular collisions at the microscopic scale. But, the calculations are messy and rather involved. Here I choose a different route to estimate the coefficient functions.

Focusing on a particular particle, its dynamics due to inter-molecular collisions is well captured by the Langevin equation,

$$\frac{dp}{dt} = -\gamma p + f(t), \tag{18}$$

where γ is due to viscosity and $f(t)$ is the random forces due to collisions. It is straightforward to show that γ is related to the mobility, $\mu_p = q/(\gamma M)$. The random force has a white-noise spectrum,

$$\langle f(t)f(t')\rangle = \Lambda\, \delta(t-t'), \tag{19}$$

where $\Lambda = 2\gamma^2 M^2 D$ is linearly proportional to the diffusion constant D. Integrate the Langevin equation to obtain the time dependence of momentum,

$$\langle \Delta p\rangle = -\gamma p\Delta t + \int_t^{t+\Delta t} dt' \langle f(t')\rangle = -\gamma p \Delta t. \tag{20}$$

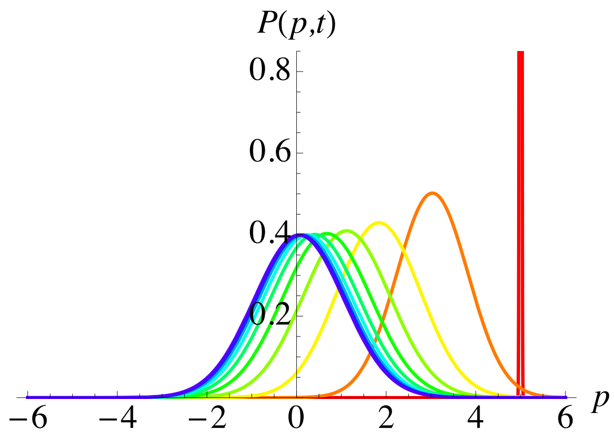

Figure 2: Thermalization – time evolution of the probability distribution $P(p,t)$ from the Fokker-Plank equation in Langevin limit.The initial probability distribution $P(p,0) = \delta(p - p_0)$ (red curve) is sharp with the same momentum p_0, gradually dissipating (from red to blue curves) into the Maxwell-Boltzmann distribution and reaching thermal equilibrium.

By comparison, the mean of momentum change within Δt is

$$A(p) \equiv \lim_{\Delta t \to 0} \frac{\langle \Delta p \rangle}{\Delta t} = -\gamma p. \tag{21}$$

One can also compute the variance of the momentum change,

$$\begin{aligned}\langle (\Delta p)^2 \rangle &= \gamma^2 p^2 (\Delta t)^2 + \int_t^{t+\Delta t} dt_1 \int_t^{t+\Delta t} dt_2 \ \langle f(t_1) f(t_2) \rangle \\ &= \gamma^2 p^2 (\Delta t)^2 + \Lambda \Delta t.\end{aligned} \tag{22}$$

The first term can be ignored because it is of order $(\Delta t)^2$. The second term gives a constant variance of the momentum change,

$$B(p) \equiv \lim_{\Delta t \to 0} \frac{\langle (\Delta p)^2 \rangle}{\Delta t} = \Lambda = 2\gamma^2 M^2 D. \tag{23}$$

The Fokker-Plank equation now takes a simpler form,

$$\frac{\partial P}{\partial t} = \gamma \frac{\partial}{\partial p}(pP) + \gamma^2 M^2 D \, \frac{\partial^2 P}{\partial p^2}. \tag{24}$$

The above partial differential equation can be solved analytically and the probability density for momentum distribution is

$$P(p,t) = \frac{1}{\sqrt{2\pi\Delta(t)}} \exp\left[-\frac{\left(p - p_{int}\right)^2}{2\Delta(t)} \right], \tag{25}$$

$$p_{int}(t) = p_0\, e^{-\gamma t}, \qquad \Delta(t) = \gamma M^2 D \left(1 - e^{-2\gamma t}\right) \tag{26}$$

The time evolution of the probability distribution is shown in Fig. 2. In the long time limit, the memory of the initial momentum p_0 is washed away and the variance reaches a constant value,

$$\langle (\Delta p)^2 \rangle = \gamma M^2 D. \tag{27}$$

Equipartition theorem gives $\langle (\Delta p)^2 \rangle = M\tau$. Combined with $\mu_p = q/(\gamma M)$, we arrive at the Einstein relation again, $D = \mu_p \tau / q$. As one can tell from the analytic solution, thermalization is rather similar to diffusion except the time dependences of the drift and variance are different.

• diffusion process

By now, you should appreciate the power of Fokker-Plank equation. In fact, the idea can be generalized to include both generalized coordinates and momenta at the same time. To describe a system with a collection of random variables $\boldsymbol{X}(t) = (X_1, X_2, ..., X_n)$. If the following two conditions are satisfied, the stochastic dynamics of $\boldsymbol{X}(t)$ is called diffusion process.

The first condition is that the process must be Markovian. In other words, the conditional probability

$$P(\boldsymbol{x}, t | \boldsymbol{x}_i, t_i; \boldsymbol{x}_{i-1}, t_{i-1}; \ldots; \boldsymbol{x}_0, t_0) = P(\boldsymbol{x}, t; \boldsymbol{x}_i, t_i) \tag{28}$$

that $\boldsymbol{X}(t) = \boldsymbol{x}$, given that $\boldsymbol{X}(t_k) = \boldsymbol{x}_k$,..., $\boldsymbol{X}(t_0) = \boldsymbol{x}_0$ with $t_0 < t_1 < ... < t_i < t$, depends only on (x_i, t_i). The above argument may seem rather abstract to you at first glance but it is the foundation of the master equation we wrote down in previous sections. In layman language, there is no memory effect in the chain of the stochastic events.

The second condition is the existence of the means and variances for all variables in the short time limit,

$$A_i(\boldsymbol{x}) \equiv \lim_{\Delta t \to 0} \frac{\langle \Delta x_i \rangle}{\Delta t}, \tag{29}$$

$$B_{ij}(\boldsymbol{x}) \equiv \lim_{\Delta t \to 0} \frac{1}{\Delta t} \langle \Delta x_i \Delta x_j \rangle. \tag{30}$$

When both conditions are satisfied, starting from the integral master equation and expanding it in Taylor series, the Fokker-Plank equation reads,

$$\frac{\partial P}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}\Big[A(\boldsymbol{x}) P(\boldsymbol{x}, t)\Big] + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j}\Big[B_{ij}(\boldsymbol{x}) P(\boldsymbol{x}, t)\Big]. \tag{31}$$

Note that the Fokker-Plank equation is also known as the forward Kolmogorov equation. It can be applied to a Brownian particle in one dimension subjected to external force. Introduce the random variable $\boldsymbol{X} = (x, p)$. By applying the same reasoning, one can compute the means and variances,

$$\begin{aligned} A_1 &= \lim_{\Delta t \to 0} \frac{1}{\Delta t} \langle \Delta x \rangle = \frac{p}{M}, \\ A_2 &= \lim_{\Delta t \to 0} \frac{1}{\Delta t} \langle \Delta p \rangle = qE(x) - \gamma p, \\ B_{22} &= \lim_{\Delta t \to 0} \frac{1}{\Delta t} \langle (\Delta p)^2 \rangle = \Lambda, \end{aligned} \tag{32}$$

all other terms vanishes at order of Δt. Thus, the generalized diffusion process satisfies the Fooker-Plank equation,

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{p}{M} P\right] - \frac{\partial}{\partial p}\left[\big(qE - \gamma p\big) P\right] + \gamma M \tau \frac{\partial^2 P}{\partial p^2}, \tag{33}$$

where we have exploited the Einstein relation to eliminate $\Lambda = 2\gamma^2 M^2 D = 2\gamma M \tau$. This equation is called the Klein-Kramers equation.

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