The Fokker-Planck equation

We will

1. Derive the Fokker-Planck equation which is an expression for $\partial P/\partial t$.
2. Make use of this to show that Brownian dynamics gives

$$P(x) \propto e^{-U(x)/T},$$

by demonstrating that

$$\frac{\partial P}{\partial t} = 0 \quad \text{if} \quad P(x) \propto e^{-U(x)/T}.$$

Derivation of the Fokker-Planck equation

Consider starting from some probability distribution $P(x, 0)$ at time $t = 0$. The change to this distribution with time comes from two terms:

$$
\begin{aligned}
P(x, \Delta_t) = P(x, 0) \quad &- \quad \int d\tilde{x}\; D(x - \tilde{x}, \Delta_t | x, 0)\; P(x, 0) \\
&+ \quad \int d\tilde{x}\; D(x, \Delta_t | x - \tilde{x}, 0)\; P(x - \tilde{x}, 0). \qquad (1)
\end{aligned}
$$

Here $D(x - \tilde{x}, \Delta_t | x, 0)$ describes the dynamics, it is the probability that the particle which was at x at $t = 0$ is at $x - \tilde{x}$ at time Δ_t.
The second integral is the probability that the particle originally at $x - \tilde{x}$ will be found at x at time Δ_t.

The first integral is simplified with the use of

$$\int d\tilde{x}\; D(x - \tilde{x}, \Delta_t | x, 0) = 1, \qquad (2)$$

which is just a statement that the particle originally at x has to be somewhere a time Δ_t later.

Derivation of the Fokker-Planck equation…cont'd

With $\partial P(x,0)/\partial t \approx [P(x,\Delta_t) - P(x,0)]/\Delta_t$ one finds

$$\frac{\partial P(x,0)}{\partial t}\Delta_t = -P(x,0) + \int d\tilde{x}\; D(x,\Delta_t|x-\tilde{x},0)\; P(x-\tilde{x},0).$$

With

$$f(x) = D(x+\tilde{x},\Delta_t|x,0)\; P(x,0),$$

this is

$$\frac{\partial P(x,0)}{\partial t}\Delta_t = -P(x,0) + \int d\tilde{x}\; f(x-\tilde{x}).$$

Derivation of the Fokker-Planck equation...cont'd

With $f(x) = D(x+\tilde{x}, \Delta_t | x, 0)\; P(x,0)$ and the expansion

$$f(x-\tilde{x}) = \sum_{n=0}^{\infty} \frac{(-\tilde{x})^n}{n!} \frac{\partial^n}{\partial x^n} f(x), \qquad \text{this gives}$$

$$\begin{aligned}
&\frac{\partial P(x,0)}{\partial t} = \\
= \quad & -\frac{P(x,0)}{\Delta_t} + \sum_n \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[P(x,0) \frac{1}{\Delta_t} \int d\tilde{x}\; \tilde{x}^n D(x+\tilde{x}, \Delta_t | x, 0) \right] \\
\approx \quad & -\frac{\partial}{\partial x} \left[P(x,0) M_1 \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[P(x,0) M_2 \right],
\end{aligned}$$

where

$$M_n = \frac{1}{\Delta_t} \int d\tilde{x}\; \tilde{x}^n D(x+\tilde{x}, \Delta_t | x, 0),$$

and the $n=0$ term in the sum cancels the $P(x,0)$ term. This is the Fokker-Planck equation.

The Fokker-Planck equation

Summary:

The Fokker-Planck equation describes the change of the probability distribution function with time:

$$\frac{\partial P(x,0)}{\partial t} \approx -\frac{\partial}{\partial x}\left[P(x,0)M_1\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[P(x,0)M_2\right],$$

where

$$M_n = \frac{1}{\Delta_t}\int d\tilde{x}\; \tilde{x}^n D(x+\tilde{x},\Delta_t|x,0).$$

Application of the Fokker-Planck equation

What is the stationary probability distribution for a particle in a one dimensional potential $U(x)$ at temperature T, with Brownian dynamics?

We then need to evaluate the integrals over $D(x + \tilde{x}, \Delta_t | x, 0)$, related to the dynamics,

$$x(\Delta_t) = x(0) + \frac{\Delta_t}{\alpha} F + \eta \Delta_t.$$

Write as a delta function!

$$D(x+\tilde{x}, \Delta_t | x, 0) = \delta\left(x + \frac{\Delta_t}{\alpha} F + \eta\Delta_t - (x + \tilde{x})\right) = \delta\left(\frac{\Delta_t}{\alpha} F + \eta\Delta_t - \tilde{x}\right).$$

The relevant quantities are M_1 and M_2 *averaged over the random noise*:

$$M_n = \frac{1}{\Delta_t}\left\langle \int d\tilde{x}\, \tilde{x}^n\, \delta\left(\frac{\Delta_t}{\alpha} F + \eta\Delta_t - \tilde{x}\right)\right\rangle = \frac{1}{\Delta_t}\left\langle \left(\frac{\Delta_t}{\alpha} F + \eta\Delta_t\right)^n \right\rangle.$$

Application of the Fokker-Planck equation. . . cont'd

$$\textit{With} \qquad M_n = \frac{1}{\Delta_t}\left\langle \left(\frac{\Delta_t}{\alpha}F + \eta\Delta_t\right)^n \right\rangle \qquad \textit{and}$$

$$F = -\partial U/\partial x, \qquad \langle\eta\rangle = 0, \qquad \langle\eta^2\rangle = \frac{2T}{\alpha\Delta_t},$$

we get, to lowest order in Δ_t,

$$M_1 = -\frac{1}{\alpha}\frac{\partial U}{\partial x} + \frac{1}{\Delta_t}\langle\eta\rangle\Delta_t = -\frac{1}{\alpha}\frac{\partial U}{\partial x},$$

and

$$M_2 = \frac{1}{\Delta_t}\left[\left(-\frac{\Delta_t}{\alpha}\frac{\partial U}{\partial x}\right)^2 - 2\frac{\Delta_t}{\alpha}\frac{\partial U}{\partial x}\langle\eta\rangle\Delta_t + \langle\eta^2\rangle\Delta_t^2\right] = \frac{2T}{\alpha}.$$

Stationary solution

Our equation is

$$\frac{\partial P}{\partial t} \approx -\frac{\partial}{\partial x}\left[P M_1\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[P M_2\right].$$

With

$$M_1 = -\frac{1}{\alpha}\frac{\partial U}{\partial x}, \quad M_2 = \frac{2T}{\alpha},$$

this becomes

$$\frac{\partial P}{\partial t} \approx \frac{1}{\alpha}\frac{\partial}{\partial x}\left[P\frac{\partial U}{\partial x}\right] + \frac{T}{\alpha}\frac{\partial^2 P}{\partial x^2},$$

Stationary solution. . . cont'd

We now want to demonstrate that $P \propto e^{-U/T}$ is the stationary solution to the F-P equation, i.e. that it gives $\partial P/\partial t = 0$. First note:

$$P \propto e^{-U/T}, \quad \frac{\partial P}{\partial x} = -\frac{1}{T}\frac{\partial U}{\partial x}P, \quad \frac{\partial^2 P}{\partial x^2} = \left[\frac{1}{T^2}\left(\frac{\partial U}{\partial x}\right)^2 - \frac{1}{T}\frac{\partial^2 U}{\partial x^2}\right] P.$$

We then have

$$\frac{\partial}{\partial x}\left[P\frac{\partial U}{\partial x}\right] = \frac{\partial P}{\partial x}\frac{\partial U}{\partial x} + P\frac{\partial^2 U}{\partial x^2} = -\frac{1}{T}\left(\frac{\partial U}{\partial x}\right)^2 P + \frac{\partial^2 U}{\partial x^2}P.$$

and we arrive at

$$\frac{\partial P}{\partial t} \approx \frac{1}{\alpha}\frac{\partial}{\partial x}\left[P\frac{\partial U}{\partial x}\right] + \frac{T}{\alpha}\frac{\partial^2 P}{\partial x^2} = 0.$$