A. Steady State Motion of a Brownian Particle

- Recall the conditions that gave us the Smoluchowski Equation for the steady state motion of a Brownian particle. Start with the FPE:

\[ \frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left( \frac{\Delta x}{\Delta t} \right) P(x,t) + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left\{ \frac{\langle \Delta x^2 \rangle}{\Delta t} \right\} P(x,t) \]

(10.1)

- Assuming the Brownian particle diffuses in a potential \( U(x) \) and at steady state (i.e. \( \frac{dp}{dt} = 0 \)):

\[ \Delta x = -\Delta \]

(10.2)

- For one dimensional motion we also have

\[ 2D\Delta t = 2BkT\Delta t \]

(10.3)

- With (10.2) and (10.3) the FPE (10.1) becomes

\[ \frac{\partial P(x,t)}{\partial t} = B \frac{\partial}{\partial x} \left\{ \frac{dU}{dx} P(x,t) \right\} + BkT \frac{\partial^2}{\partial x^2} P(x,t) \]

(10.4)

- Suppose the diffusive motion occurs free of a potential \( U(x) \). That is, suppose \( U(x) = 0 \). Then (10.4) becomes:

\[ \frac{\partial P(x,t)}{\partial t} = BkT \frac{\partial^2 P(x,t)}{\partial x^2} \]

(10.5)

which is the free diffusion equation.

B. Solution of the Free Diffusion Equation: Initial Value Problem

- Suppose no boundary conditions constrain the motion of the Brownian particle. In this case we need only consider the initial condition. Assume a delta-function initial distribution, i.e.:

\[ P(x,0) = \delta(x - x_0) \]

(10.6)

- Define the Fourier transform (FT) of \( P(x,t) \)

\[ U(s,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} P(x,t)e^{isx}dx = FT\{P(x,t)\} \]

(10.7)

- Recall the general relationship

\[ FT\left( \frac{\partial^n P(x,t)}{\partial x^n} \right) = (-is)^n U(s,t) \]

(10.8)
• Next take the FT of equation (10.5). Using (10.7) and (10.8) the result is
\[
\frac{\partial U(s,t)}{\partial t} = -s^2 D U(s,t) \tag{10.9}
\]

• The solution is:
\[
U(s,t) = U(s,0)e^{-Ds^2t} \tag{10.10}
\]

• We need to determine U(s,0). According to equation (10.7)
\[
U(s,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} P(x,0)e^{ixx} dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x-x_0)e^{ixx} dx = \frac{e^{jxx_0}}{\sqrt{2\pi}} \tag{10.11}
\]

• Now we take the inverse Fourier transform of the expression in (10.11):
\[
P(x,t) = \int_{-\infty}^{+\infty} U(s,t)e^{-ixx} ds = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-s^2Dt} e^{jxx_0} e^{-ixx} ds
\]
\[
= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-s^2Dt} e^{jx(x_0-x)} ds = \frac{2}{\sqrt{2\pi}} \int_{0}^{+\infty} e^{-s^2Dt} \cos[js(x_0-x)] ds
\]
\[
= \frac{1}{\sqrt{2Dt}} e^{-(x-x_0)^2/4Dt} \tag{10.12}
\]

• After normalizing the result is
\[
P(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-(x-x_0)^2/4Dt} \tag{10.13}
\]

• With Equation (10.13) we obtain the expected results:
\[
\langle x \rangle = \int_{-\infty}^{+\infty} xP(x,t) dx = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{+\infty} xe^{-(x-x_0)^2/4Dt} dx = 0
\]
\[
\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2P(x,t) dx = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{+\infty} x^2 e^{-(x-x_0)^2/4Dt} dx = 2Dt \tag{10.14}
\]