Final

Sunday, December 6, 2020 4:10 PM

1. **25 points** A Fokker-Plank equation describes the diffusion of a particle in a potential $U(x)$, with

?

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 p}{\partial x^2} + \frac{1}{\zeta}\frac{\partial}{\partial x}\left(n\frac{\partial U}{\partial x}\right) \tag{1}$$

should p be n?

For $U(x) = -fx$, with reflecting boundary conditions at $x = \pm L/2$, analytically determine the steady state solution for $n_\infty(x)$. Numerically integrate the Fokker Plank equation using any method you choose (for any nonzero ζ and f you choose), and show that your predicted steady state solution is recovered as $t \to \infty$.

$$\text{BC: } \left.\frac{dn}{dx}\right]_{x=\pm\frac{L}{2}} = 0 \qquad U(x) = -fx$$

steady state @ $\frac{\partial n}{\partial t} = 0$ or $\cancel{\frac{\partial p}{\partial t} = 0}$?

$$0 = D\frac{\partial^2 n}{\partial x^2} + \frac{1}{\gamma}\frac{\partial}{\partial x}\left(n\frac{\partial U}{\partial x}\right) = \frac{\partial}{\partial x}\underbrace{J(x)}_{\text{probability flux}} = 0$$

I have trouble drawing ζ symbol so let it be γ.

$$\frac{\partial n}{\partial t} = \frac{-fx}{\gamma}\frac{\partial n}{\partial t} + D\frac{\partial^2 n}{\partial x^2}$$

Probably can't do this.

Let $fx \equiv F$

$$\tau(x) \equiv \langle T(x)\rangle = \int dx' \, g_0(x', x) \quad \{\text{passage time}\}$$

$$-\frac{F}{\gamma}\frac{d\tau(x)}{dx} + D\frac{d^2\tau(x)}{dx^2} = -1$$

$n(x = \pm\frac{L}{2}) = 0$

$\gamma \qquad \partial x \qquad\qquad \partial x$

BC $\left(\frac{\partial \tau(x)}{\partial x}\right)_{x=\pm\frac{L}{2}} = 0$, $\tau\left(x=\pm\frac{L}{2}\right) = 0$

$$\tau(x) = \frac{\gamma^2 D}{F^2}\left[\exp\left(\frac{FL}{\gamma D}\right) - \exp\left(\frac{Fx}{\gamma D}\right) + \frac{\gamma(x-L)}{F}\right]$$

$$\therefore \int_0^L \tau(x)\,dx = \frac{\delta^2}{D}\left(\frac{\exp\left[\frac{FL}{\gamma D}\right] - 1 - FL/\gamma D}{\left(FL/\gamma D\right)^2}\right)$$

Do I even need this?

At a reflecting boundary, there is ~~zero~~ flux:

$$\vec{J}\cdot\hat{N} = 0\Big]_{x=+\frac{1}{2}}, \quad \vec{J}\cdot -\hat{N} = 0\Big]_{x=-\frac{1}{2}}$$

normal to boundary

$$\frac{\partial n}{\partial t} = \vec{\nabla}\cdot\vec{J} = LP$$

assuming particle is initially @ x_0:

$$n(\vec{x}, 0) = \delta(\vec{x} - \vec{x}_0)$$

$$\frac{d}{dx} J(x) = \frac{d}{dx}\left[D\frac{\partial n}{\partial x} + \frac{1}{\gamma} n \frac{\partial U}{\partial x}\right] = 0 \quad @\ x = \pm\frac{L}{2}$$

$$\therefore n_{\text{steady state}} \propto \exp\left(\frac{-U(x)}{\gamma D}\right)$$

$$= C \exp\left[-\frac{U(x)}{\ldots}\right]$$

$$n_{\substack{\text{steady}\\ \text{state}}} \equiv n_s = \underset{\substack{\uparrow\\ \text{some}\\ \text{constant}}}{C} \exp\left[-\frac{U(x)}{\gamma D}\right]$$

known equilibrium distribution: $P(x) = \exp(-\beta U(x))$

need Einstein relation: $D = k_B T \Gamma$

$$\boxed{n_s = C \exp\left[-\frac{fx}{\gamma D}\right]}$$

Let $\alpha = \dfrac{f}{\gamma D}$

so

$n_s = C e^{-\alpha x}$

$$C \exp\left[\frac{f/2}{\gamma D}\right] = 0$$

$$C \exp\left[\frac{-f/2}{\gamma D}\right] = 0$$