TFY 4275: Classical Transport Theory

Solution (sketch) V2008

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Problem 1

a) Ordinary diffusion : $\langle x^2(t) \rangle \sim 2Dt$
(linear in time)

b) Anomalous diffusion corresponds to $\langle x^2(t) \rangle$ scales non-linearly with time.

- sub-diffusion : $\langle x^2 \rangle$ increases slower than t
  Can be caused by long waiting times
  Non-Markovian
- super-diffusion: $\langle x^2 \rangle$ increases faster than t
  May be caused by long jumps.
  Markovian

c) $$\langle |x|^\delta \rangle = \int_{-\infty}^{\infty} dx\, |x|^\delta \mathcal{L}_\alpha(x) = 2 \int_0^{\infty} dx\, x^\delta \mathcal{L}_\alpha(x)$$

The integrand of this integral scales like

$$x^{\delta-(\alpha+1)}$$

For the integral to converge one must have

$$\delta-(\alpha+1) < -1$$

that is, if $\underline{\delta < \alpha}$.

If $\mathcal{L}_\alpha(x) \to p(x) \sim x^{-(\alpha+1)}$ (and otherwise well behaived) nothing will change, and the above condition still applies. $\langle |x|^\delta \rangle$ will still be finite when $\alpha \geq 2$ if $\delta < \alpha$.

d) From the previous sub-problem it follows that $\langle x^2 \rangle$ and $\langle t \rangle$ are finite if

$$\mu > 2$$
$$\gamma > 1$$

Hence:

1) Ordinary diff
2) sub-diffusion
3) can be anything
4) ordinary diffusion
5) super-diffusion
6) Super-diffusion

Problem 2

a) Jump size prob

$$p_1(\xi) = p_+ \,\delta(\xi - \Delta x) + p_- \,\delta(\xi + \Delta x) + (1 - p_+ - p_-)\,\delta(\xi)$$

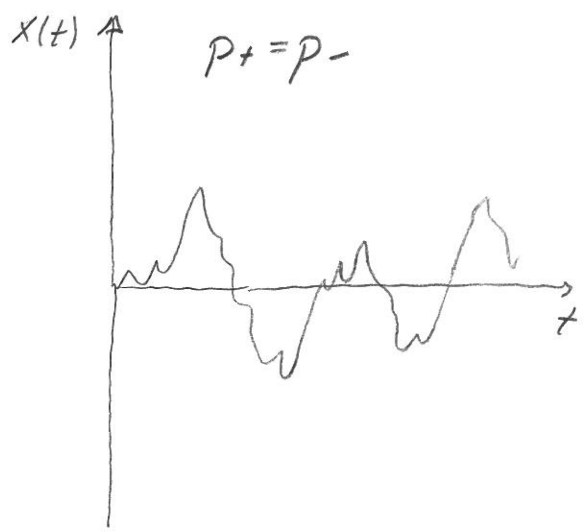
$$\hat{p}_1(k) = p_+ e^{-ik\Delta x} + p_- e^{ik\Delta x} + 1 - p_+ - p_-$$

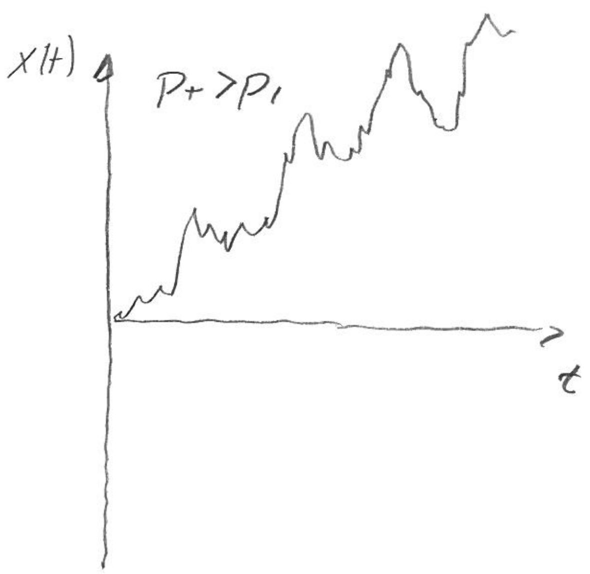
$$= 1 + p_+ (e^{-ik\Delta x} - 1) + p_- (e^{ik\Delta x} - 1)$$

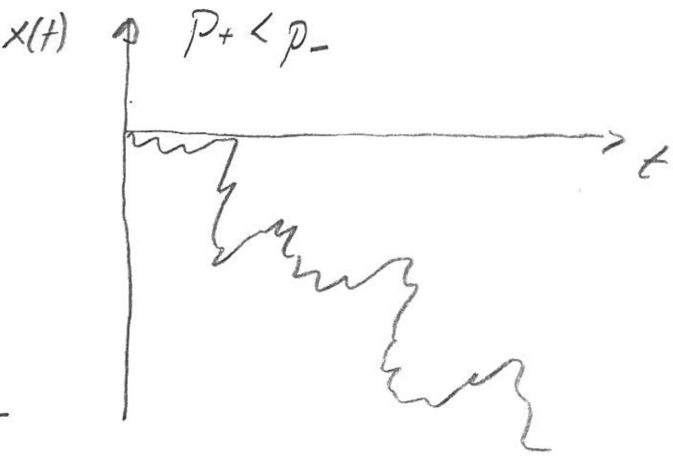
b) $\langle \xi \rangle = \int d\xi \; \xi \, p_1(\xi) = (p_+ - p_-)\,\Delta x$

Average drift velocity:

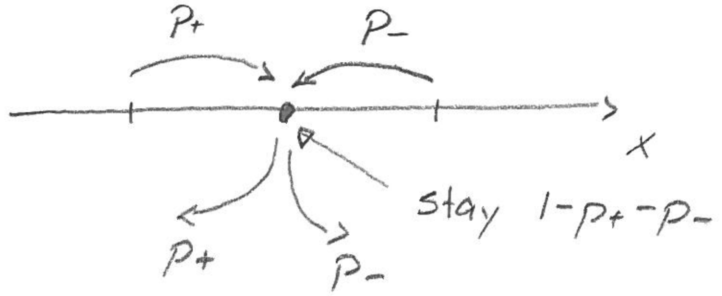
$$V_{drift} = \frac{\langle \xi \rangle}{\Delta t} = (p_+ - p_-)\,\frac{\Delta x}{\Delta t} \leq \frac{\Delta x}{\Delta t}$$







c)



$$P(x,t+\Delta t) = \underbrace{+p_+ P(x-\Delta x,t) + p_- P(x+\Delta x,t)}_{\text{in-flow}}$$
$$\underbrace{-p_+ P(x,t) - p_- P(x,t)}_{\text{out-flow}}$$
$$+P(x,t)$$

$$= P(x,t) + p_+\left[P(x-\Delta x,t) - P(x,t)\right] + p_-\left[P(x+\Delta x,t) - P(x,t)\right]$$

d)

$$P(x,t+\Delta t) \simeq P(x,t) + \Delta t\, \partial_t P(x,t) + \dots$$

To first order in Δt we have

$$\partial_t P(x,t) = r_+\left[P(x-\Delta x,t) - P(x,t)\right] + r_-\left[P(x+\Delta x,t) - P(x,t)\right], \quad r_\pm = \frac{p_\pm}{\Delta t}$$

This is the Master eq. for the process.

e) $$f(x\pm\Delta x,t) = f(x,t) \pm \Delta x\, \partial_x f(x,t) + \frac{\Delta x^2}{2!}\partial_x^2 f(x,t) + \dots$$

$$\partial_t f(x,t) = r_+\left[f(x,t) - \Delta x\,\partial_x f(x,t) + \frac{\Delta x^2}{2!}\partial_x^2 f(x,t) + \dots - f(x,t)\right]$$
$$+ r_-\left[f(x,t) + \Delta x\,\partial_x f(x,t) + \frac{\Delta x^2}{2!}\partial_x^2 f(x,t) + \dots - f(x,t)\right]$$

$$= -(r_+ - r_-)\Delta x\,\partial_x f(x,t) + (r_+ + r_-)\frac{\Delta x^2}{2!}\partial_x^2 f(x,t) + \dots$$

Hence to second order in Δx the given eq. follows with

$$v = (r_+ - r_-)\Delta x = (p_+ - p_-)\frac{\Delta x}{\Delta t}$$

$$D = (r_+ + r_-)\frac{\Delta x^2}{2!} = (p_+ + p_-)\frac{\Delta x^2}{2\Delta t}$$

This is the Fokker-Planck eq.
Specially when $p_+ = p_- = 1/2$

$$v = 0$$
$$D = \frac{\Delta x^2}{2\Delta t}$$

as we saw in the lectures in the symmetric case.

f] The v-term is a drift term (diffusion-advection eq.). This term can be transfomed "away" by going to a movable reference frame ($x - vt$). In this frame one has just the regular diffusion eq. Hence, the solution is the one given.

g] $$\langle x(t)\rangle = \int_{-\infty}^{\infty} dx \; x \, f(x,t)$$

$$u = x - x_0 - vt \qquad du = dx$$

$$= \frac{1}{\sqrt{4\pi D t}} \int_{-\infty}^{\infty} du \, (u + x_0 + vt) \, e^{-u^2/4Dt}$$

$$= \frac{1}{\sqrt{4\pi D t}} (x_0 + vt) \sqrt{\pi \, 4Dt}$$

$$= x_0 + vt$$

$$\langle x^2(t)\rangle = \int_{-\infty}^{\infty} dx \; x^2 f(x,t)$$

$$= \frac{1}{\sqrt{4\pi D t}} \int_{-\infty}^{\infty} du \, \underbrace{(u + x_0 + vt)^2}_{u^2 + 2u(x_0+vt) + (x_0+vt)^2} \, e^{-u^2/4Dt}$$

$$= \frac{1}{\sqrt{4\pi D t}} \left[\frac{4Dt}{2} + (x_0 + vt)^2 \right] \sqrt{\pi \, 4Dt}$$

$$= 2Dt + (x_0 + vt)^2$$

$$\sigma_x(t) = \left[\langle x^2(t)\rangle - \langle x\rangle^2 \right]^{1/2} = \sqrt{2Dt}$$

Note: The change in the details of the RW does not change the scaling!

Alternatively these results may be obtained from the FP equation. Multiply the FP eq. by x and integrate over all space:

$$\int_{-\infty}^{\infty} dx \; x \, \partial_t f(x,t) = -v \int_{-\infty}^{\infty} dx \; x \, \partial_x f(x,t) + D \int_{-\infty}^{\infty} dx \; x \, \partial_x^2 f(x,t)$$

$$\partial_t \langle x(t) \rangle = -v \left[\cancel{x f(x,t)}^{\,0} \right] \Big|_{x=-\infty}^{\infty} + v \int_{-\infty}^{\infty} dx \; f(x,t)$$

$$+ D \left[\cancel{x \, \partial_x f(x,t)}^{\,0} \right] \Big|_{x=-\infty}^{\infty} - D \int_{-\infty}^{\infty} \cancel{dx \, \partial_x f(x,t)}^{\,0}$$

$$= v$$

The solution of this eq. is as before

$$\langle x(t) \rangle = vt + x_0$$

Where we have used that $\langle x(t=0) \rangle = x_0$.

In a similar way, one may derive an eq. for $\langle x^2(t) \rangle$ by multiplying the FP eq. by x^2 and integrating over all space.

Problem 3

a) Shortly after $t=0$ the positive ions will start moving towards the wall in order to try to "cancel" the effect of the negative potential.
For long times the concentrations $C_\pm(x)$ will reach stationary solutions.
Far away from the wall one should have, $C_\pm(x=\infty) = C_0$, i.e. the initial concentrations.

b) The Fokker-Planck eq:

$$\partial_t C_\pm(x) = -\partial_x [\mu_\pm F_\pm(x) C_\pm(x)] + D_\pm \partial_x^2 C_\pm(x)$$

Stationary solution when $\partial_t C_\pm(x) = 0$:

$$\partial_x [\mu_\pm F_\pm(x) C_\pm(x)] = D_\pm \partial_x^2 C_\pm(x)$$

Integrating one time gives

$$\partial_x C_\pm(x) = \frac{\mu_\pm}{D_\pm} F_\pm(x) C_\pm(x) + \gamma_1$$

$$= \mp \frac{e}{k_B T} \frac{d\phi(x)}{dx} C_\pm(x) + \gamma_1$$

$\gamma_1 = 0$ since $\partial_x C_\pm(x)|_{x=\infty} = 0$ and $\partial_x \phi(x)|_{x=\infty} = 0$.
so that the eq. is separable :

$$\frac{\partial_x C_\pm(x)}{C_\pm(x)} = \mp \frac{e}{k_B T} \frac{d\phi}{dx}$$

Integrating once more gives:

$$\ln C_\pm(x) = \mp \frac{e}{k_B T} \phi(x) + \mathcal{H}_2$$

$$C_\pm(x) = \mathcal{H} \exp\left(\mp \frac{e}{k_B T} \phi(x)\right), \quad \mathcal{H} = e^{\mathcal{H}_2}$$

Boundary conditions $C_\pm(x=\infty) = C_0$, $\phi(x=\infty) = 0 \Rightarrow \mathcal{H} = C_0$

$$C_\pm(x) = C_0 \exp\left(\mp \frac{e}{k_B T} \phi(x)\right)$$

c) The electrical potential:

$$-\varepsilon \frac{d^2\phi(x)}{dx^2} = e\left[C_+(x) - C_-(x)\right]$$

$$\varepsilon \partial_x^2 \phi(x) = -eC_0\left[e^{-e\phi/k_BT} - e^{e\phi/k_BT}\right]$$

$$\partial_x^2\phi(x) = \frac{2eC_0}{\varepsilon} \sinh\left(\frac{e\phi(x)}{k_BT}\right)$$

d) Linearize the eq. for the electrical potential:

$$\partial_x^2 \phi(x) = \frac{2eC_0}{\varepsilon}\left(\frac{e\phi}{k_BT} + \dots\right) \simeq \frac{2e^2C_0}{\varepsilon k_BT} \phi(x)$$

$$\partial_x^2 \phi(x) - k^2 \phi(x) = 0 \qquad k^2 = \frac{2e^2C_0}{\varepsilon k_BT}$$

Solution

$$\phi(x) = Ae^{kx} + Be^{-kx}$$

When $x \to \infty$, $\phi(x) \to 0$ which implies that $A = 0$. The boundary condition at $x=0$ gives $B = -\phi_0$. Hence

$$\phi(x) = -\phi_0 e^{-kx} = \underline{-\phi_0 e^{-x/\lambda}}$$

where

$$\lambda = k^{-1} = \sqrt{\frac{\varepsilon k_B T}{2e^2 c_0}}$$

e) Charge density:

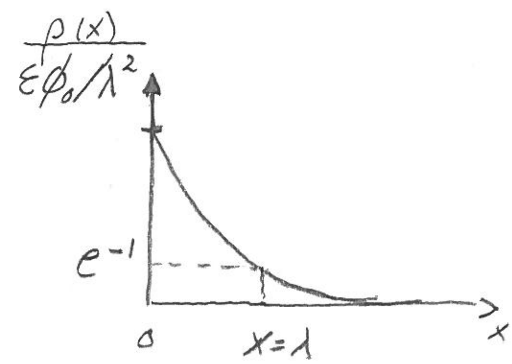
$$\rho(x) = e\left[c_+(x) - c_-(x)\right] = -2ec_0 \sinh\left(\frac{e\phi(x)}{k_B T}\right)$$

Linearized charge density:

$$\rho(x) \simeq -2ec_0 \frac{e\phi(x)}{k_B T}$$

$$= 2\frac{e^2 c_0}{k_B T} \phi_0 e^{-x/\lambda}$$

$$= \underline{\frac{\varepsilon \phi_0}{\lambda^2} e^{-x/\lambda}}$$



λ sets the scale over which $\rho(x)$ has dropped to e^{-1} of its value at the wall. Since $\rho(x) = 0$, far away from the wall, a screening effect is present. It is thus natural to call λ a screening length.