TFY 4275 : CLASSICAL TRANSPORT THEORI

Solution Exam May 2009

Problem 1

a) The master-eqation is a fundamental eq. that gives the rate of change of the probability density, say $p(y_2,t)$, due to transitions <u>into</u> the state y_2 from <u>all</u> other states y_1 and the transions <u>out</u> of state y_2 into other states y_1.

A general form is

$$\frac{\partial p(y_2,t)}{\partial t} = \int dy_1 \left[W(y_2,y_1) P(y_1,t) - W(y_1,y_2) P(y_2,t) \right]$$

where $W(y_1,y_2)$ denotes the transition prob. (per unit time) that the system changes y_2 to y_1.

The master eq. is derived from the Chapman-Kolmogorov equation, and thus the master-eq describes Markov processes.

b) The change of the number of mice in room A; should equal the "flow" <u>into</u> room A, minus the <u>out-flow</u>. Hence

$$N_A(t+\Delta t) - N_A(t) = \frac{2}{3} N_B(t) + \frac{1}{2} N_C(t) - N_A(t)$$

$$N_A(t+\Delta t) = \frac{2}{3} N_B(t) + \frac{1}{2} N_C(t) \qquad (1a)$$

Here the factor 2/3 in front of $N_B(t)$ comes from the fact that 2 out of 3 doors leads from room B to A.

Similarly, one gets

$$N_B(t+\Delta t) = \frac{2}{3} N_A(t) + \frac{1}{2} N_C(t) \qquad (1b)$$

$$N_C(t+\Delta t) = \frac{1}{3} N_A(t) + \frac{1}{3} N_B(t) \qquad (1c)$$

c) The master-eq. for the house of the mice follows from Eqs.(1) by dividing through by N, adding to both sides $\vec{p}(t)$ and dividing by Δt. This gives:

$$\partial_t \vec{p}(t) = \Gamma \vec{p}(t) \qquad (2a)$$

where

$$\Gamma = \frac{1}{\Delta t} \begin{pmatrix} -1 & 2/3 & 1/2 \\ 2/3 & -1 & 1/2 \\ 1/3 & 1/3 & -1 \end{pmatrix} \qquad (2b)$$

d) From the master-eq. it follows:

$$\frac{1}{\Delta t}\left[\vec{\rho}(t+\Delta t)-\vec{\rho}(t)\right] = \Gamma\vec{\rho}(t)$$

$$\vec{\rho}(t+\Delta t) = (\Delta t\,\Gamma + 1)\,\vec{\rho}(t) \equiv T\vec{\rho}(t) \qquad (3)$$

Hence

$$T = \Delta t\,\Gamma + 1 = \begin{pmatrix} 0 & 2/3 & 1/2 \\ 2/3 & 0 & 1/2 \\ 1/3 & 1/3 & 0 \end{pmatrix}$$

e) The interpretation of the matrix element T_{ij} is the transition probability to go from room <u>j to i</u> (different in general from that from i to j).

Conservation of # mice requires that

$$\sum_i \rho_i(t) = 1$$

for <u>all</u> times. Hence from Eq. (3) it follows that

$$1 = \sum_i \rho_i(t+\Delta t) = \sum_i \left[\sum_j T_{ij}\rho_j(t)\right]$$

$$= \sum_j \left[\sum_i T_{ij}\right]\rho_j(t) \qquad \text{changing order of summation}$$

$$\Rightarrow \quad \sum_i T_{ij} = 1.$$

That is, the column sum of T is one which physically means that the prob. for going from room j to <u>any</u> of the other rooms is one. T given in subproblem d satisfies this property.

f] The steady-state means that

$$\vec{\bar{p}} = T\vec{\bar{p}}$$

Assume

$$\vec{\bar{p}} = \alpha \begin{pmatrix} 1 \\ x \\ y \end{pmatrix}$$

where α is a normalization constant

$$\begin{pmatrix} 1 \\ x \\ y \end{pmatrix} = \begin{pmatrix} 2/3\, x + 1/2\, y \\ 2/3 + 1/2\, y \\ 1/3 + 1/3\, x \end{pmatrix}$$

$$\left.\begin{array}{rl} x - 1/2\, y &= 2/3 \\ -1/3\, x + y &= 1/3 \end{array}\right\} \Rightarrow \frac{5}{6}x = \frac{5}{6} \Rightarrow \left\{\begin{array}{l} x = 1 \\ y = 2/3 \end{array}\right.$$

Hence

$$\underline{\vec{\bar{p}} = \frac{1}{8}\begin{pmatrix} 3 \\ 3 \\ 2 \end{pmatrix}}$$

g] $\bar{p}_A : \bar{p}_B : \bar{p}_C = 3:3:2$

This ratio is the <u>same</u> as the ratio between the doors:

$D_A : D_B : D_C = 3:3:2$

Problem 2

a) D is the diffusion constant and has unit m^2/s. $p(x,t|x_0,t_0)$ gives the probability for finding the particle at position x at time t given that it was at x_0 at t_0.

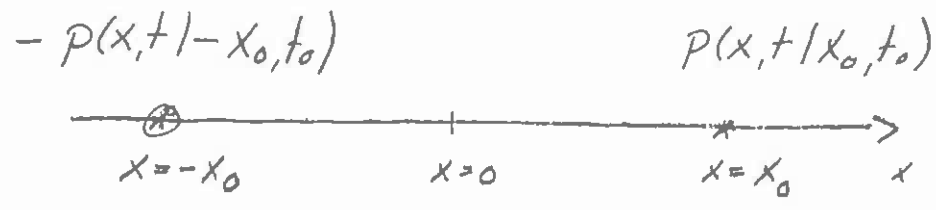
$$\lim_{t \to t_0} p(x,t|x_0,t_0) = \delta(x-x_0)$$

The point (x_0,t_0) is the source point.

b) Since particles are always absorbed at position $x=0$, it means that probability for being at this position is zero, i.e.

$$u(x,t|x_0,t_0)\Big|_{x=0} = 0$$

c) $u(x,t|x_0,t_0)$ will always be zero if we place a source of negative amplitude (this is called a sink) at location $x=-x_0$. This is due to the symmetry property of the propagator with respect to $x=0$.



Diffusion sink
"the image"

d] From the configuration from 2c we have $(t > t_0 = 0)$

$$u(x,t|x_0,t_0) = p(x,t|x_0,t_0) - p(x,t|-x_0,t_0)$$

$$= \frac{1}{\sqrt{4\pi Dt}} \left\{ e^{-\frac{(x-x_0)^2}{4Dt}} - e^{-\frac{(x+x_0)^2}{4Dt}} \right\}$$

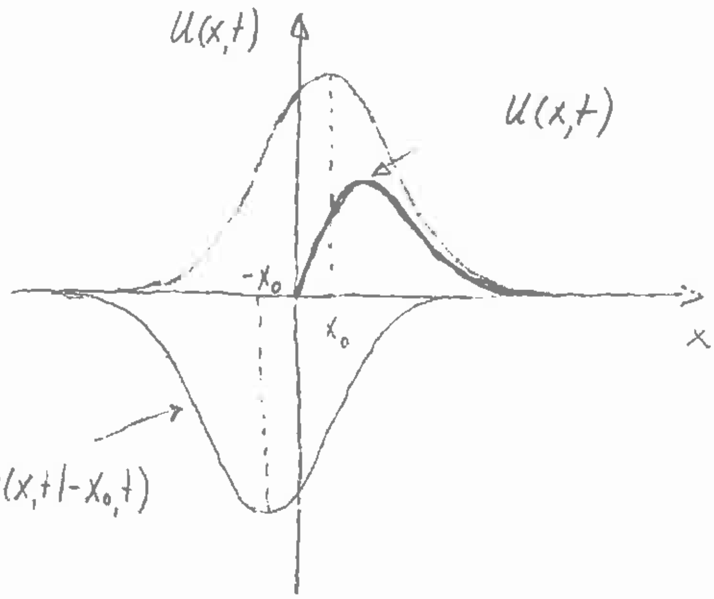
$$= \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x^2+x_0^2)}{4Dt}} \left\{ e^{xx_0/2Dt} - e^{-xx_0/2Dt} \right\} \quad (4)$$

In the long time limit one has

$$\{ \quad \} \simeq \frac{x x_0}{Dt}$$

so that

$$u(x,t|x_0,t_0) \simeq \frac{1}{\sqrt{4\pi Dt}} \frac{x x_0}{Dt} e^{-\frac{(x^2+x_0^2)}{4Dt}} \quad (5)$$



e] Fick's 1st law says that the concentration current is $\vec{J} = -D\nabla c(x,t)$ at position x at time t where $c(x,t)$ denotes the concentration.

Hence, in our case, $D\,\partial_x u(x,t|x_0,t_0)|_{x=0}$ is the probability current flowing to the left at position $x=0$. That is, the "probability" corresponding to particles falling off the plateau.

Hence:

$$f(0,t|x_0,t_0) = +D\,\partial_x u(x,t|x_0,t_0)\Big|_{x=0}$$

f] From Eq. (4) it follows:

$$f(0,t|x_0,t_0) = \frac{D}{\sqrt{4\pi D t}}\left\{ e^{-\frac{(x-x_0)^2}{4Dt}}\left[\frac{-2(x-x_0)}{4Dt}\right] - e^{-\frac{(x+x_0)^2}{4Dt}}\left[\frac{-2(x+x_0)}{4Dt}\right]\right\}\Bigg|_{x=0}$$

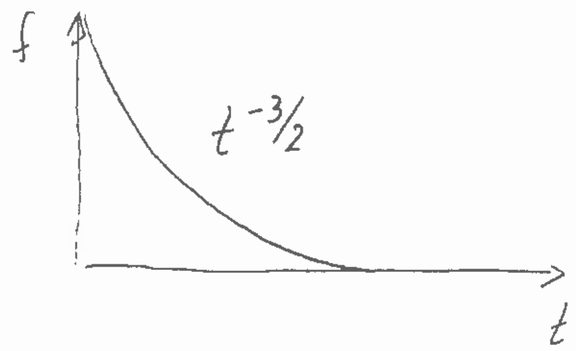
$$= \frac{D}{\sqrt{4\pi D t}}\,\frac{x_0}{Dt}\,e^{-\frac{x_0^2}{4Dt}}$$

$$= \frac{x_0}{\sqrt{4\pi D t^3}}\,e^{-\frac{x_0^2}{4Dt}}$$

g] $$\langle t \rangle = \int_0^\infty dt\, t\, \underbrace{f(0,t|x_0,t_0)}_{\sim t^{-3/2}} = \infty$$

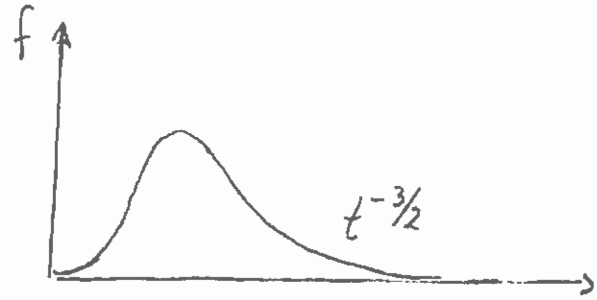
The reason that $\langle t \rangle = \infty$ comes from the fact that the particle can make infinitly long excursions to the right of the starting-point before reaching the cliff. This results in the fat-tailed waiting time distribution.

i] $x_0 \to 0^+$



A pure power-law

ii] $x_0 > 0$ and finite



The distribution goes throug a maximum.

When x_0 is finite it takes some time to reach the barrier. This is seen as $f(0,t|x_0,t_0)$ going throug a maximum.

h) i) $\sqrt{Dt} \gg x_0$

$$f(0,t|x_0,t_0) \simeq \frac{x_0}{\sqrt{4\pi D t^3}}$$

We see that the starting point does not matter for the functional form.

ii) $\sqrt{Dt} \ll x_0$

$$f(0,t|x_0,t_0) \simeq 0$$

The particle has not had time to reach the barrier.

i) The survival probability:

$$S(t|x_0,t_0) = 1 - \int_0^t dt' \, f(0,t|x_0,t_0)$$

$$= 1 - \int_0^t dt' \frac{x_0}{\sqrt{4\pi D t^3}} \exp\left\{-\frac{x_0^2}{4Dt'}\right\}$$

Make the change of integration variable

$$u^2 = \frac{x_0^2}{4Dt} \Rightarrow t = \frac{x_0^2}{4Du^2}$$

$$dt = \frac{x_0^2}{4D}(-2u^{-3})\,du = -2\frac{x_0^2}{4Du^3}\,du$$

$$\frac{x_0}{\sqrt{4\pi D t^3}} = \frac{x_0}{\sqrt{4\pi D \left(\frac{x_0^2}{4Du^2}\right)^3}}$$

$$= \frac{1}{\sqrt{\pi}} \frac{x_0}{\sqrt{\frac{1}{(4D)^2} \frac{x_0^6}{u^6}}}$$

$$= \frac{1}{\sqrt{\pi}} \frac{x_0}{\frac{x_0^3}{4Du^3}}$$

$$= \frac{1}{\sqrt{\pi}} \frac{4Du^3}{x_0^2}$$

Therefor :

$$dt \frac{x_0}{\sqrt{4\pi D t^3}} = du\,(-2) \frac{x_0^2}{4Du^3} \frac{1}{\sqrt{\pi}} \frac{4Du^3}{x_0^2}$$

$$= -\frac{2}{\sqrt{\pi}}\, du$$

Hence, by collecting terms one gets:

$$S(t\,|\,x_0,t_0) = 1 - \left(-\frac{2}{\sqrt{\pi}}\right) \int_{\infty}^{\frac{x_0}{\sqrt{4Dt}}} du\; e^{-u^2}$$

$$= 1 - \frac{2}{\sqrt{\pi}} \int_{\frac{x_0}{\sqrt{4Dt}}}^{\infty} du\; e^{-u^2}$$

$$= \frac{2}{\sqrt{\pi}} \int_0^{\frac{x_0}{\sqrt{4Dt}}} du \; e^{-u^2} \qquad [\text{Using } \operatorname{erf}(\infty) = 1]$$

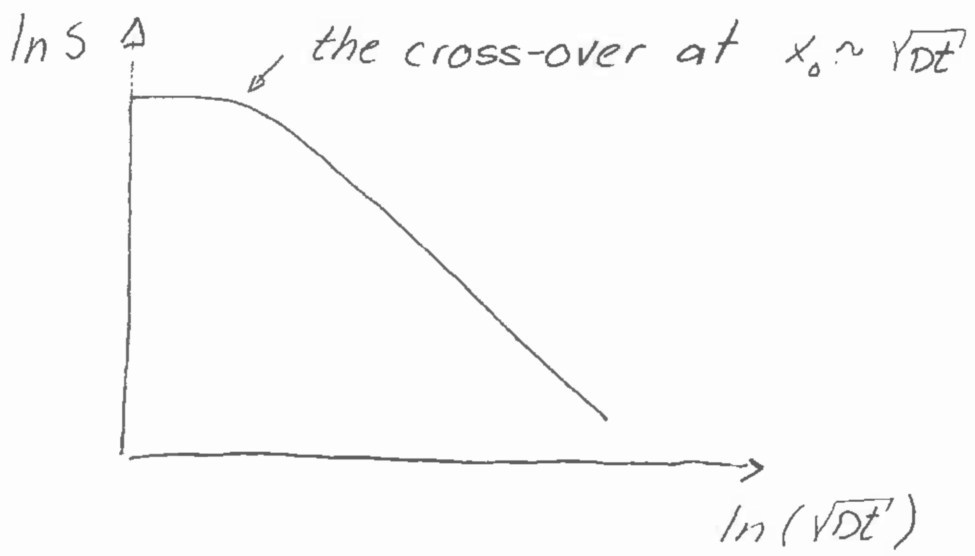
$$= \operatorname{erf}\left(\frac{x_0}{\sqrt{4Dt}} \right)$$

j) Using the expansions of the error function:

i) $\sqrt{Dt} \ll x_0 \quad : \quad S(t \mid x_0, t_0) \simeq 1.$

ii) $\sqrt{Dt} \gg x_0 \quad : \quad S(t \mid x_0, t_0) \simeq \frac{2}{\sqrt{\pi}} \frac{x_0}{\sqrt{4Dt}} \sim \frac{x_0}{\sqrt{Dt}}$

k)



It takes time to reach the barrier, so for small diffusion length $\sqrt{Dt} \ll x_0$, $S \simeq 1$, and no particles have reached the barrier. However when $\sqrt{Dt} \gg x_0$, the starting point for the particles is irrelevant and S will drop with time, as more and more part. reach $x=0$.