

TFY 4275 : CLASSICAL TRANSPORT THEORY
Solution Exam May 2009

Problem 1

a) The master-equation is a fundamental eq. that gives the rate of change of the probability density, say $P(y_2, t)$, due to transitions into the state y_2 from all other states y_1 and the transitions out of state y_2 into other states y_1 .

A general form is

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

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-equ. describes Markov processes.

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

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

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

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

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

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

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:

$$\partial_t \vec{p}(t) = \Pi \vec{p}(t) \quad (2a)$$

where

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

d) From the master-eq. it follows:

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

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

Hence

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

e) The interpretation of the matrix element \mathcal{T}_{ij} is the transition probability to go from room j to i (different in general from that from i to j).

Conservation of # mice requires that

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

for all times. Hence from Eq. (3) it follows that

$$\begin{aligned} 1 &= \sum_i \rho_i(t+\Delta t) = \sum_i \left[\sum_j \mathcal{T}_{ij} \rho_j(t) \right] \\ &= \sum_j \left[\sum_i \mathcal{T}_{ij} \right] \rho_j(t) \quad \text{changing} \\ &\hspace{15em} \text{order of} \\ &\hspace{15em} \text{summation} \end{aligned}$$

$$\Rightarrow \sum_i \mathcal{T}_{ij} = 1.$$

That is, the column sum of \mathcal{T} is one which physically means that the prob. for going from

room j to any of the other rooms is one.
 T given in subproblem d satisfies this property.

f] The steady-state means that

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

Assume

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

where α is a normalization constant

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

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

Hence

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

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

This ratio is the same 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 .

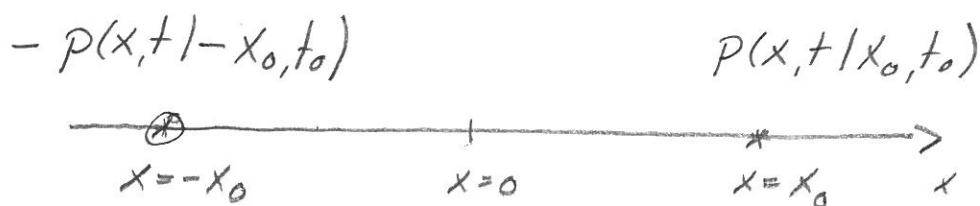
$$\lim_{t \rightarrow t_0} p(x, t | x_0, t_0) = \delta(x - x_0)$$

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
 $(t > t_0 = 0)$

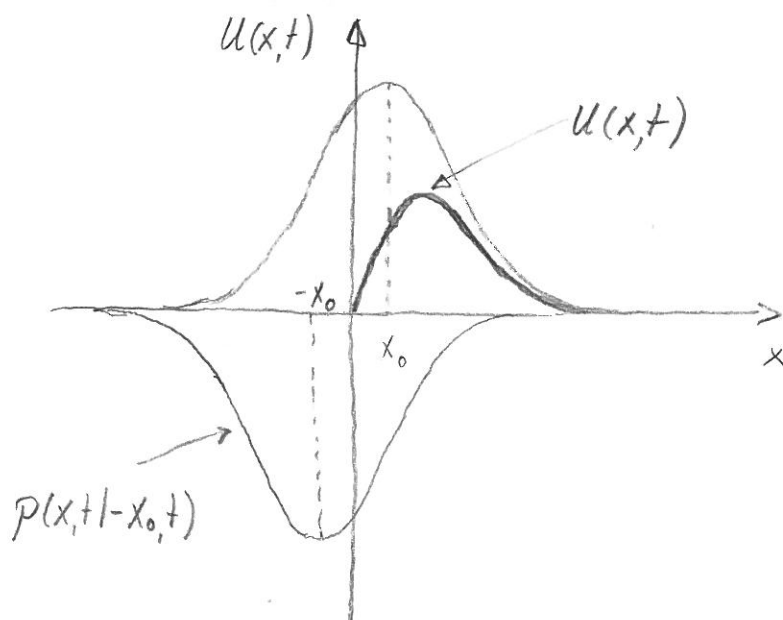
$$\begin{aligned}
 u(x, t | x_0, t_0) &= p(x, t | x_0, t_0) - p(x, t | -x_0, t_0) \\
 &= \frac{1}{\sqrt{4\pi Dt}} \left\{ e^{-\frac{(x-x_0)^2}{4Dt}} - e^{-\frac{(x+x_0)^2}{4Dt}} \right\} \\
 &= \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x^2+x_0^2)}{4Dt}} \left\{ e^{xx_0/2Dt} - e^{-xx_0/2Dt} \right\} \quad (4)
 \end{aligned}$$

In the long time limit one has

$$\{ \} \approx \frac{xx_0}{Dt}$$

so that

$$u(x, t | x_0, t_0) \approx \frac{1}{\sqrt{4\pi Dt}} \frac{xx_0}{Dt} e^{-\frac{(x^2+x_0^2)}{4Dt}} \quad (5)$$



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:

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

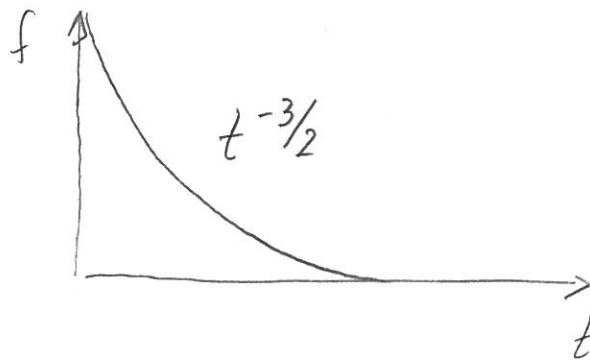
f] From Eq. (4) it follows:

$$\begin{aligned} f(0, t | x_0, t_0) &= \frac{D}{\sqrt{4\pi Dt}} \left\{ e^{-\frac{(x-x_0)^2}{4Dt}} \left[\frac{-2(x-x_0)}{4Dt} \right] \right. \\ &\quad \left. - e^{-\frac{(x+x_0)^2}{4Dt}} \left[\frac{-2(x+x_0)}{4Dt} \right] \right\} \Big|_{x=0} \\ &= \frac{D}{\sqrt{4\pi Dt}} \frac{x_0}{Dt} e^{-\frac{x_0^2}{4Dt}} \\ &= \frac{x_0}{\sqrt{4\pi D t^3}} e^{-\frac{x_0^2}{4Dt}} \end{aligned}$$

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

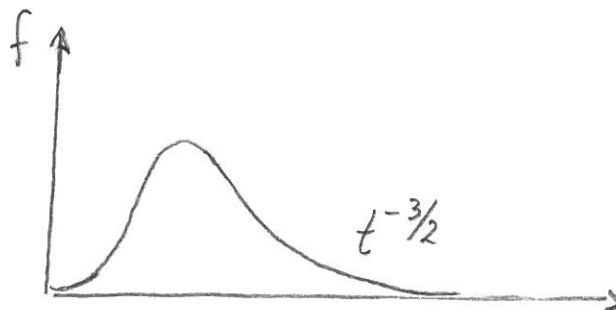
The reason that $\langle t \rangle = \infty$ comes from the fact that the particle can make infinitely long excursions to the right of the starting-point before reaching the cliff. This results in the fat-tailed waiting time distribution.

$$i) x_0 \rightarrow 0^+$$



A pure power-law

$$ii) x_0 > 0 \text{ and finite}$$



The distribution goes through 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 through a maximum.

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

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

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

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

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

The particle has not had time to reach the barrier.

ii) The survival probability:

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

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

Make the change of integration variable

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

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

$$\begin{aligned}
\frac{x_0}{\sqrt{4\pi Dt^3}} &= \frac{x_0}{\sqrt{4\pi D \left(\frac{x_0^2}{4Du^2}\right)^3}} \\
&= \frac{1}{\sqrt{\pi}} \frac{x_0}{\sqrt{\frac{1}{(4D)^2} \frac{x_0^6}{u^6}}} \\
&= \frac{1}{\sqrt{\pi}} \frac{x_0}{\frac{x_0^3}{4Du^3}} \\
&= \frac{1}{\sqrt{\pi}} \frac{4Du^3}{x_0^2}
\end{aligned}$$

Therefore :

$$\begin{aligned}
dt \frac{x_0}{\sqrt{4\pi Dt^3}} &= du (-2) \frac{x_0^2}{4Du^3} \frac{1}{\sqrt{\pi}} \frac{4Du^3}{x_0^2} \\
&= -\frac{2}{\sqrt{\pi}} du
\end{aligned}$$

Hence, by collecting terms one gets:

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

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

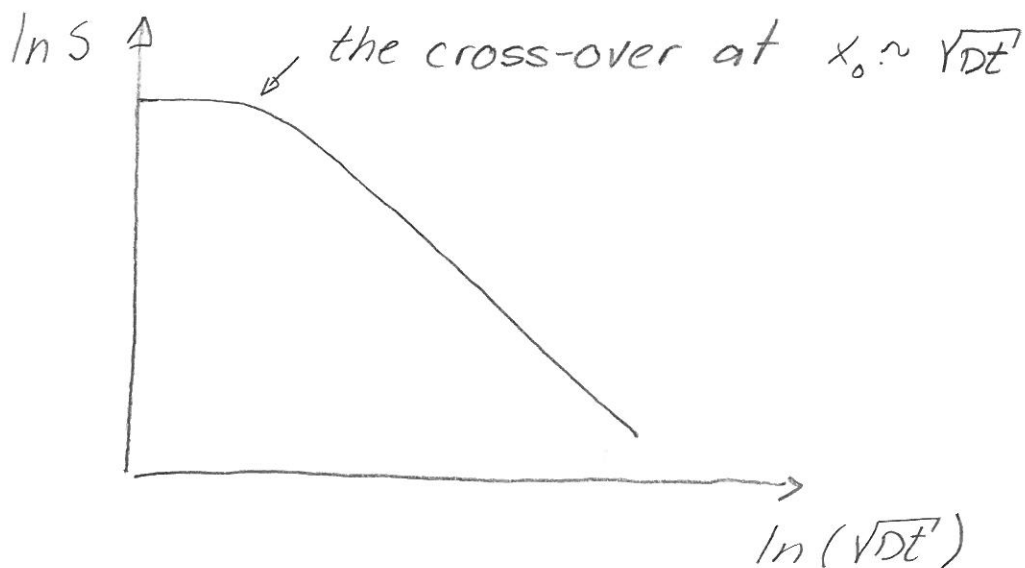
$$= \text{erf} \left(\frac{x_0}{\sqrt{4Dt}} \right)$$

j) Using the expansions of the error function:

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

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

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 $x=0$.