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Solution to the exam in
TFY4275/FY8907 CLASSICAL TRANSPORT THEORY

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This solution consists of 5 pages.

Problem 1.

a) Two examples of diffusion problems under windy conditions or in a river. The situation $q_- \neq_+$ is generally true when advection is playing a role (in addition to diffusion).

By considering the "flow" of particles into node n from time t to $t + \Delta t$ (see lecture notes for details):

$$P(n, t + \Delta t) = P(n, t)\left[1 - q_+ - q_-\right] + P(n - 1, t)q_+ + P(n + 1, t)q_-. \tag{1}$$

b) Now we take the limit $\Delta t \to 0$. To this end, we expand the left-hand-side of Eq. (1) around time t to first order to obtain

$$P(n, t) + \Delta t \frac{\partial P(n, t)}{\partial t} + \mathcal{O}(\Delta t^2) = P(n, t)\left[1 - q_+ - q_-\right] + P(n - 1, t)q_+ + P(n + 1, t)q_-. \tag{2}$$

Now by introducing, $q_\pm = k_\pm \Delta t$, into the above equation, and dividing the result by Δt, one is lead to

$$\frac{\partial P(n, t)}{\partial t} = k_- P(n + 1, t) + k_+ P(n - 1, t) - \left[k_- + k_+\right] P(n, t), \tag{3}$$

which is what we should show.

c) To take the continuous spatial limit, we let $n\Delta x \to x$, where x is the continuous spatial coordinate. In this limit, $P(n, t)$ should be interpreted as the probability of being in an interval of length Δx about $n\Delta x$. Hence, we have the relation $P(n, t) = f(x, t)\Delta x$ [and $(P(n \pm 1, t) = f(x \pm \Delta x, t)\Delta x$] from which it follows from Eq. (3) after Taylor expanding $f(x \pm \Delta x)$ to second order around x

$$\frac{\partial f(x, t)}{\partial t} = -\nu \frac{\partial f(x, t)}{\partial x} + D \frac{\partial^2 f(x, t)}{\partial x^2}, \tag{4a}$$

where

$$\nu = (k_+ - k_-)\Delta x = (q_+ - q_-)\frac{\Delta x}{\Delta t}, \tag{4b}$$

and

$$D = \frac{1}{2}(k_+ + k_-)\Delta x^2 = (q_+ + q_-)\frac{\Delta x^2}{2\Delta t}. \tag{4c}$$

The coefficients, ν and D, are physically interpreted as *drift velocity* and *diffusion coefficients*, respectively [check the units].

d) In the special limit $k_- = k_+ = k = q/\Delta t$ one obtains from Eqs. (4)(b) and (c) that

$$\nu = 0, \tag{5a}$$

and

$$D = k\Delta x^2 = 2q\frac{\Delta x^2}{2\Delta t}. \tag{5b}$$

Notice that even though in Eq. (4a) assumed a continuous representation of position and time, the nature of the physical problem implies that Δx and Δt are finite. The values for Δx and Δt are of the order of the mean free path and mean free time, respectively.

Problem 2.

a) In order to obtain a differential equation for $\langle n \rangle$, we start by multiply Eq. (3) by n and summing the resulting equation from $-\infty$ to ∞. By using that

$$\langle n \rangle (t) = \sum_{-\infty}^{\infty} nP(n,t), \tag{6}$$

we arrive at

$$\frac{\partial \langle n \rangle (t)}{\partial t} = k_+ - k_-. \tag{7}$$

Using a similar approach, where the only difference is that we now multiply by n^2, leads to the following equation:

$$\frac{\partial \left\langle n^2 \right\rangle (t)}{\partial t} = 2\langle n \rangle (k_+ - k_-) + (k_+ + k_-). \tag{8}$$

b) under the assumptions that $\langle n \rangle (t)$ and $\left\langle n^2 \right\rangle (t)$ are both zero at $t = 0$, we can solve Eqs. (6) and (8) readily to obtain:

$$\langle n \rangle (t) = (k_+ - k_-)t, \tag{9a}$$

and

$$\left\langle n^2 \right\rangle (t) = (k_+ - k_-)^2 t^2 + (k_+ + k_-)t. \tag{9b}$$

Hence, we get that

$$\begin{aligned} \left\langle \delta n^2 \right\langle (t) &= \left\langle n^2 \right\rangle (t) - [\langle n \rangle (t)]^2 \\ &= (k_+ + k_-)t, \end{aligned} \tag{10a}$$

which is *linear* in time as expected for diffusion. Alternatively, this latter result can be expressed in terms of the dimension-less probabilities $q_\pm$ as

$$\left\langle \delta n^2 \right\rangle (t) = (q_+ + q_-)\frac{t}{\Delta t} = (q_+ + q_-)N, \tag{10b}$$

where $N = t/\Delta t$ is the number of steps of length Δt corresponding to time t. In passing we note that in the limit $k_- = k_+$, $\langle n \rangle (t) = 0$ for all times and $\left\langle n^2 \right\rangle (t) \propto t$, also this as expected.

c) The generating function is defined as

$$G(s,t) = \sum_{n=-\infty}^{\infty} P(n,t)s^n, \qquad 0 < |s| \leq 1. \tag{11}$$

By multiplying the master equation (2) by s^n and summing the resulting equation from $-\infty$ to ∞, one is arrives at

$$\frac{\partial G(s,t)}{\partial s} = k_+ sG(s,t) + \frac{k_-}{s}G(s,t) - (k_- + k_+)G(s,t). \tag{12}$$

In arriving at this result we have used that the order of time-differentiation and summation do commute. Moreover, the terms of this equation containing $P(n \pm 1, t)$ have been multiplied by $s/s = 1$ in order to get the "correct" powers of s to use the definition of the generating function. For instance this means that $\sum_{-\infty}^{\infty} P(n-1,t)s^n = sG(s,t)$. Since, $k_\pm$ is a constant and s is independent of t the differential equation, (12) is solved straightforwardly with the result

$$G(s,t) = \exp\left[\left(\frac{k_-}{s} + k_+ s - k_- - k_+\right) t\right], \tag{13}$$

where we have used that $G(s, t = 0) = 1$, due to the initial condition $P(n, 0) = \delta_{n,0}$. This result is that should be derived.

d) From the generating function, moments of the pdf, $P(n, t)$ can be derived via

$$\left\langle n^k \right\rangle (t) = \left.\left[\left(s\frac{\partial}{\partial s}\right)^k G(s,t)\right]\right|_{s=1}. \tag{14}$$

To show this, we start by noting that (assuming $k \leq n$)

$$\begin{aligned}
s^k \frac{\partial^k G(s,t)}{\partial s^k} &= s^k \frac{\partial^k}{\partial s^k} \sum_{n=-\infty}^{\infty} P(n,t)s^n \\
&= s^k \sum_{n=-\infty}^{\infty} P(n,t)\frac{\partial^k}{\partial s^k}s^n \\
&= s^k \sum_{n=-\infty}^{\infty} P(n,t)\frac{n!}{(n-k)!}s^{n-k} \\
&= \sum_{n=-\infty}^{\infty} P(n,t)s^n \frac{n!}{(n-k)!}
\end{aligned}$$

This result is derived *via* induction, but will not done here.

By direct calculations, using Eq. (14), the results obtained in Eqs. (9a) and (9b) can be re-established using the generating function method.

Problem 3.

a) For the diffusion problem in the half-space $x \geq 0$, where the boundary is reflecting, the proper boundary conditions (at $x = 0$) reads $\partial_x p(x = 0, t|x_0, t_0) = 0$. Since the domain Ω is only bounded at one side, the method of images, similar to what is used in electro statics, can be used. This method amounts to removing the boundary, but compensating for this action by placing a source term *outside* the region of interest so that the proper boundary condition on the original boundary, $\partial\Omega$, is satisfied for all times. In our particular case, where the boundary is reflecting, the image source term is placed in the region $x < 0$ at position $x = -x_0$. Since we now have no boundary (*i.e.* free-diffusion) the solution to the problem is the sum of the free-space propagators from the two sources. The (conditional) probability density function for the half-space problem reads

$$p(x,t|x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left[-\frac{(x-x_0)^2}{4D(t-t_0)}\right] + \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left[-\frac{(x+x_0)^2}{4D(t-t_0)}\right], \qquad x \geq 0. \tag{15}$$

Obviously this is a solution of the diffusion equations, since each of the two terms, satisfy the equations. Moreover, from this form it is also straightforward to show that $\partial_x p(x = 0, t|x_0, t_0) = 0$, something that also shows the correctness of the assumption of equal source strength for the source and image-source.

b) If we have two reflecting walls, at $x = 0$ and $x = a < \infty$, the particles will be reflected many times from the boundaries. In the long time limit, the probability of for finding the particle *anywhere* in the interval $0 \leq x \leq a$ will be the same. Hence the probability density function should be independent of x — a uniform distribution. Since it should be a normalized function on the interval $[0, a]$, it should satisfy

$$\lim_{t\to\infty} p(x,t|x_0,t_0) = \frac{1}{a}. \tag{16}$$

This is what our physical intuition is telling us.

c) By direct calculations it follows readily, using the given expressions for $v_n(x)$ [Eq. (8) in the exam set], that

$$D\partial_x^2 v_n(x) = \lambda_n v_n(x), \tag{17a}$$

with

$$\lambda_n = -D\left(\frac{n\pi}{a}\right)^2, \tag{17b}$$

for all $n = 0, 1, 2, \ldots$. We also notice that

$$\partial_x v_n(x) \propto -\frac{n\pi}{a} \sin\left[n\pi\frac{x}{a}\right] \tag{18}$$

which all vanish at $x = 0$ (as they should).

d) By substituting the expansion

$$p(x,t|x_0,t_0) = \sum_{n=0}^{\infty} \alpha_n(t|x_0,t_0) v_n(x), \tag{19}$$

into the diffusion equation one gets,

$$\sum_{n=0}^{\infty} \partial_t \alpha_n(t|x_0,t_0) v_n(x) = D \sum_{n=0}^{\infty} \alpha_n(t|x_0,t_0) \partial_x^2 v_n(x) = \sum_{n=0}^{\infty} \alpha_n(t|x_0,t_0) \lambda_n v_n(x), \tag{20}$$

where we have used the the time- and spatial-derivatives commute with the summation over n. In the latest transition of Eq. (21) we have used the eigen-equation (17b).

Now multiplying Eq. (21) by $v_m(x)$, integrating the resulting equation from $x = 0$ to a, leads to

$$\sum_{n=0}^{\infty} \partial_t \alpha_n(t|x_0,t_0) \langle v_m | v_n \rangle = \sum_{n=0}^{\infty} \alpha_n(t|x_0,t_0) \lambda_n \langle v_m | v_n \rangle, \tag{21}$$

and after using the orthonormality condition $\langle v_m | v_n \rangle = \delta_{mn}$ gives the final differential equation for the expansion coefficients

$$\partial_t \alpha_m(t|x_0,t_0) = \lambda_m \, \alpha_m(t|x_0,t_0). \tag{22}$$

The solution of Eq. (23) is

$$\alpha_m(t|x_0,t_0) = e^{\lambda_m(t-t_0)} \beta_m(x_0,t_0), \tag{23}$$

where $\beta_m(x_0,t_0)$ is time-independent constants. The factor $e^{\lambda_m(-t_0)}$ was included in this way for later convenience, and you could have absorbed it into the definition of β_m if you so wished.

e) The initial condition for $p(x,t|x_0,t_0)$ says that $p(x,t_0|x_0,t_0) = \delta(x - x_0)$ which implies that

$$\sum_{n=0}^{\infty} \beta_n(x_0,t_0) v_n(x) = \delta(x - x_0). \tag{24}$$

Again taking the scalar product with $v_m(x)$ and using the orthogonality condition results in the determination of the coefficients $\beta_m(x_0,t_0)$ (assuming $x_0 \in [0,a]$):

$$\beta_m(x_0,t_0) = v_m(x). \tag{25}$$

Thus the final expression for the propagator becomes

$$p(x,t|x_0,t_0) = \sum_{n=0}^{\infty} e^{\lambda_n(t-t_0)} v_n(x_0) v_n(x). \tag{26}$$

f) The long time limit of $p(x,t|x_0,t_0)$ is easily derived by noticing that all $\lambda_n < 0$ for $n > 0$. Hence when $t \to \infty$ only the term $n = 0$ will contribute (since $\lambda_0 = 0$). Therefore, one has that

$$\lim_{t\to\infty} p(x,t|x_0,t_0) = e^{\lambda_0(t-t_0)} v_0(x_0) v_0(x) = \frac{1}{a}. \tag{27}$$

This results conforms our initial intuition, but now the result has been derived formally. Moreover, with Eq. (26), the full time-development from the initial condition to the long time limit can be studied.