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Exam in TFY4275/FY8907 CLASSICAL TRANSPORT THEORY

May 20, 2011
09:00–13:00

Allowed help: Alternativ **D**
Authorized calculator and mathematical formula book

This problem set consists of 4 pages.

This exam consists of three problems each containing several sub-problems. Each of the sub-problems will be given approximately equal weight during grading (if noting else is said to indicate otherwise).

Problem 3 may seem somewhat lengthy, but the calculations are not too time consuming.

I (or a substitute) will be available for questions related to the problems themselves (though not the answers!). The first round (of two), I plan to do a round 10am, and the other one, about two hours later.

The problems are given in English only. Should you have any language problems related to the exam set, do not hesitate to ask. For your answers, you are free to use either English or Norwegian.

Good luck to all of you!

Problem 1.

We will now revisit the (asymmetric) random walk problem in one-dimension. It will be assumed that the walker starts from the position $x = 0$ at time $t = 0$. Within the time interval, Δt, the walker may move with a fixed step length Δx to the left with probability $q_- = k_-\Delta t$, and to the right with probability $q_+ = k_+\Delta t$, where $k_\pm > 0$ denote the jump rates. Note that we in general have $q_+ + q_- \leq 1$ and $q_+ \neq q_-$.

a) Give at least two examples of physical circumstances which naturally lead to $k_- \neq k_+$ (or $q_- \neq q_+$). Write down the master equation for this problem (in discrete space and time). Express your answer in terms of $q_\pm$.

b) Take the limit $\Delta t \to 0$ (continuous time) limit of the master equation and show that in this limit it can be written

$$\frac{\partial P(n,t)}{\partial t} = k_- P(n+1,t) + k_+ P(n-1,t) - (k_- + k_+)P(n,t), \tag{1}$$

where $P(n,t)$ denotes the probability for the particle to be at position n at time t. [Note that Eq. (1) is also a master equation, but now in continuous time.]

We will now as well take the continuous spatial limit, $\Delta x \to 0$, of Eq. (1). This is achieved by letting the discrete position $n\Delta x$ be associated with the continuous spacial coordinate x ($n\Delta x \to x$). Let $f(x,t)$ denote the probability density for finding the particle at position x at time t.

c) Show that in the continuous space limit the master equation (1) turns into the Fokker-Plank equation

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

Identify the coefficients ν and D and express them in terms of $k_\pm$, Δx and Δt. What is the physical significance of these coefficients (*i.e.* of ν and D)?

d) Check the expressions for ν and D for the special case $k_+ = k_-$. Do you find your answers reasonable?

Problem 2.

In the lectures we solved the Fokker-Planck equation, Eq. (2), in closed form. Moreover, this solution was used to calculate the scaling of the second moment, $\left\langle \delta x^2 \right\rangle$ ("the spatial fluctuations"), with time.

Now we shall derive the same scaling relations, however, using two alternative approaches which both are based upon the master equation (1).

a) Obtain differential equations for $\langle n \rangle$ and $\left\langle n^2 \right\rangle$ expressed in terms of $k_\pm$ and the dependent variables alone. [Hint: use Eq. (1)].

b) Solve both equations under the assumptions that $\langle n \rangle (t)$ and $\left\langle n^2 \right\rangle (t)$ are both zero at $t = 0$. Use these results to find an expression for the fluctuations $\left\langle n^2 \right\rangle (t) - [\langle n \rangle (t)]^2$, and make sure that the scaling is as expected.

With access to the generating function for the probability distribution, $P(n,t)$, moments of any order can be easily calculated. For a spatially discrete probability distribution it is defined as [1]

$$G(s,t) = \sum_{n=-\infty}^{\infty} P(n,t)s^n, \qquad 0 < |s| \le 1. \tag{3}$$

c) Derive the differential equation satisfied by the generating function and show that it has the solution

$$G(s,t) = \exp\left[\left(\frac{k_-}{s} + k_+ s - k_- - k_+\right)t\right]. \tag{4}$$

d) Establish the relation

$$\left\langle n^k \right\rangle(t) = \left[\left(s\frac{\partial}{\partial s}\right)^k G(s,t)\right]\bigg|_{s=1}, \tag{5}$$

and use this result to calculate $\langle n \rangle(t)$ and $\left\langle n^2 \right\rangle(t)$. Compare your results to what was found in subproblem 2b.

Problem 3.

In this problem we will consider one-dimensional free diffusion within a constrained spatial region Ω. Hence, we aim at finding the conditional probability density function, $p(x,t|x_0,t_0)$, that obeys the diffusion equation

$$\partial_t p(x,t|x_0,t_0) = D\partial_x^2 p(x,t|x_0,t_0), \tag{6a}$$

subject to the initial condition

$$p(x,t_0|x_0,t_0) = \delta(x-x_0), \tag{6b}$$

with x and x_0 in Ω.

In this problem the boundary of the domain Ω, denoted $\partial\Omega$, will be assumed to be *reflecting*. The appropriate reflecting boundary condition to be satisfied on $\partial\Omega$ is

$$D\partial_x p(x,t|x_0,t_0) = 0, \qquad \text{for } x \in \partial\Omega. \tag{6c}$$

We now intend to solve Eqs. (6) for two geometries — the half-space and a finite domain.

First we will assume $\Omega = [0,\infty)$, *i.e.* the particle can diffuse freely in the half-space $x \ge 0$ with a reflecting boundary at $x = 0$. Moreover, in this case one should have the boundary condition $\lim_{x\to\infty} p(x,t|x_0,t_0) = 0$.

a) Show that the solution to this half-space problem (that can be derived by the method of images) can be written as

$$p(x,t|x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}}\exp\left[-\frac{(x-x_0)^2}{4D(t-t_0)}\right] + \frac{1}{\sqrt{4\pi D(t-t_0)}}\exp\left[-\frac{(x+x_0)^2}{4D(t-t_0)}\right], \qquad x \ge 0. \tag{7}$$

What is the physical interpretation of this solution?

[1] This is the discrete analogy of $G(k,t) = \int dx\, P(x,t)\exp(ikx)$, but with $s = \exp(ik)$.

We will now consider $\Omega = [0, a]$ where $a > 0$, that is, free diffusion within a finite domain of length a and reflecting boundaries at $x = 0$ and $x = a$.

b) Based on the physics of the problem, what is to be expected for $\lim_{t\to\infty} p(x, t|x_0, t_0)$?

To formally derive a solution to the finite domain free diffusion problem is quite a bit harder than for the equivalent half-space problem.

To this end, we will expend $p(x, t|x_0, t_0)$ in *eigenfunctions* of the diffusion operator $D\partial_x^2$. This method follows very closely what is done in quantum mechanics [2]. However, only the eigenfunctions that are consistent with the reflecting boundary conditions, Eq. (6c), at $x = 0$ and $x = a$ will be included in the expansion. The relevant eigenfunctions can be shown to be (you do not have to show this though)

$$v_n(x) = \begin{cases} \sqrt{\frac{1}{a}}, & \text{for } n = 0, \\ \sqrt{\frac{2}{a}} \cos\left[n\pi \frac{x}{a}\right], & \text{for } n = 1, 2, 3, \ldots, \end{cases} \tag{8}$$

which are *orthonormal* with respect to the scalar product (on the interval $[0, a]$)

$$\langle f|g\rangle = \int_0^a dx\, f(x)g(x), \tag{9}$$

that is, the eigenfunctions satisfy $\langle v_m|v_n\rangle = \delta_{mn}$.

In terms of these eigenfunctions one may write

$$p(x, t|x_0, t_0) = \sum_{n=0}^{\infty} \alpha_n(t|x_0, t_0) v_n(x), \tag{10}$$

where $\alpha_n(t|x_0, t_0)$ are expansion coefficients to be determined.

c) Show that $v_n(x)$ satisfies the eigenequation (for the diffusion operator)

$$D\partial_x^2 v_n(x) = \lambda_n v_n(x), \tag{11a}$$

with

$$\lambda_n = -D\left(\frac{n\pi}{a}\right)^2, \tag{11b}$$

for all $n = 0, 1, 2, \ldots$.

d) Find the differential equation satisfied by $\alpha_m(t|x_0, t_0)$ and demonstrate that its solution is

$$\alpha_n(t|x_0, t_0) = e^{\lambda_n(t-t_0)}\beta_n(x_0, t_0), \tag{12}$$

where $\beta_n(x_0, t_0)$ are time-independent constants.

e) Determine $\beta_n(x_0, t_0)$ and show that the final solution of the free diffusion problem with reflecting boundary at $x = 0$ and $x = a$ (valid for $t > t_0$) can be written as

$$p(x, t|x_0, t_0) = \sum_{n=0}^{\infty} e^{\lambda_n(t-t_0)} v_n(x_0) v_n(x). \tag{13}$$

f) Finally obtain the long time behavior of $p(x, t|x_0, t_0)$, and compare this analytical prediction to what you obtained based on your physical intuition in subproblem 3b.

[2] This similarity is not unexpected since the time-dependent Schrödinger equation essentially is a diffusion equation in complex time.