NTNU **Institutt for fysikk**

Contact during the exam:
Professor Ingve Simonsen
Telephone: 9 34 17 or 470 76 416

Exam in TFY4275/FY8907 CLASSICAL TRANSPORT THEORY

May 15, 2009
09:00–13:00

Allowed help: Alternativ **D**

Authorized calculator and mathematical formula book

This problem set consists of 5 pages, plus an Appendix of one page.

This exam consists of two problems each containing several sub-problems. Each of the sub-problem will be given approximately equal weight during grading. For your information, I estimate that you will spend about twice the amount of time on the 2nd problem relative the 1st.

I will be available for questions related to the problems themselves (though not the answers!). The first round (of two), I plan to do around 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.

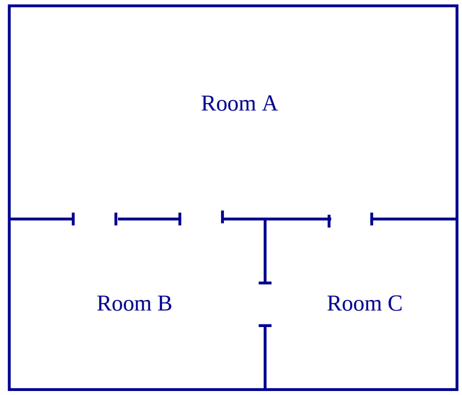

Figure 1: Floor plan for the house of the mice

In this problem we will consider an ensemble of *trained* mice living in a house as shown in the figure above (Fig. 1). A bell rings at a regular interval, Δt, (considered short compared to the lifetime of the mice). Each time it rings, the mice are trained and will change room. When they change rooms, they are *equally* likely to pass through any of the doors of the room they currently are in.

a) Explain in words what the master-equation is and how it is derived. If the master equation is appropriate for describing the underlying stochastic process, what can in general be said about the properties of the process.

Let us denote the total (time-independent) number of mice for N and the number of mice in room A at time t for, $N_A(t)$, and similarly for room B and C. Moreover, we define the (density) state vector for the system by

$$\boldsymbol{\rho}(t) = \begin{pmatrix} \rho_A(t) \\ \rho_B(t) \\ \rho_C(t) \end{pmatrix} = \frac{1}{N} \begin{pmatrix} N_A(t) \\ N_B(t) \\ N_C(t) \end{pmatrix},$$

where $\rho_i(t) = N_i(t)/N$ $(i = A, B, C)$ denotes the fraction of mice being present at room i at time t.

b) From the continuity of the number of mice (assuming that none of them die during the time of the study) obtain expressions for $N_i(t+\Delta t)$ $(i = A, B, C)$ in terms of the other $N_i(t)$'s.

c) Obtain the master-equation for the house of the mice when assuming that the time interval between rings is Δt. Express your answer in terms of $\partial_t \boldsymbol{\rho}(t) = (\boldsymbol{\rho}(t+\Delta t) - \boldsymbol{\rho}(t))/\Delta t$ and determine the matrix, $\boldsymbol{\Gamma}$, that appears on the right hand side of the equation. Make sure that you explain properly your way of reasoning.

d) Demonstrate that one also may write $\boldsymbol{\rho}(t+\Delta t) = \mathbf{T}\boldsymbol{\rho}(t)$ where $\mathbf{T}$ is the so-called transfer matrix given by

$$\mathbf{T} = \begin{pmatrix} 0 & 2/3 & 1/2 \\ 2/3 & 0 & 1/2 \\ 1/3 & 1/3 & 0 \end{pmatrix}.$$

e) What is the interpretation of the matrix elements T_{ij}? Based on this interpretation, what property for the elements of $\mathbf{T}$ does the conservation of probability (or mice) imply?

f) What is the steady-state (or stationary) solution, $\bar{\boldsymbol{\rho}} = \lim_{t\to\infty} \boldsymbol{\rho}(t)$, of the equation $\boldsymbol{\rho}(t + \Delta t) = \mathbf{T}\boldsymbol{\rho}(t)$.

g) In the steady state, what is the ratio between the densities of the three rooms $\bar{\rho}_A : \bar{\rho}_B : \bar{\rho}_C$? How are these ratios related to the number of doors, D_i $(i = A, B, C)$, of the various rooms.

Problem 2.

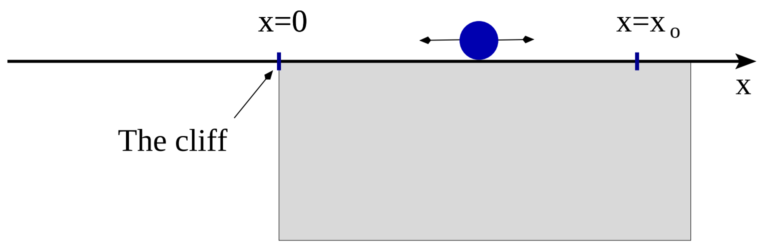

Figure 2: The diffusing particle in the absorbing semi-infinite interval $(0, \infty)$, *i.e.* the "cliff problem".

We consider a general (one-sided) barrier crossing problem where the so-called *first-passage* and *survival* probabilities appear. This problem is devoted to a step-by-step derivation of central properties of such systems, including the two probabilities given above.
To set the stage, let us consider a diffusing particle that starts from position $x = x_0 > 0$ at time $t = t_0$. A steep cliff is located at $x = 0$, and a flat plateau is present in the region $x > 0$. The particle will fall down from the plateau when it arrives at the cliff at $x = 0$ (for the first time). In more typical physics terms, one says that the particle is absorbed, *i.e.* we have an *absorbing boundary condition* at $x = 0$. Notice that the particle is *only* allowed to diffuse in the positive x-region of our coordinate system (*i.e.* at the plateau).

The questions we are concerned about are : (*i*) What is the distribution of waiting times for the particle to fall off the cliff (being absorbed at the cliff) — known as the *first-passage* probability; and (*ii*) what is the probability that the particle has *not* fallen off the plateau after a time t — the *survival* probability.

In electrostatic boundary value problems for the electric potential, *e.g.*, a charged sphere located above a conducting grounded plane, one introduces an image charge distribution below the plane of given strength and located so that the appropriate boundary conditions at the surface of the plane is satisfied. This powerful approach is known as the *method of images* (or image method). Notice in particular that the image charge is introduced in order to satisfy the boundary condition at (in our example) the surface of the grounded plane and that the total potential from the two charges is only valid in the region above the plane.
Here we will apply a similar image method to our diffusion problem with absorbing boundary condition.

From the lectures we recall that the propagator in free space for a diffusing particle starting from x_0 at time t_0 is

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

a) What is the meaning of the quantity D present in Eq. (1), and what is its physical unit? Give a physical interpretation of the propagator $p(x,t|x_0,t_0)$. What happens to $p(x,t|x_0,t_0)$ in the limit $t \to t_0$ (from above)? Based on this limit, argue what is so special about the point (x_0,t_0) in the xt-plane (what is the physical meaning of this point)?

Let $u(x,t|x_0,t_0)$ denote the probability density for the diffusing particle with the absorbing boundary conditions at $x = 0$ (the "cliff-problem") described above. Here (as before) x_0 and t_0 denote the starting point and time of the particle, respectively. [Often this problem is referred to as the problem of a diffusion particle in the absorbing semi-infinite interval $(0,\infty)$. If you should find it easier, you may from hereon (without loss of generality) set $t_0 = 0$.]

b) Argue why the absorbing boundary conditions at $x = 0$ implies the boundary condition $u(x = 0,t|x_0,t_0) = 0$?

c) Use the method of images to find the location and strength of the *image* diffusion source (or sink) so that the boundary condition $u(x = 0,t|x_0,t_0) = 0$ (at $x = 0$) is satisfied for *all* times. Make a figure of your suggested configuration.

d) For your suggested configuration, obtain an expression for $u(x,t|x_0,t_0)$ valid for $x \geq 0$ and $t > t_0$. Also derive an approximate expression for $u(x,t|x_0,t_0)$ in the long time limit ($t \gg t_0$, $\sqrt{Dt} \gg x_0$). Make a sketch of your solution $u(x,t|x_0,t_0)$ (for $x \geq 0$ and $t > t_0$) and also indicate the two fundamental propagators from which $u(x,t|x_0,t_0)$ can be constructed.

e) Argue why the first-passage probability to the origin ($x = 0$), $f(0,t|x_0,t_0)$, is given by

$$f(0,t|x_0,t_0) = D\,\frac{\partial}{\partial x}u(x,t|x_0,t_0)\bigg|_{x=0}. \tag{2}$$

What is the physical interpretation of this equation?

f) From Eq. (2) (or by other means) calculate $f(0,t|x_0,t_0)$ in the long time limit and show that

$$f(0,t|x_0,t_0) = \frac{x_0}{\sqrt{4\pi Dt^3}} \exp\left\{-\frac{x_0^2}{4Dt}\right\}. \tag{3}$$

g) What is the average waiting time $\langle t \rangle$ for first-passage to the origin, and how do you rationalize this finding? Make a sketch of $f(0,t|x_0,t_0)$ for (*i*) $x_0 \to 0^+$ and (*ii*) $x_0 > 0$ and finite. What is the main difference between these two cases, and how should one interpret this difference?

h) The diffusion length of the particle is given by $\sqrt{Dt}$. Discuss and find expressions for the first-passage probability $f(0,t|x_0,t_0)$ in the two limits (*i*) $\sqrt{Dt} \gg x_0$ and (*ii*) $\sqrt{Dt} \ll x_0$. These two limits separate two physically very different regimes. What is the physical significance of the two regimes?

The survival probability $S(t|x_0, t_0)$ measures the probability that the diffusing particle has *not* been absorbed (at $x = 0$) by time t. Hence, it is given by

$$S(t|x_0, t_0) = 1 - \int_0^t dt' f(0, t'|x_0, t_0), \tag{4}$$

where the last term of Eq. (4) measures the (total) probability of being absorbed up to time t. [Moreover, it can be shown that this definition is equivalent to $S(t|x_0, t_0) = \int_0^\infty dx\, u(x, t|x_0, t_0)$.]

i) Show that the survival probability is given by

$$S(t|x_0, t_0) = \operatorname{erf}\left(\frac{x_0}{\sqrt{4Dt}}\right), \tag{5}$$

where $\operatorname{erf}(\cdot)$ denotes the so-called error function (see the appendix).

j) Find approximations for $S(t|x_0, t_0)$ valid when (*i*) $\sqrt{Dt} \ll x_0$ and (*ii*) $\sqrt{Dt} \gg x_0$.

k) Make a sketch of a log-log graph of $S(t|x_0, t_0)$ *vs.* $\sqrt{Dt}$ where the two regimes are apparent. What are the physical reasons why the two regimes are so different?

Mathematics:

- The Fourier Transform:

$$\hat{f}(k) = \int_{-\infty}^{\infty} dx\, f(x) e^{-ikx}$$

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \hat{f}(k) e^{ikx}$$

- The Lévy distribution

$$\hat{\mathcal{L}}\alpha(k) = \exp(-a|k|\alpha)$$

- Sin hyperbolicus

$$\sinh(x) = \frac{e^x - e^{-x}}{2}$$

- The error function

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x du\, e^{-u^2}$$

- Taylor expansions

$$f(x+\delta) \simeq f(x) + \delta f'(x) + \frac{\delta^2}{2!} f''(x) + \dots$$

$$\sinh(x) \simeq x + \frac{x^3}{3!} + O(x^5)$$

$$\mathrm{erf}(x) \simeq \begin{cases} \frac{2}{\sqrt{\pi}} e^{-x^2} \left[x + \frac{2x^3}{1\cdot 3} + \frac{4x^5}{1\cdot 3\cdot 5} + \cdots \right], & x \ll 1 \\ 1 - \frac{e^{-x^2}}{\sqrt{\pi} x} \left[1 - \frac{1}{2x^2} - \cdots \right], & x \gg 1 \end{cases}$$

- Some integrals

$$\int_{-\infty}^{\infty} dx\, e^{-\left(ax^2+2bx+c\right)} = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2-ac}{a}\right), \qquad a > 0$$

$$\int_{-\infty}^{\infty} dx\, x\, e^{-\left(ax^2+2bx+c\right)} = \frac{-b}{a} \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2-ac}{a}\right), \qquad a > 0$$

$$\int_{-\infty}^{\infty} dx\, x^2\, e^{-\left(ax^2+2bx+c\right)} = \frac{a+2b^2}{2a^2} \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2-ac}{a}\right), \qquad a > 0$$