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Solution to the exam in
TFY4275/FY8907 CLASSICAL TRANSPORT THEORY

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This solution consists of 8 pages.

Problem 1.

a) The constant N is a normalization constant and is determined from

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{0}^{\infty} \mathrm{d}t\, \psi(x,t) = 1. \tag{10}$$

Evaluating the integrals leads to

$$\begin{aligned} 1 &= N \int_{-\infty}^{\infty} \mathrm{d}x \, \exp\left(-\frac{|x|}{a}\right) \int_{0}^{\infty} \mathrm{d}t \, \exp\left(-\frac{t}{\tau}\right) \\ &= 2N \underbrace{\int_{0}^{\infty} \mathrm{d}x \, \exp\left(-\frac{x}{a}\right)}_{a} \underbrace{\int_{0}^{\infty} \mathrm{d}t \, \exp\left(-\frac{t}{\tau}\right)}_{\tau} \\ &= 2Na\tau. \end{aligned} \tag{11}$$

Hence, the normalization constant becomes

$$N = \frac{1}{2a\tau}, \tag{12}$$

so that the final form of the joint jump distribution reads

$$\psi(x,t) = \frac{1}{2a\tau} \exp\left(-\frac{|x|}{a} - \frac{t}{\tau}\right). \tag{13}$$

The marginal distributions are obtained from $\psi(x,t)$ as

$$p_x(x) = \int_{0}^{\infty} \mathrm{d}t\, \psi(x,t) = \frac{1}{2a} \exp\left(-\frac{|x|}{a}\right), \tag{14}$$

and

$$p_t(t) = \int_{-\infty}^{\infty} \mathrm{d}x\, \psi(x,t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right). \tag{15}$$

The integrals were here evaluated similarly to those use to obtain N.

In passing we note that $\psi(x,t)$ is a product of the Laplace distribution for the jump-size and an exponential waiting time distribution.

b) The diffusion constant, D, of the CTRW model is determined from

$$D = \frac{\langle x^2 \rangle}{2\langle t \rangle}. \tag{16}$$

so one has to calculate the proper moments of the marginal distributions. By direct calculations one obtains

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, x^2 p_x(x) = \frac{1}{a}\int_0^{\infty} \mathrm{d}x\, x^2 \exp\left(-\frac{x}{a}\right) = 2a^2 \tag{17}$$

and

$$\langle t \rangle = \int_0^{\infty} \mathrm{d}t\, t p_t(t) = \frac{1}{\tau}\int_0^{\infty} \mathrm{d}t\, t \exp\left(-\frac{t}{\tau}\right) = \tau. \tag{18}$$

Therefore, the diffusion constant becomes

$$D = \frac{\langle x^2 \rangle}{2\langle t \rangle} = \frac{a^2}{\tau}. \tag{19}$$

Problem 2.

a) Due to the translation invariance of the surface, the width $w(t)$ can not depend on the spatial coordinate x. Therefore, in addition to time t, only a dependence on the constants D and Γ is expected. We observe that

$$[t] = T \tag{20a}$$

$$[D] = \frac{L^2}{T} \tag{20b}$$

$$[\Gamma] = [\eta]^2 LT = \frac{L^3}{T} \tag{20c}$$

where L and T are length and time-scales, respectively. Lets start by defining

$$w^2(t; D, \Gamma) = t^\alpha D^\beta \Gamma^\gamma F(\kappa), \tag{21}$$

where F is a dimensionless function of a dimensionless argument κ. Using that $[w^2] = L^2$ and equating powers of L and T gives the following set of equations, respectively,

$$\begin{aligned} 2 &= 2\beta + 3\gamma \\ 0 &= \alpha - \beta - \gamma. \end{aligned} \tag{22}$$

Equation (22) represents two equations in three unknowns, so a unique solution does not exist. Therefore, we try to put $\gamma = 0$, something that is motivated by Eq. (6). With the choice $\gamma = 0$, it follows from Eq. (22) that $\alpha = \beta = 1$ so that $w^2(t) \propto Dt$ that is consistent with Eq. (6). However, from the point of view of dimensional analysis, one may multiply this result by a dimensionless function, so that we get

$$w^2(t) = DtF(\kappa), \tag{23}$$

which is the form one should demonstrate (where κ is assumed dimensionless as well).

To find the form of κ, we start by assuming that $\kappa = t^{\alpha'} D^{\beta'} \Gamma^{\gamma'}$. From $[\kappa] = 1$ one is lead to the set of equations $0 = 2\beta' + 3\gamma'$ and $0 = \alpha' - \beta' - \gamma'$, which has the solution

$$\beta' = -\frac{3}{2}\gamma', \qquad \alpha' = -\frac{\gamma'}{2}, \tag{24}$$

valid for arbitrary value of γ'. For simplicity putting $\gamma' = -2\gamma''$ it follows that a dimensionless combination is $\left(D^3 t/\Gamma^2\right)^{\gamma''}$. Hence, a good choice for κ is

$$\kappa = \frac{D^3 t}{\Gamma^2}, \tag{25}$$

[or the inverse of this (i.e. $\gamma'' = -1$), or any other integer power......].

b) Since the Edwards-Wilkinson equation is linear, it follows that the height is proportional to the noise η, and so is the surface width. Moreover, due to the properties of the noise, Eq. (4b), it follows that $\eta \propto \sqrt{\Gamma}$. Therefore, we have that $w^2(t) \propto \Gamma$ and the unknown function F thus becomes

$$F(\kappa) = C\kappa^{-1/2}, \tag{26}$$

where C is some unknown (dimensionless) constant. Therefore, from Eq. (23) with Eqs. (25) and (26) it follows that

$$w^2(t) = C\Gamma\sqrt{\frac{t}{D}}. \tag{27}$$

The constant C we still have to determine, but from dimensional analysis and linearity of the problem the functional form (27) is predicted. This explicitly demonstrates the power of dimensional analysis.

c) The general solution for the height $h(x,t)$ follows from the principle of superposition and can be written in terms of the fundamental solution $p(x,t|x_0,t_0)$ as

$$\begin{aligned} h(x,t) &= \int_0^t \mathrm{d}t_0 \int_{-\infty}^{\infty} \mathrm{d}x_0 \, p(x,t|x_0,t_0)\eta(x_0,t_0) \\ &= \int_0^t \mathrm{d}t_0 \int_{-\infty}^{\infty} \mathrm{d}x_0 \, \frac{\exp\left(-\frac{(x-x_0)^2}{4D(t-t_0)}\right)}{\sqrt{4\pi D(t-t_0)}} \eta(x_0,t_0). \end{aligned} \tag{28}$$

The physical interpretation of this expression is that the effect of the source of amplitude $\eta(x_0,t_0)$ at position x_0 at time t_0 is at the observation point (x,t) represented by $p(x,t|x_0,t_0)\eta(x_0,t_0)$. Due to the linearity of the problem, we may add all such possible contributions for sources active up till time t, something that is taken into account by the spatial and temporal integrals over the source coordinates in Eq. (28).

d) From Eq. (28) the surface width can be calculated explicitly in the following way:

$$
\begin{aligned}
w^2(t) &= \langle h^2(x,t) \rangle \\
&= \int_0^t \mathrm{d}t_0 \int_{-\infty}^{\infty} \mathrm{d}x_0 \, \frac{\exp\left(-\frac{(x-x_0)^2}{4D(t-t_0)}\right)}{\sqrt{4\pi D(t-t_0)}} \int_0^t \mathrm{d}t_0' \int_{-\infty}^{\infty} \mathrm{d}x_0' \, \frac{\exp\left(-\frac{(x-x_0')^2}{4D(t-t_0')}\right)}{\sqrt{4\pi D(t-t_0')}} \underbrace{\langle \eta(x_0,t_0)\eta(x_0',t_0') \rangle}_{2\Gamma\delta(x_0-x_0')\delta(t_0-t_0')} \\
&= \Gamma \int_0^t \mathrm{d}t_0 \int_{-\infty}^{\infty} \mathrm{d}x_0 \, \frac{1}{2\pi D(t-t_0)} \exp\left(-\frac{(x-x_0)^2}{2D(t-t_0)}\right)
\end{aligned}
\tag{29}
$$

where we in the last transition have taken into account the properties of the noise.

Performing the integrals give

$$
w^2(t) = \Gamma \int_0^t \mathrm{d}t_0 \, \frac{1}{2\pi D(t-t_0)} \underbrace{\int_{-\infty}^{\infty} \mathrm{d}x_0 \, \exp\left(-\frac{(x-x_0)^2}{2D(t-t_0)}\right)}_{\sqrt{2\pi D(t-t_0)}} = \sqrt{\frac{2}{\pi}} \Gamma \sqrt{\frac{t}{D}}. \tag{30}
$$

In obtaining this result, we have used that the spatial integral is of the Gaussian type and can thus be evaluated straightforwardly.

From Eq. (30) it follows that the result is consistent with what was obtained by dimensional analysis, and the "missing constant" we find to be $\sqrt{2/\pi}$.

Problem 3.

a) Fick's two empirical laws read:

1. Fick's 1st law states that the particle current density is given by $\mathbf{J} = -D\boldsymbol{\nabla} p(\mathbf{x}, t|\mathbf{x}_0, t_0)$ [for the meaning of the symbols see below]
2. Fick's 2nd law:

$$
\frac{\partial p(\mathbf{x}, t|\mathbf{x}_0, t_0)}{\partial t} = D\nabla^2 p(\mathbf{x}, t|\mathbf{x}_0, t_0),
$$

   that is the diffusion equation.

Note that Fick's 1st law is general and does also apply to situations where D varies in space. However, the 2nd law (as stated above) only applies to situations where D is constant.

If D is not constant, then one instead has to start from the continuity equation of particles

$$
\frac{\partial p(\mathbf{x}, t|\mathbf{x}_0, t_0)}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} = 0,
$$

in order to derive the appropriate diffusion equation.

Combining this result with the 1st law gives the diffusion equation satisfied for a spatially dependent D;

$$
\begin{aligned}
\frac{\partial p(\mathbf{x}, t|\mathbf{x}_0, t_0)}{\partial t} &= \boldsymbol{\nabla} \cdot \{D\boldsymbol{\nabla} p(\mathbf{x}, t|\mathbf{x}_0, t_0)\} \\
&= [\boldsymbol{\nabla} D(\mathbf{x})] \cdot \boldsymbol{\nabla} p(\mathbf{x}, t|\mathbf{x}_0, t_0) + D(\mathbf{x})\nabla^2 p(\mathbf{x}, t|\mathbf{x}_0, t_0).
\end{aligned}
$$

The above relation is the diffusion equation in media where the "diffusion constant" is spatially dependent, $D(\mathbf{x})$.

b) The boundary conditions at $x = \pm\infty$ is that (for all finite x_0)

$$\lim_{x\to\pm\infty} p(x, t|x_0, 0) = 0 \tag{31}$$

At $x = 0$, the boundary condition says that the current density should be continuous at this point. This means that one should have for all times t

$$J(0^+, t) = J(0^-, t), \tag{32a}$$

where $x^\pm$ means $x \pm \eta$ where η is a positive infinitesimal number, and

$$J(x, t) = -D(x)\frac{\partial p(x, t|x_0, 0)}{\partial x}. \tag{32b}$$

If the latter condition is not satisfied, particles will "pile up" at $x = 0$, something that is not physical. Note that it is not sufficient that $p(x, t|x_0, 0)$ is continuous at this point.

c) To identify the time-scale t_* we proceed as follows; Let $\ell(t)$ be the distance (the "diffusion length") from the starting point x_0 that the diffusing particles on average has reached at time t. For the approximation $p(x, t|x_0, 0) \approx p_+(x, t|x_0, 0)$ to hold, one should require [when the particle starts at $x = x_0$ at time $t = 0$]

$$\ell(t) \ll x_0, \qquad \text{for } t \ll t_*. \tag{33}$$

For $\ell(t)$ we will use the standard deviation, *i.e.*

$$\ell(t) \simeq \sigma(t) = \sqrt{2D_+t}. \tag{34}$$

To identify the time t_*, we solve the equation $\ell(t_*) = x_0$ to find that

$$t_* = \frac{x_0^2}{2D_+}. \tag{35}$$

So we expect that the approximation $p(x, t|x_0, 0) \approx p_+(x, t|x_0, 0)$ should hold for times $t \ll t_* = x_0^2/(2D_+)$. Later we will explicitly check this results.

d) Following the problem set, we start by assuming a solution on the form

$$p(x, t|x_0, 0) = \begin{cases} A_-p_-(x, t|x_0, 0), & x < 0 \\ A_+p_+(x, t|x_0, 0), & x \geq 0 \end{cases}, \tag{36}$$

where the $A_\pm$ are function independent of spacial coordinates. We denote the denoting the relevant (particle) current density by

$$J_\pm(x, t) = -D_\pm\frac{\partial p_\pm(x, t|x_0, 0)}{\partial x}, \tag{37}$$

where the subscripts denote which domain that they apply [+ for $x > 0$ and $-$ for $x < 0$.] To determine the functions $A_\pm$, we will use the boundary conditions at x_0 that states that :

$$J_-(0^-, t) = J_+(0^+, t), \qquad \text{for all } t. \tag{38}$$

Substituting the expressions for $p_\pm(x, t|x_0, 0$ into Eq. (38) and with the use of the definition (37) it follows that

$$A_- \frac{-x_0}{2t} p_-(0, t|x_0, 0) = A_+ \frac{-x_0}{2t} p_+(0, t|x_0, 0), \tag{39}$$

or after some straightforward mathematical manipulation

$$A_- = A_+ \sqrt{\frac{D_-}{D_+}} \exp\left\{ \frac{(D_+ - D_-)x_0^2}{4D_+D_-t} \right\}. \tag{40}$$

So for given A_+ (determined by normalization, see sub-problem f), we see that A_- is a function of time.

In the limit $D_- = D_+$, it follows immediately form Eq. (40) that $A_- = A_+$ as is to be expected.

e) So with relation (40), it follows

$$p(x, t|x_0, 0) = \begin{cases} \frac{A_+}{\sqrt{4\pi D_+ t}} \exp\left\{ \frac{(D_+ - D_-)x_0^2}{4D_+D_-t} - \frac{(x-x_0)^2}{4D_-t} \right\}, & x < 0 \\ \frac{A_+}{\sqrt{4\pi D_+ t}} \exp\left\{ -\frac{(x-x_0)^2}{4D_+t} \right\}, & x \geq 0 \end{cases}, \tag{41}$$

In order to demonstrate that $p(x, t|x_0, 0) \approx p_+(x, t|x_0, 0)$ for $t \ll t_*$, we need to demonstrate that then the solution $p(x, t|x_0, 0) \approx 0$ for $x < 0$. To this end, we study the exponent [see Eq. (41) for $x < 0$]

$$\frac{(D_+ - D_-)x_0^2}{4D_+D_-t} - \frac{(x - x_0)^2}{4D_-t} = -\frac{D_+(x - x_0)^2 - (D_+ - D_-)x_0^2}{4D_+D_-t}.$$

It now follows by recalling that here $x < 0$ and (by assumption) $x_0 > 0$

$$\begin{aligned} \frac{D_+(x - x_0)^2 - (D_+ - D_-)x_0^2}{4D_+D_-t} &\gg \frac{D_+(x - x_0)^2 - (D_+ - D_-)x_0^2}{4D_+D_-t_*} \\ &= \frac{D_+(x - x_0)^2 - (D_+ - D_-)x_0^2}{2D_-x_0^2} \\ &= \frac{1}{2}\frac{D_+}{D_-}\left(\frac{x}{x_0} - 1\right)^2 - \frac{1}{2}\left(\frac{D_+}{D_-} - 1\right) \\ &> \frac{1}{2}\frac{D_+}{D_-} - \frac{1}{2}\frac{D_+}{D_-} + \frac{1}{2} \\ &= \frac{1}{2}. \end{aligned} \tag{42}$$

Since the exponent of the exponential function contained in the expression for $p(x,t|x_0,0)$ when $x<0$ is much smaller than $1/2$ when $t \ll t_*$ and $x_0>0$, one may conclude that for the same time region

$$p(x,t|x_0,0) \ll 1, \qquad \text{for } x<0. \tag{43}$$

Hence, we have mathematically demonstrated our original argument obtained from general principles.

f) The function A_+ is determined by the normalization condition of the probability density function, *i.e.*

$$\int_{-\infty}^{\infty} \mathrm{d}x\, p(x,t|x_0,0) = 1, \qquad \forall t. \tag{44}$$

This implies since $A_\pm$ do not depend on the spatial coordinates:

$$A_- \int_{-\infty}^{0} \mathrm{d}x\, p_-(x,t|x_0,0) + A_+ \int_{0}^{\infty} \mathrm{d}x\, p_+(x,t|x_0,0) = 1 \tag{45}$$

Now we calculate the following integrals

$$\begin{aligned}\int_{0}^{\infty} \mathrm{d}x\, p_\pm(x,t|x_0,0) &= \frac{1}{\sqrt{\pi}} \int_{-\frac{x_0}{\sqrt{4D_\pm t}}}^{\infty} \mathrm{d}w\, \exp\left(-w^2\right) \\ &= \frac{1}{2} - \frac{1}{2}\mathrm{erf}\left(-\frac{x_0}{\sqrt{4D_\pm t}}\right),\end{aligned} \tag{46a}$$

where we have made a change of variable to

$$w = \frac{x-x_0}{\sqrt{4D_\pm t}}, \tag{46b}$$

and introduced the error-function (see appendix of the problem set).

Moreover, since $p_\pm(x,t|x_0,0)$ both are normalized on the entire real axis, we have that

$$\begin{aligned}\int_{-\infty}^{0} \mathrm{d}x\, p_\pm(x,t|x_0,0) &= 1 - \int_{0}^{\infty} \mathrm{d}x\, p_\pm(x,t|x_0,0) \\ &= \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(-\frac{x_0}{\sqrt{4D_\pm t}}\right).\end{aligned} \tag{47}$$

Therefore, from the normalization condition, Eq. (45), it follows

$$\begin{aligned}1 &= A_- \int_{-\infty}^{0} \mathrm{d}x\, p_-(x,t|x_0,0) + A_+ \int_{0}^{\infty} \mathrm{d}x\, p_+(x,t|x_0,0) \\ &= A_-\left[\frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(-\frac{x_0}{\sqrt{4D_- t}}\right)\right] + A_+\left[\frac{1}{2} - \frac{1}{2}\mathrm{erf}\left(-\frac{x_0}{\sqrt{4D_+ t}}\right)\right] \\ &= \frac{A_+}{2}\left\{\left[\sqrt{\frac{D_-}{D_+}}\exp\left\{\frac{(D_+-D_-)x_0^2}{4D_+D_- t}\right\}\right]\left[1+\mathrm{erf}\left(-\frac{x_0}{\sqrt{4D_- t}}\right)\right] + 1 - \mathrm{erf}\left(-\frac{x_0}{\sqrt{4D_+ t}}\right)\right\},\end{aligned} \tag{48}$$

so that the final expression for the time-dependent function A_+ reads

$$A_+(t) = 2\left\{1 - \operatorname{erf}\left(-\frac{x_0}{\sqrt{4D_+t}}\right) + \left[\sqrt{\frac{D_-}{D_+}}\exp\left\{\frac{(D_+ - D_-)x_0^2}{4D_+D_-t}\right\}\right]\left[1 + \operatorname{erf}\left(-\frac{x_0}{\sqrt{4D_-t}}\right)\right]\right\}^{-1}. \tag{49}$$

In the limit, $D_+ = D_-$ it follows that $A_+(t) = 1$ for all times, as expected!