PHYSICS 210B : NONEQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

(1) Consider the following stochastic differential equation,

$$dx = -\beta x\, dt + \sqrt{2\beta(a^2 - x^2)}\, dW(t) \ ,$$

where $x \in [-a, a]$.

(i) Find the corresponding Fokker-Planck equation.

(ii) Find the normalized steady state probability $\mathcal{P}(x)$.

(iii) Find and solve for the eigenfunctions $P_n(x)$ and $Q_n(x)$. *Hint: learn a bit about Chebyshev polynomials.*

(iv) Find an expression for $\langle x^3(t)\, x^3(0)\rangle$, assuming $x_0 \equiv x(0)$ is distributed according to $\mathcal{P}(x_0)$.

Solution:

(a) From §3.3.4 of the notes, assuming the stochastic differential equation is in the Itô form (parameter α=0),

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}(fP) + \frac{1}{2}\,\frac{\partial^2}{\partial x^2}(g^2 P) \quad ,$$

with $f(x) = -\beta x$ and $g(x) = \sqrt{2\beta(a^2 - x^2)}$. Thus,

$$\frac{\partial P}{\partial t} = \beta \frac{\partial}{\partial x}(xP) + \beta\, \frac{\partial^2}{\partial x^2}\big[(a^2 - x^2)\, P\big] \quad .$$

At the boundaries $x = \pm a$ the diffusion constant vanishes, and the drift is into the interval, hence *the boundaries are reflecting*.

(b) We set the LHS of the FPE to zero to find the steady state solution. Assuming no currents at the boundaries, we have $P(x, t \to \infty) = \mathcal{P}(x)$, where the equilibrium distribution $\mathcal{P}(x)$ satisfies the first order equation

$$0 = x\,\mathcal{P} + \frac{d}{dx}\big[(a^2 - x^2)\,\mathcal{P}\big] \quad .$$

This may be rewritten as

$$\frac{d}{dx} \ln\big[(a^2 - x^2)\,\mathcal{P}\big] = -\frac{x}{a^2 - x^2} = \frac{d}{dx}\, \tfrac{1}{2} \ln(a^2 - x^2) \quad ,$$

and therefore

$$\mathcal{P}(x) = \frac{1}{\pi}\, \frac{1}{\sqrt{a^2 - x^2}} \quad ,$$

which is normalized with $\int\limits_{-a}^{a} dx\, \mathcal{P}(x) = 1$.

(c) The eigenfunctions $P_n(x)$ satisfy $\mathcal{L}\,\mathcal{P}_n(x) = -\lambda_n P_n(x)$, with $Q_n(x) = P_n(x)/\mathcal{P}(x)$ satisfying $\mathcal{L}^\dagger Q_n = -\lambda_n Q_n$. It is useful to measure distances in units of a and times in units of β^{-1}. Then the FPE is $\partial_t P = \mathcal{L}\,P$, where our Fokker-Planck operator is

$$\mathcal{L} = \frac{d}{dx}\,x + \frac{d^2}{dx^2}\,(1-x^2) \quad .$$

The eigenfunctions $Q_n(x)$ satisfy $\mathcal{L}^\dagger Q_n = -\lambda_n\,Q_n$. Thus,

$$(1-x)^2\,\frac{d^2Q_n}{dx^2} - x\,\frac{dQ_n}{dx} = -\lambda_n Q_n \,.$$

This is Chebyshev's equation. The solution are the Chebyshev polynomials $T_n(x)$, and the eigenvalues are $\lambda_n = n^2$. The eigenfunctions $P_n(x)$ are given by $P_n(x) = \mathcal{P}(x)\,Q_n(x)$, with $\mathcal{P}(x) = \pi^{-1}(1-x^2)^{-1/2}$.

A good place to learn about Chebyshev polynomials is Wikipedia. The Chebyshev polynomials of the first kind are an orthonormal family of functions $\{T_n(x)\}$ on the interval $x \in [-1,1]$, satisfying the recurrence relation

$$T_0(x) = 1 \qquad , \qquad T_1(x) = x \qquad , \qquad T_{n+1}(x) = 2x\,T_n(x) - T_{n-1}(x) \quad .$$

They satisfy the differential equation

$$(1-x^2)\frac{d^2T_n}{dx^2} - x\,\frac{dT_n}{dx} + n^2\,T_n = 0 \quad .$$

There are several generating functions for the $\{T_n(x)\}$:

$$\frac{1-tx}{1-2tx+t^2} = \sum_{n=0}^\infty t^n\,T_n(x)$$

$$e^{tx}\cos\!\left(t\sqrt{1-x^2}\right) = \sum_{n=0}^\infty \frac{t^n}{n!}\,T_n(x)$$

$$-\tfrac{1}{2}\ln\!\left(1-2tx+t^2\right) = \sum_{n=1}^\infty \frac{t^n}{n}\,T_n(x) \quad .$$

The orthogonality relation is

$$\frac{1}{\pi}\int\limits_{-1}^{1}\frac{dx}{\sqrt{1-x^2}}\,T_m(x)\,T_n(x) = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n = 0 \\ \frac{1}{2} & \text{if } m = n \neq 0 \quad . \end{cases}$$

The first few $T_n(x)$ are

$$\begin{aligned}
T_0(x) &= 1 & T_6(x) &= 32x^6 - 48x^4 + 18x^2 - 1 \\
T_1(x) &= x & T_7(x) &= 64x^7 - 112x^5 + 56x^3 - 7x \\
T_2(x) &= 2x^2 - 1 & T_8(x) &= 128x^8 - 256x^6 + 160x^4 - 32x^2 + 1 \\
T_3(x) &= 4x^3 - 3x & T_9(x) &= 256x^9 - 576x^7 + 432x^5 - 120x^3 + 9x \\
T_4(x) &= 8x^4 - 8x^2 + 1 & T_{10}(x) &= 512x^{10} - 1280x^8 + 1120x^6 - 400x^4 + 50x^2 - 1 \\
T_5(x) &= 16x^5 - 20x^3 + 5x & T_{11}(x) &= 1024x^{11} - 2816x^9 + 2816x^7 - 1232x^5 + 220x^3 - 11x \quad .
\end{aligned}$$

The general solution of the Fokker-Planck equation is then

$$P(x,t) = \sum_{n=0}^{\infty} A_n \, \mathcal{P}(x) \, T_n(x) \, e^{-n^2 t} \quad .$$

The coefficients A_n are obtained from initial data $P(x,0)$, *viz.*

$$A_0 = \int_{-1}^{1} \! dx \; P(x,0) \qquad , \qquad A_{n>0} = 2 \int_{-1}^{1} \! dx \; P(x,0) \, T_n(x) \quad .$$

(d) From the conclusion of §4.2.4 of the notes, we have that

$$P(x,t \,|\, x_0, 0) = \sum_n Q_n(x_0) \, P_n(x) \, e^{-\lambda_n t} \quad ,$$

where $P_0(x) = \mathcal{P}(x)$ and $P_{n>0}(x) = \sqrt{2} \, T_n(x) \, \mathcal{P}(x)$. Thus, assuming x_0 is distributed according to $\mathcal{P}(x_0)$,

$$\big\langle x^3(t) \, x^3(0) \big\rangle = \int_{-1}^{1} \! dx_0 \; \mathcal{P}(x_0) \, x_0^3 \int_{-1}^{1} \! dx \; P(x,t \,|\, x_0, 0) = \sum_n \big| \big\langle \, x^3 \, | \, P_n \, \big\rangle \big|^2 \, e^{-n^2 t} \quad ,$$

where

$$\big\langle \, x^3 \, | \, P_n \, \big\rangle = \sqrt{2} \int_{-1}^{1} \! dx \; \mathcal{P}(x) \, x^3 \, T_n(x) = \tfrac{1}{\sqrt{2}} \Big(\tfrac{1}{4} \, \delta_{n,3} + \tfrac{3}{4} \, \delta_{n,1} \Big) \quad ,$$

since $x^3 = \frac{1}{4} \, T_3(x) + \frac{3}{4} \, T_1(x)$. Thus,

$$\big\langle x^3(t) \, x^3(0) \big\rangle = \tfrac{1}{32} \, e^{-3t} + \tfrac{9}{32} \, e^{-t} \quad .$$

Note that $\big\langle x^6(0) \big\rangle = \frac{5}{16}$, which agrees with the calculation

$$\big\langle x^6(0) \big\rangle = \int_{-1}^{1} \! dx_0 \; \mathcal{P}(x_0) \, x_0^6 = \frac{1}{\pi} \int_0^{\pi} \! d\theta \; \cos^6\theta = \frac{1}{2^6} \binom{6}{3} = \frac{5}{16} \quad .$$

(2) A diffusing particle is confined to the interval $[0, L]$. The diffusion constant is D and the drift velocity is v_{D}. The boundary at $x = 0$ is absorbing and that at $x = L$ is reflecting.

(a) Calculate the mean and mean square time for the particle to get absorbed at $x = 0$ if it starts at $t = 0$ from $x = L$. Examine in detail the cases $v_{\mathrm{D}} > 0$, $v_{\mathrm{D}} = 0$, and $v_{\mathrm{D}} < 0$.

(b) Compute the Laplace transform of the distribution of trapping times for the cases $v_D > 0$, $v_D = 0$, and $v_D < 0$, and discuss the asymptotic behaviors of these distributions in the limits $t \to 0$ and $t \to \infty$.

Solution:

(a) We studied first passage problems in §4.2.5. The distribution function for exit times is given by $-\partial_t G(x,t)$, where $G(x,t) = \int\limits_0^L dx'\, P(x',t\,|\,x,0)$ satisfies the backward FPE,

$$\frac{\partial G}{\partial t} = D\,\frac{\partial^2 G}{\partial x^2} + v_D\,\frac{\partial G}{\partial x} = \mathcal{L}^\dagger G \quad .$$

The boundary conditions are $G(0,t) = 0$ and $\partial_x G(x,t)\big|_{x=L} = 0$. The mean n^{th} power of the exit time, $T_n(x) = \langle t_x^n \rangle$, therefore satisfies

$$\begin{aligned}\mathcal{L}^\dagger\, T_n(x) &= \mathcal{L}^\dagger \int\limits_0^\infty dt\; t^n \bigg(-\frac{\partial G(x,t)}{\partial t}\bigg) = n\,\mathcal{L}^\dagger \int\limits_0^\infty dt\; t^{n-1}\, G(x,t) \\ &= n \int\limits_0^\infty dt\; t^{n-1}\,\frac{\partial G(x,t)}{\partial t} = -n\, T_{n-1}(x) \quad ,\end{aligned}$$

with $\mathcal{L}^\dagger\, T_1(x) = -1$, *i.e.* $T_0(x) = \langle t_x^0 \rangle = 1$.

With $x=0$ absorbing and $x=L$ reflecting, we have

$$T_1(x) = \frac{1}{D}\int\limits_0^x \frac{dy}{\psi(y)} \int\limits_y^L dz\; \psi(z) \quad ,$$

where $\psi(x) = \exp\big(v_D x/D\big)$ (use Eqn. 4.53 with $A = v_D$ and $B = 2D$). We then have

$$T_1(x) = \frac{D}{v_D^2}\,\big(1 - e^{-v_D x/D}\big)\, e^{v_D L/D} - \frac{x}{v_D} \quad .$$

One can check that this solution satisfies the boundary conditions $T_1(0) = 0$ and $T_1'(L) = 0$.

It is convenient to define the length scale $\ell = D/|v_D|$ and the time scale $\tau = D/v_D^2$. We henceforth measure all lengths in units of ℓ and all times in units of τ. We therefore measure the moments T_n in units of τ^n. The mean escape time is

$$T_1 = e^{\sigma L} - e^{\sigma(L-x)} - \sigma x \quad ,$$

where $\sigma = \text{sgn}(v_D)$. Note that for $\sigma > 0$ the drift is away from the absorbing boundary, and the mean escape time is $T_1 \sim e^L$, where L is the length in units of $D/|v_D|$. This grows exponentially with $|v_D|$. When $\sigma < 0$ the exponential terms are dominated by the linear term for $L-x \gg 1$, and $T_1 \approx x$, or in dimensionful units, $T_1 \approx x/v_{\rm D}$, which says the particle exits in a time similar to what would expect for $D=0$, when there is pure ballistic motion. When $v_{\rm D}=0$ our length and time scales are divergent, which means the dimensionless quantities L and x are infinitesimal. We then expand to get $T_1 = \frac{1}{2}x(2L-x)$. Restoring units recovers $T_1 = x(2L-x)/2D$ in terms of dimensionful quantities.

To find $T_2(x)$, we solve $\mathcal{L}^\dagger\, T_2(x) = -T_1(x)$. This means that the dimensionless $T_2(x)$ satisfies

$$T_2'' + \sigma\, T_2' = 2\Big[e^{\sigma(L-x)} - e^{\sigma L} + \sigma x\Big] \quad .$$

We can solve this by a spatial Laplace transform on the interval $x \in [0,\infty)$, later imposing the conditions $T_2(0) = T_2'(L) = 0$. We define

$$\check{T}_2(\alpha) = \int\limits_0^\infty \! dx\, T_2(x)\, e^{-\alpha x} \quad .$$

Then

$$\begin{aligned}\int\limits_0^\infty \! dx\, T_2''(x)\, e^{-\alpha x} &= -T_2'(0) - \alpha\, T_2(0) + \alpha^2\, \check{T}_2(\alpha)\\ \int\limits_0^\infty \! dx\, T_2'(x)\, e^{-\alpha x} &= -T_2(0) + \alpha\, \check{T}_2(\alpha) \quad .\end{aligned}$$

Assuming Re $\alpha+\sigma > 0$, we have

$$\int\limits_0^\infty \! dx\, \Big[e^{\sigma(L-x)} - e^{\sigma L} + \sigma x\Big]\, e^{-\alpha x} = \frac{e^{\sigma L}}{\alpha+\sigma} - \frac{e^{\sigma L}}{\alpha} + \frac{\sigma}{\alpha^2} \quad .$$

We therefore have

$$\alpha(\alpha+\sigma)\, \check{T}_2(\alpha) = A + \frac{e^{\sigma L}}{\alpha+\sigma} - \frac{e^{\sigma L}}{\alpha} + \frac{\sigma}{\alpha^2} \quad ,$$

where we have used $T_2(0)=0$, and where the constant $A \equiv T_2'(0)$, which is yet to be determined. Therefore

$$T_2(x) = 2 \oint \frac{d\alpha}{2\pi i} \left\{ \frac{A}{\alpha(\alpha+\sigma)} - \frac{\sigma\, e^{\sigma L}}{\alpha^2(\alpha+\sigma)^2} + \frac{\sigma}{\alpha^3(\alpha+\sigma)} \right\} e^{\alpha x} \quad .$$

We now employ the method of partial fractions:

$$\begin{aligned}\frac{1}{\alpha(\alpha+\sigma)} &= \frac{1}{\sigma}\bigg(\frac{1}{\alpha} - \frac{1}{\alpha+\sigma}\bigg) = \frac{\sigma}{\alpha} - \frac{\sigma}{\alpha+\sigma}\\ \frac{1}{\alpha^2(\alpha+\sigma)^2} &= \bigg(\frac{1}{\alpha} - \frac{1}{\alpha+\sigma}\bigg)^2 = \frac{1}{\alpha^2} + \frac{1}{(\alpha+\sigma)^2} - \frac{2\sigma}{\alpha} + \frac{2\sigma}{\alpha+\sigma}\\ \frac{1}{\alpha^3(\alpha+\sigma)} &= \frac{1}{\alpha^2}\bigg(\frac{\sigma}{\alpha} - \frac{\sigma}{\alpha+\sigma}\bigg) = \frac{\sigma}{\alpha^3} - \frac{\sigma}{\alpha}\bigg(\frac{\sigma}{\alpha} - \frac{\sigma}{\alpha+\sigma}\bigg) = \frac{\sigma}{\alpha^3} - \frac{1}{\alpha^2} + \frac{\sigma}{\alpha} - \frac{\sigma}{\alpha+\sigma} \quad .\end{aligned}$$

We can now basically read off the form for $T_2(x)$:

$$T_2(x) = 2\,\sigma A\big(1 - e^{-\sigma x}\big) + 2\,e^{\sigma L}\big(2 - 2\,e^{-\sigma x} - \sigma x - \sigma x\,e^{-\sigma x}\big) + x^2 - 2\,\sigma x + 2 - 2\,e^{-\sigma x} \quad .$$

To fix A, we set $T_2'(L) = 0$:

$$T_2'(L) = 2A\,e^{-\sigma L} + 4L - 4\sinh L \qquad \Rightarrow \qquad A\,e^{-\sigma L} = 2\sinh L - 2L \quad .$$

Then

$$\begin{aligned} T_2(L) &= L^2 - 4 + 2\,(1 - 3\sigma L)\,e^{\sigma L} + 2\,e^{2\sigma L} \\ &= \tfrac{5}{12}\,L^4 + \tfrac{3}{10}\,\sigma L^5 + \mathcal{O}(L^6) \quad , \end{aligned}$$

where the second line says that in $v_{\rm D} \to 0$ limit we have $T_2(L) = 5L^4/12D^2$ (with appropriate dimensions). Note again that for $\sigma = +1$, when the drift is away from the absorbing boundary, the mean square escape time behaves to leading order as $T_2(L) \sim (D/v_{\rm D}^2)\exp(2Lv_{\rm D}/D)$, whereas when $\sigma = -1$ and the drift is toward the absorbing boundary, the mean square escape time behaves as a power law $T_2(L) \simeq (L/v_{\rm D})^2$.

(b) The probability distribution of exit times is $W(x,t) = -\partial G(x,t)/\partial t$, where

$$G(x,t) = \int\limits_0^L \! dx'\,P(x',t\,|\,x,0) \quad ,$$

as discussed in §4.2.5 of the notes. The Laplace transform $\check{W}(x,z)$ therefore satisfies

$$\mathcal{L}^\dagger\,\check{W}(x,z) = z\,\check{W}(x,z) \quad ,$$

with boundary conditions

$$\check{W}(0,z) = 1 \quad , \quad \frac{\partial \check{W}(x,z)}{\partial x}\bigg|_{x=L} = 0 \quad .$$

The first of these boundary conditions comes from the fact that $W(0,t) = \delta(t)$, since a particle starting at the left boundary is immediately absorbed. The resulting equation for $\check{W}(x,z)$,

$$D\,\frac{\partial^2 \check{W}}{\partial x^2} + v_{\rm D}\,\frac{\partial \check{W}}{\partial x} - z\,\check{W} = 0 \quad ,$$

has the general solution $\check{W}(x,z) = A_+\,e^{\lambda_+ x} + A_-\,e^{\lambda_- x}$, where

$$\lambda_\pm(z) = -\frac{v_{\rm D}}{2D} \pm \sqrt{\left(\frac{v_{\rm D}}{2D}\right)^2 + \frac{z}{D}} \quad .$$

Accounting for the boundary conditions, we have

$$\check{W}(x,z) = \frac{\lambda_+\,e^{\lambda_+ L}\,e^{\lambda_- x} - \lambda_-\,e^{\lambda_- L}\,e^{\lambda_+ x}}{\lambda_+\,e^{\lambda_+ L} - \lambda_-\,e^{\lambda_- L}} \quad .$$

Define

$$\ell \equiv \frac{D}{|v_{\rm D}|} \quad , \quad \tau \equiv \frac{D}{v_{\rm D}^2} \quad , \quad u \equiv \sqrt{1+4\tau z} \quad \Rightarrow \quad z = \frac{u^2-1}{4\tau} \quad .$$

Then the eigenvalues $\lambda_\pm$ are

$$\lambda_\pm = \begin{cases} (-1 \pm u)/2\ell & \text{if } v_{\rm D} > 0 \\ \pm\sqrt{z/D} & \text{if } v_{\rm D} = 0 \\ (1 \pm u)/2\ell & \text{if } v_{\rm D} < 0 \quad . \end{cases}$$

For $v_{\rm D} = 0$, we have

$$\check{W}(x,z) = \frac{e^{x\sqrt{z/D}} + e^{(2L-x)\sqrt{z/D}}}{1 + e^{2L\sqrt{z/D}}} \quad .$$

The closest pole to $z = 0$ lies at $2L\sqrt{z/D} = i\pi$, which means $z = -\pi^2 D/4L^2$. Upon taking the inverse Laplace transform, and evaluating at $x = L$ for convenience, we find $W(L,t) \sim e^{-\pi^2 Dt/4L^2}$, which says that the characteristic escape time is $t_{\rm esc} \sim L^2/D$, as we found in part (a).

When $v_{\rm D} \neq 0$, it is helpful to eliminate z in favor of the variable u defined above. For $v_{\rm D} > 0$, we have

$$\check{W}(x,z) = \frac{(1+u)\, e^{-u(L-x)/2\ell} - (1-u)\, e^{u(L-x)/2\ell}}{(1+u)\, e^{-uL/2\ell} - (1-u)\, e^{uL/2\ell}}\, e^{-x/2\ell} \quad .$$

The pole in the denominator occurs for

$$e^{uL/\ell} = \frac{1+u}{1-u} \quad \Rightarrow \quad \frac{L}{2\ell}\, u = \tanh^{-1} u \quad .$$

Assuming $L \gg \ell$, the solution lies at $u = 1 - \varepsilon$ with $\varepsilon \simeq 2\, e^{-L/\ell}$, hence

$$z = \frac{u^2-1}{4\tau} \simeq -\frac{1}{\tau}\, e^{-L/\ell} \quad .$$

Thus, $W(L,t) \sim e^{-\gamma t}$ with $\gamma^{-1} \simeq \tau\, e^{L/\ell}$ exponentially large in L/ℓ, as found in part (a).

When $v_{\rm D} < 0$, we have

$$\check{W}(x,z) = \frac{(1+u)\, e^{u(L-x)/2\ell} - (1-u)\, e^{-u(L-x)/2\ell}}{(1+u)\, e^{uL/2\ell} - (1-u)\, e^{-uL/2\ell}}\, e^{x/2\ell} \quad .$$

The poles of the denominator lie at values of u such that

$$e^{uL/\ell} = \frac{1-u}{1+u} \quad .$$

With $u = -iw$, this yields $(L/2\ell)\, w = -\tan^{-1} w$, whose only solution lies at $w = 0$. In fact, this pole is cancelled by the numerator.