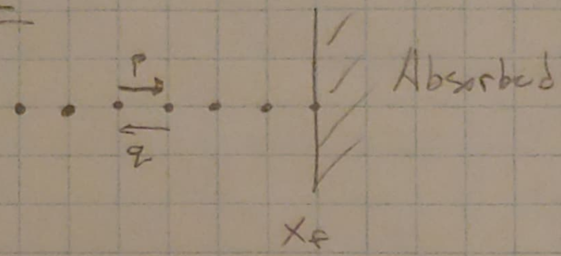
## Problem 1

### 1.1




Prob to be absorbed at $x_f$, when starting from $x_0$

$$P^{x_f}(x_0) = q\, P^{x_f}(x-a) + p\, P^{x_f}(x+a)$$

With initial conditions $P^{x_f}(x_f) = 1$,

$P^{x_f}(L) = 0$,

where $L$ is some far away distance.

Make the usual guess that $P^{x_f}(x_0) = \lambda^{x_0}$

It feels weird to write like this when doing discrete steps, so

$$x \to n \qquad a \to 1$$

$$P^{n_f}(n_0) = q\, P^{n_f}(n_0-1) + p\, P^{n_f}(n_0+1)$$

$$\lambda^{n_0} = q\lambda^{n_0-1} + p\lambda^{n_0+1} \qquad \text{divide by } \lambda^{n_0-1}$$

$$0 = q + p\lambda^2 - \lambda$$

$$\lambda = \frac{-b \pm \sqrt{b^2-4ac}}{2a} = \frac{1 \pm \sqrt{1-4pq}}{2p} \qquad q = 1-p$$

$$\lambda = \frac{1 \pm \sqrt{1-4p(1-p)}}{2p} = \frac{1 \pm \sqrt{1-4p+4p^2}}{2p} = \frac{1 \pm \sqrt{(1-2p)^2}}{2p}$$

$$\lambda = 1 \quad \text{or} \quad \frac{q}{p}$$

1.1 (cont.) $\lambda = 1$ or $\frac{q}{p}$

Then we have $P^{n_f}(n_0) = A + B\left(\frac{q}{p}\right)^{n_0}$

Apply B.C.'s $P^{n_f}(n_f) = 1$, $P^{n_f}(L) = 0$

$$A + B\left(\frac{q}{p}\right)^{n_f} = 1 \qquad A = -B\left(\frac{q}{p}\right)^{L}$$

$$B\left(\frac{q}{p}\right)^{n_f} - \left(\frac{q}{p}\right)^{L} = 1$$

$$B = \frac{1}{\left(\frac{q}{p}\right)^{n_f} - \left(\frac{q}{p}\right)^{L}} \qquad A = \frac{\left(\frac{q}{p}\right)^{L}}{\left(\frac{q}{p}\right)^{L} - \left(\frac{q}{p}\right)^{n_f}}$$

$$P^{n_f}(n_0) = \frac{\left(\frac{q}{p}\right)^{L}}{\left(\frac{q}{p}\right)^{L} - \left(\frac{q}{p}\right)^{n_f}} + \frac{1}{\left(\frac{q}{p}\right)^{n_f} - \left(\frac{q}{p}\right)^{L}}\left(\frac{q}{p}\right)^{n_0} = \frac{\left(\frac{q}{p}\right)^{n_0} - \left(\frac{q}{p}\right)^{L}}{\left(\frac{q}{p}\right)^{n_f} - \left(\frac{q}{p}\right)^{L}}$$

Now we want to send $L$ away. $L \to -\infty$

For $p > q$: $$\frac{\left(\frac{q}{p}\right)^{n_0} - \left(\frac{p}{q}\right)^{-L}}{\left(\frac{q}{p}\right)^{n_f} - \left(\frac{p}{q}\right)^{-L}} \approx \frac{-\left(\frac{p}{q}\right)^{-L}}{-\left(\frac{p}{q}\right)^{-L}} = 1$$

small compared to $\left(\frac{p}{q}\right)^{\infty}$

~~For $p = q$:~~ $\cancel{\frac{n_0}{n_f}}$

For $q > p$: $$\frac{\left(\frac{q}{p}\right)^{n_0} - \cancel{\left(\frac{p}{q}\right)^{-L}}}{\left(\frac{q}{p}\right)^{n_f} - \cancel{\left(\frac{p}{q}\right)^{-L}}} = \frac{\left(\frac{q}{p}\right)^{n_0}}{\left(\frac{q}{p}\right)^{n_f}} = \left(\frac{q}{p}\right)^{n_0 - n_f}$$

1.1 (cont.)

Probability to Fall Off : $P^{n_f}_{(n_0)} = \begin{cases} 1, & p > q \\ \left(\frac{q}{p}\right)^{n_0 - n_f} & p < q \end{cases}$

Probability to not Fall Off : $\sim P^{n_f}_{(n_0)} = 1 - P^{n_f}_{(n_0)}$

Problem 1 (cont.)

1.2 Steal some results from class

$$T(n_0) = q\,T(n_0-1) + p\,T(n_0+1) + \tau$$

Is the time to be absorbed.

"Guess" $T(n_0) = A + B\left(\frac{q}{p}\right)^{n_0} - \frac{\tau n_0}{p-q}$

B.C.'s: $T(n_t) = 0$, $T(L) = 0$

$$A + B\left(\frac{q}{p}\right)^{n_t} = \frac{\tau n_t}{p-q} \qquad A + B\left(\frac{q}{p}\right)^{L} = \frac{\tau L}{p-q}$$

Subtract equations

$$B\left[\left(\frac{q}{p}\right)^{n_t} - \left(\frac{q}{p}\right)^{L}\right] = \frac{\tau(n_t-L)}{p-q} \longrightarrow B = \frac{\tau(n_t-L)}{p-q}\,\frac{1}{\left(\frac{q}{p}\right)^{n_t} - \left(\frac{q}{p}\right)^{L}}$$

$$A = \frac{\tau n_t}{p-q} - \frac{\tau(n_t-L)}{p-q}\,\frac{\left(\frac{q}{p}\right)^{n_t}}{\left(\frac{q}{p}\right)^{n_t} - \left(\frac{q}{p}\right)^{L}}$$

$$T(n_0) = \frac{\tau n_t}{p-q} - \frac{\tau(n_t-L)}{p-q}\,\frac{(q/p)^{n_t}}{(q/p)^{n_t} - (q/p)^{L}} + \frac{\tau(n_t-L)}{p-q}\,\frac{(q/p)^{n_0}}{(q/p)^{n_t} - (q/p)^{L}} - \frac{\tau n_0}{p-q}$$

$$T(n_0) = \frac{\tau}{p-q}\left[n_t - n_0 + \frac{n_t-L}{(q/p)^{n_t} - (q/p)^{L}}\left((q/p)^{n_0} - (q/p)^{n_t}\right)\right]$$

1.2 (cont.)

Now we send $L \to -\infty$ and check our cases.

$$T(n_0) = \frac{\tau}{p-q}\left[n_f - n_0 + \frac{n_f - L}{(q/p)^{n_f} - (q/p)^L}\left((q/p)^{n_0} - (q/p)^{n_f}\right)\right]$$

For $p > q$: $\left(\frac{q}{p}\right)^L \to \left(\frac{p}{q}\right)^{-L} \underset{L\to-\infty}{\to} \infty$

$$T(n_0) = \frac{\tau}{p-q}\left[n_f - n_0\right]$$

given we fall off, we divide by $P^{n_0}(n_0) = 1$

For $q = p$: we blow up, and $T(n_0)$ goes to $\infty$.

This doesn't seem physical, but I believe it's because as our distribution spreads out (drift $= 0$), one of the tails provides a flux through the absorption boundary. However, the other tail can spread out forever. Hence, our mean first passage time isn't well defined because those lost souls could wonder all the way back, and be absorbed a significant time later. The computer can give an answer because we artificially explude some trajectories that have gone "far enough".

For $(p < q)$: We run into the same issue. We get runaways.

Problem 2

2.1 The probability that we don't decay until time $t$ is the probability that we didn't decay at any time step before $t$.

$$S(t) = \underbrace{(1-r_1 dt - r_2 dt)}_{1st\ step}(1-r_1 dt - r_2 dt)\dots\underbrace{(1-r_1 dt - r_2 dt)}_{N\ th\ step}$$

As we take $dt \to 0$, this looks like an exponential.

$$S(t) = (1-(r_1+r_2)dt)^N \qquad \text{where } N = t/dt$$

$$S(t) = \left(e^{-(r_1+r_2)dt}\right)^N$$

$$S(t) = e^{-(r_1+r_2)t}$$

2.2 Probability to decay via 1 is the probability that we haven't decayed for previous timesteps, and we do decay in the next step.

$$\rho_1(t)dt = S(t)\,\Gamma_1\,dt$$

$$\rho_1(t)\,dt = e^{-(\Gamma_1+\Gamma_2)t}\,\Gamma_1\,dt$$

For the probability to decay via 1, we integrate for all time.

$$P_1(t\to\infty) = \int_0^\infty e^{-\Gamma_1+\Gamma_2 t}\,\Gamma_1\,dt = \frac{\Gamma_1}{-(\Gamma_1+\Gamma_2)}\,e^{-(\Gamma_1+\Gamma_2)t}\Big|_0^\infty$$

$$\boxed{P_1(t\to\infty) = \frac{\Gamma_1}{\Gamma_1+\Gamma_2}}$$

2.3 Mean decay time:

$$\rho_1(t) = e^{-(r_1+r_2)t} r_1 dt \Big/ \frac{r_1}{r_1+r_2}$$

Given we decay via 1

$$\langle t \rangle = \int_0^\infty t\rho_1(t)\,dt = \int_0^\infty (r_1+r_2)\,e^{-(r_1+r_2)t}\,t\,dt$$

Integrate by parts: $\int u\,dv = uv - \int v\,du$

let $u = t$ $\quad du = dt \quad dv = e^{-(r_1+r_2)t} \quad v = \frac{-e^{-(r_1+r_2)t}}{r_1+r_2}$

$$\langle t \rangle_1 = (r_1+r_2)\left[\frac{-t\,e^{-(r_1+r_2)t}}{r_1+r_2}\Big|_0^\infty - \int_0^\infty \frac{-e^{-(r_1+r_2)t}}{r_1+r_2}\,dt\right.$$

$$\langle t \rangle_1 = \frac{r_1+r_2}{r_1+r_2}\;\frac{e^{-(r_1+r_2)t}}{r_1+r_2}\Big|_0^\infty = \frac{1}{r_1+r_2}$$

$$\boxed{\langle t \rangle_1 = \frac{1}{r_1+r_2}}$$

by symmetry, for $\langle t_2 \rangle$ $\quad r_1 \to r_2, \; r_2 \to r_1$

$$\langle t \rangle_2 = \frac{1}{r_2+r_1} = \langle t \rangle_1 \quad !$$

$$P_1(t) = \int_0^t e^{-(r_1+r_2)t'} r_1\,dt' = -\frac{r_1}{r_1+r_2}\,e^{-(r_1+r_2)t'}\Big|_0^t$$

$$P_1(t) = \frac{r_1}{r_1+r_2}\left[1 - e^{-(r_1+r_2)t}\right]$$

By symmetry, $P_2(t) = \frac{r_2}{r_1+r_2}\left[1 - e^{-(r_1+r_2)t}\right]$

## Problem 3

**3.1** The Smoluchowski Equation is

$$\frac{\partial P}{\partial t} = -\frac{\partial J}{\partial x},$$

where $$J = D\left[\frac{f(x)}{k_B T} P - \frac{\partial P}{\partial x}\right],$$

and $$f(x) = -\frac{dU(x)}{dx}$$

For our molecule, $U(r) = \frac{a k_B T r^2}{2} \longrightarrow f(r) = -a k_B T r$

Plugging this into the Smoluchowski Eq., we get

$$\frac{\partial P(r,t)}{\partial t} = -\frac{\partial}{\partial r}\left[D\left(\frac{-a k_B T r}{k_B T} P(r,t) - \frac{\partial}{\partial r} P(r,t)\right)\right]$$

$$= aD\frac{\partial}{\partial r}\left[r P(r,t)\right] + D\frac{\partial^2 P(r,t)}{\partial r^2}$$

For the steady-state solution, we require

$$\frac{\partial P}{\partial t} = 0 \longrightarrow -arP(r) = \frac{\partial}{\partial r} P(r)$$

"Guess" that a Gaussian distribution will work. Try the Boltzmann distribution.

$$P(r) = \frac{1}{Z} e^{-\beta U(r)} = \frac{1}{Z} e^{-\beta a k_B T r^2/2} = \frac{1}{Z} e^{-ar^2/2}$$

Test ✓

$$-arP(r) = \frac{-ar\, e^{-ar^2/2}}{Z} \qquad \frac{\partial}{\partial r} P(r) = \frac{-ar\, e^{-ar^2/2}}{Z}$$

3.1 (cont.)

Find the proper normalization.

$$1 = \int_0^\infty P(r)\,dr \rightarrow Z = \int_0^\infty e^{-ar^2/2}\,dr$$

Only $r > 0$.

Use a table for this one. It involves the error function.

$$Z = \sqrt{\frac{\pi}{2a}}\,\mathrm{erf}\left(\sqrt{\frac{a}{2}}\,r\right)\Big|_0^\infty$$

$\mathrm{erf}(\infty) = 1$
$\mathrm{erf}(0) = 0$

$$Z = \sqrt{\frac{\pi}{2a}}$$

$$\boxed{P^{ss}(r) = \sqrt{\frac{2a}{\pi}}\,e^{-ar^2/2}}$$

Can you find the dynamical solution $P(r,t)$?

It should be possible, but very difficult. I can guess at its form. It should be a function that starts as a delta function at $r_0$ $(r(t=0))$, and then spreads out to the half Gaussian we have.

3.2 $\dfrac{d\tilde{x}}{dt} = \mu\left(F(x) + \xi(t)\right)$, where $\xi(t)$ satisfies

$\xi(t) = 0$, and $\langle \xi(t)\,\xi(t')\rangle = \Gamma\,\delta(t-t')$.

For our molecule, we have $F(r) = -ak_BT r$.

$$\mu = D/k_BT$$

$$\boxed{\frac{dr}{dt} = \frac{D}{k_BT}\left[-ak_BT\,r + \xi(t)\right]}$$

$$\frac{dr}{dt} = -aDr + \xi(t)$$

$$\dot{r} + aDr = \xi(t) \qquad \text{multiply by } e^{aDt}$$

$$\dot{r}e^{aDt} + aDre^{aDt} = \xi(t)\,e^{aDt}$$

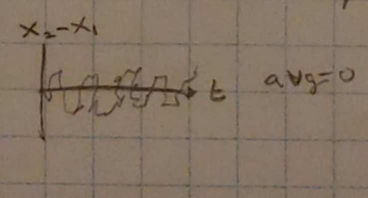
$$\frac{d}{dt}\left(r e^{aDt}\right) = \xi(t)\,e^{aDt}$$

$$r(t) = e^{-aDt}\left[\int_0^t dt\; e^{aDt}\,\xi(t) + C\right]$$

To find $C$, we cant take $t \to 0$. Then $C = r(0)$.

$$r(t) = r_0 e^{-aDt} + e^{-aDt}\int_0^t dt'\; e^{aDt'}\,\xi(t')$$

Taking $\langle r(t)\rangle$ will just give us $r_0 e^{-aDt}$, which is no good. Then $\langle r(t\to\infty)\rangle \to 0$, which I interpret as the atoms can switch sides as much as they like, so on average they spend as much time separated left to right as right to left.



## 3.2 (cont.)

Let's try to take $\sqrt{\langle r(t) r(t) \rangle}$.

$$\langle r(t)^2 \rangle = \left\langle \left( r_0 e^{-aDt} + e^{-aDt} \int_0^t dt' \, e^{aDt'} \xi(t') \right)^2 \right\rangle$$

$$= \left\langle r_0^2 e^{-2aDt} + 2 r_0 e^{-2aDt} \int_0^t dt' \, e^{aDt'} \xi(t') + e^{-2aDt} \int_0^t \int_0^t dt' dt'' \, e^{aDt'} e^{aDt''} \xi(t') \xi(t'') \right\rangle$$

$$= r_0^2 e^{-2aDt} + 2 r_0 e^{-2aDt} \int_0^t dt' \, e^{aDt'} \underbrace{\langle \xi(t') \rangle}_{=0}$$

$$+ e^{-2aDt} \int_0^t \int_0^t dt' dt'' \, e^{aD(t'+t'')} \underbrace{\langle \xi(t') \xi(t'') \rangle}_{= \Gamma \delta(t''-t')}$$

$$\langle r(t)^2 \rangle = r_0^2 e^{-2aDt} + \Gamma e^{-2aDt} \int_0^t dt' \, e^{2aDt'}$$

$$= r_0^2 e^{-2aDt} + \Gamma e^{-2aDt} \left. \frac{e^{2aDt'}}{aD} \right|_0^t$$

$$= r_0^2 e^{-2aDt} + \frac{\Gamma}{aD} e^{-2aDt} \left( e^{2aDt} - 1 \right)$$

$$\langle r(t)^2 \rangle = r_0^2 e^{-2aDt} + \frac{\Gamma}{aD} \left( 1 - e^{-2aDt} \right)$$

For $t \to \infty$ choose $\Gamma$ such that $\langle r(t) \rangle \to \sqrt{\frac{2}{\pi a}}$

$$\frac{\Gamma}{aD} = \frac{2}{\pi a} \longrightarrow \Gamma = \frac{2D}{\pi}$$

$$\boxed{\langle r(t)^2 \rangle = r_0^2 e^{-2aDt} + \frac{2}{\pi a} \left( 1 - e^{-2aDt} \right)}$$

$$\langle r(t) \rangle \approx \sqrt{\langle r(t)^2 \rangle}$$

## 3.2 (cont.)

### Centre of Mass

$$\text{CoM} = \frac{\sum r_i m_i}{\sum m_j}$$

I didn't explicitly state it, but we've been assuming that one of the atoms was fixed in our frame of reference.

$$\text{CoM} = \frac{0 m_1 + \langle r \rangle m_2}{m_1 + m_2}$$

$$= \frac{\sqrt{r_0^2 e^{-2aDt} + \frac{2}{\pi a}\left(1 - e^{-2aDt}\right)}\, m_2}{m_1 + m_2}$$

**Variance:** $\text{var}(r) = \langle r^2 \rangle - \langle r \rangle^2$

$$= \cancel{r_0^2 e^{-2aDt}} + \frac{2}{\pi a}\left(1 - e^{-2aDt}\right) - \cancel{r_0^2 e^{-2aDt}}$$

$$\text{var}(r) = \frac{2}{\pi a}\left(1 - e^{-2aDt}\right)$$

**3.3** I don't know why, but my simulated and theoretical variance are off by a factor of $\sqrt{\pi}$

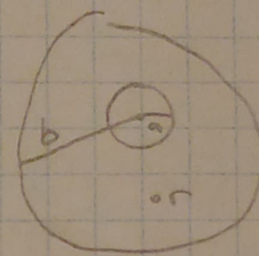
$\text{Var}^{sim}(r) = \text{Var}^{theory}(r) / \sqrt{\pi}$. I give up.

I'm not including the CoM, as it's just $\langle r \rangle$ times a constant.

Problem 4

4.1 Imagine the molecule between 2 spheres. If it touches either, it's absorbed.

start with $a<r<b$.




Absorption probability:

For the BFP $\mathcal{L}^{BFP}_{x_0} P(x,t) = 0$

$$\frac{\partial P}{\partial t}(\vec{x},t) = -\nabla\left(\mu(\vec{x},t)\, P(\vec{x},t)\right) + \nabla^2\, D(\vec{x},t) P(\vec{x},t)$$

For our situation, $\mu(\vec{x},t)=0$, and $D(\vec{x},t)=D$, so we have

$$0 = D\nabla^2 P(\vec{x},t)$$

For our spherical situation, it's natural to work in spherical coordinates

$$0 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial P}{\partial r}\right) + \theta \,\&\, \phi \text{ terms which don't matter because we're radially symmetric.}$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial P}{\partial r}\right) = 0$$

$$P(r) = A + \frac{B}{r}$$

The probability to be absorbed at a has the boundary conditions:

4.1 (cont.) $P_a(a) = 1$ $P_a(b) = 0$

$$P_a(r) = A + \frac{B}{r}$$

$$P_a(a) = 1 = A + \frac{B}{a}$$ $$P_a(b) = 0 = A + \frac{B}{b}$$

$$A = -\frac{B}{b}$$

$$1 = B\left(\frac{1}{a} - \frac{1}{b}\right)$$

$$B = \frac{1}{\frac{(b-a)}{ab}} = \frac{ab}{b-a}$$ $$A = \frac{-a}{b-a}$$

$$P_a(r) = \frac{-a}{b-a} + \frac{ab}{b-a}\frac{1}{r} = \frac{ab-ar}{(b-a)r} = \boxed{\frac{a}{r}\frac{b-r}{b-a}}$$

Time:

For the BFP, $\mathcal{L}^{BFP}\langle T\rangle = -1$ for either absorption condition.

For absorption at a $\mathcal{L}^{BFP}\langle T_a\rangle P_a = -P_a$

4.2 asks for the general absorption case, so I'm going to calculate that, and for the absorption at a case, just divide by $P_a$.

Problem 4 (cont.)

4.2 Either surface absorption time.

$$D \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dT(r)}{dr}\right) = -1$$

$$r^2 \frac{dT}{dr} = \frac{-r^3}{3D} + A$$

$$\frac{dT}{dr} = \frac{-r}{3D} + \frac{A}{r^2}$$

$$T(r) = \frac{-r^2}{6D} + \frac{-A}{r} + B$$

T has the boundary conditions $T(a) = 0 = T(b)$

$$T(a) = 0 = \frac{-a^2}{6D} - \frac{A}{a} + B \longrightarrow B - \frac{A}{a} = \frac{a^2}{6D} \quad (1)$$

$$T(b) = 0 = \frac{-b^2}{6D} - \frac{A}{b} + B \longrightarrow B - \frac{A}{b} = \frac{+b^2}{6D} \quad (2)$$

Take (1) - (2) :

$$\left(\frac{1}{b} - \frac{1}{a}\right)A = \frac{a^2 - b^2}{6D} \longrightarrow A = \frac{(b-a)\cancel{(a-b)}}{6D} \frac{ab}{\cancel{a-b}}$$

$$A = \frac{b-a}{6D} ab$$

$$B = \frac{a^2}{6D} + \frac{(b-a)}{6D} b$$

Plug back into $T(r)$

4.2 (contd.) $T(r) = \frac{-r^2}{6D} + \frac{A}{r} + B$

$$= \frac{-r^2}{6D} + \frac{b-a}{6D}\frac{a}{r} + \frac{a^2}{6D} + \frac{(b-a)b}{6D}$$

$$\boxed{T(r) = \frac{a^2 + (b-a)b - r^2}{6D} + \frac{b-a}{6D}\frac{a}{r}}$$

Given we're going to $a$. $T_a(r) = \frac{T(r)}{P_a(r)}$

$$T_a(r) = \left[\frac{a^2 + (b-a)b - r^2}{6D} + \frac{b-a}{6D}\frac{a}{r}\right]\frac{r}{a}\frac{b-a}{b-r}$$

$$= \left[\left(a^2 + (b-a)b - r^2\right)\frac{r}{a} + (b-a)\right]\frac{b-a}{b-r}\frac{1}{6D}$$

Problem 4 (cont.)

4.3 For $a \to 0$

$$T(r) \to \frac{b^2 - r^2}{6D} + 0 = \frac{b^2 - r^2}{6D}$$

$$T_a(r) \to \infty$$

Which seems reasonable. We'll never hit the point a, but we will eventually hit the outer shell b.

For $b \to \infty$

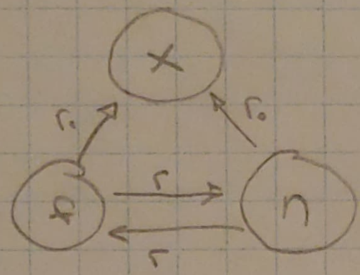
$$T(r) \longrightarrow \infty$$

$$T_a(r) \to \infty$$

This also makes sense, Some molecules may get lucky and hit a, but many more will miss and diffuse away forever. Thus the mean time to be absorbed goes to $\infty$.

Problem 5

5.1




$$\dot{P}_f = -rP_f - r_0 P_f + rP_n$$

$$\dot{P}_n = -rP_n - r_0 P_n + rP_f$$

$$\dot{P}_x = r_0 P_n + r_0 P_f$$

Solutions of the form

$$P_z(t) = Ae^{-\lambda t}$$

Then the rate matrix is

$$\hat{M} = \begin{pmatrix} -r-r_0 & r & 0 \\ r & -r-r_0 & 0 \\ r_0 & r_0 & 0 \end{pmatrix}$$

Find eigen values: $\det(\hat{M} - \mathbb{1}\lambda) = 0$

$$-\lambda\left[(-r-r_0-\lambda)^2 - r^2\right] = 0$$

We get the free answer, $\lambda = 0$.

$$(-r-r_0-\lambda)^2 = r^2$$

$$-r-r_0-\lambda = r \qquad\qquad -r-r_0-\lambda = -r$$

$$\lambda = -r_0 - 2r \qquad\qquad \lambda = -r_0$$

Find eigen vectors: $(\hat{M} - \mathbb{1}\lambda)\vec{v} = 0$

5.1 (cont.)

$\lambda_1 = 0$ $\quad v_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ by instinct. After long $t$, I have entered the refractory state.

$$\begin{pmatrix} -r-r_0 & r & 0 \\ r & -r-r_0 & 0 \\ r_0 & r_0 & 0 \end{pmatrix} \begin{pmatrix} f \\ n \\ x \end{pmatrix} = 0 \qquad \vec{v}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$r_0 f + r_0 n = 0 \longrightarrow f = -n$

$\therefore x = 1$ by normalization.

$rf - rn - r_0 n = 0 \longrightarrow f = n = 0$

$\lambda_2 = -r_0$:

$$\begin{pmatrix} -r & r & 0 \\ r & -r & 0 \\ r_0 & r_0 & r_0 \end{pmatrix} \begin{pmatrix} f \\ n \\ x \end{pmatrix} = 0 \qquad \vec{v}_2 = \begin{pmatrix} 1/2 \\ 1/2 \\ -1 \end{pmatrix}$$

$-rf + nr = 0 \longrightarrow f = n$

$r_0 f + r_0 n + r_0 x = 0 \longrightarrow 2 r_0 f = -r_0 x \longrightarrow x = -2f$

$\lambda_3 = -r_0 - 2r$:

$$\begin{pmatrix} r & r & 0 \\ r & r & 0 \\ r_0 & r_0 & r_0+2r \end{pmatrix} \begin{pmatrix} f \\ n \\ x \end{pmatrix} = 0 \qquad \vec{v}_3 = \begin{pmatrix} 1/2 \\ -1/2 \\ 0 \end{pmatrix}$$

$f = -n$

$(r_0 + 2r)x = 0 \longrightarrow x = 0$

We want to start in $n$, so make the appropriate linear combination.

$$\vec{P}(t) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ -1 \end{pmatrix} e^{-r_0 t} - \begin{pmatrix} 1/2 \\ -1/2 \\ 0 \end{pmatrix} e^{-(r_0+2r)t}$$

5.1 (contd)

Probability to be in state z at time t is

$$\vec{p}(t) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ -1 \end{pmatrix} e^{-r_0 t} - \begin{pmatrix} 1/2 \\ -1/2 \\ 0 \end{pmatrix} e^{-(r_0+2r)t} = \begin{pmatrix} P_p(t) \\ P_n(t) \\ P_x(t) \end{pmatrix}$$

Then the probability to not be in state x is

$$\sim P_x(t) = 1 - P_x(t) = \boxed{e^{-r_0 t}}$$

5.2

Up 'til now everything has been with cumulative distributions, so turn things back to probability densities.

$$\rho_x(t)\,dt = r_0 e^{-r_0 t}\,dt$$

$$\langle t \rangle_x = \int_0^\infty t r_0 e^{-r_0 t}\,dt = \boxed{\frac{1}{r_0}}$$ which makes sense.

$$\langle t^2 \rangle_x = \int_0^\infty t^2 r_0 e^{-r_0 t}\,dt =$$ let $u = t^2$, $dv = e^{-r_0 t}$, $du = 2t\,dt$, $v = \frac{e^{-r_0 t}}{-r_0}$

$$= r_0 \left[ t^2 \frac{e^{-r_0 t}}{-r_0} \Big|_0^\infty - \int_0^\infty 2t \frac{e^{-r_0 t}}{-r_0}\,dt \right]$$

$$= \frac{2}{r_0} \int_0^\infty r_0 e^{-r_0 t}\,dt = \boxed{\frac{2}{r_0^2}}$$

$$\text{var}_x = \langle t^2 \rangle - \langle t \rangle^2 = \frac{2}{r_0^2} - \frac{1}{r_0^2} = \boxed{\frac{1}{r_0^2}}$$

Fluorescent: $P_n(t) = \frac{1}{2}\left[e^{-r_0 t} - e^{-(r_0+2r)t}\right]$

$$\frac{dP_n(t)}{dt} = \frac{1}{2}\left[-r_0 e^{-r_0 t} + (r_0+2r)\,e^{-(r_0+2r)t}\right]$$

$$\langle t \rangle_f = \int_0^\infty dt\ \frac{1}{2} t \left[-r_0 e^{-r_0 t} + (r_0+2r)\,e^{-(r_0+2r)t}\right]$$

$$\langle t \rangle_f = \frac{1}{2}\left[-\frac{1}{r_0} + \frac{1}{r_0+2r}\right] = \frac{1}{2}\,\frac{\cancel{r_0} - \cancel{r_0} - 2r}{r_0^2 + 2rr_0} = \frac{-r}{r_0^2+2rr_0}$$

Somewhere, I messed up a $\ominus$ sign. $\boxed{\langle t \rangle_f = \frac{r}{r_0^2 + 2rr_0}}$

this has some expected behaviours. For example, as $r_0^2 \to 0$ $\langle t \rangle \to \frac{1}{2r_0}$. Half the time not in the refractory

5.2i (Cont.)

in the refractory period is spent in the fluorescent state.

$$\langle t^2 \rangle_f = \frac{1}{2}\int_0^\infty \left( r_0 e^{-r_0 t} + (r_0+2r) e^{-(r_0+2r)t} \right) t^2 \, dt$$

Use result from $\langle t^2 \rangle_*$ from earlier

$$\langle t^2 \rangle_f = \frac{1}{2}\left[ \frac{2}{r_0^2} - \frac{2}{(r_0+2r)^2} \right] = \frac{1}{r_0^2} - \frac{1}{(r_0+2r)^2}$$

$$= \frac{\cancel{r_0^2} + 4r^2 + 4r_0 r - \cancel{r_0^2}}{r_0^2 (r_0+2r)^2} = 4r \frac{r + r_0}{r_0^2 (r_0+2r)^2}$$

$$\mathrm{Var}_f = \langle t^2 \rangle_f - \langle t \rangle_f^2$$

$$= \frac{4r(r+r_0)}{r_0^2 (r_0+2r)^2} - \frac{4r^2}{r_0^2 (r_0+2r)^2} = \frac{4r r_0}{r_0^2 (r_0+2r)^2}$$

$$\boxed{\mathrm{Var}_f = \frac{4r}{r_0 (r_0+2r)^2}}$$