PHYSICS 210B : NONEQUILIBRIUM STATISTICAL PHYSICS
HW SOLUTIONS #4 : DIFFUSION

(1) A diffusing particle is confined to the interval $[0, L]$. The diffusion constant is D and the drift velocity is $v_{\rm D}$. 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 $v_{\rm D} > 0$, $v_{\rm D} = 0$, and $v_{\rm D} < 0$.

(b) Compute the Laplace transform of the distribution of trapping times for the cases $v_{\rm D} > 0$, $v_{\rm D} = 0$, and $v_{\rm D} < 0$, 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,

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

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

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

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 $\psi(x) = \exp\big(v_{\rm D} x / D\big)$ (use Eqn. 4.53 with $A = v_{\rm D}$ and $B = 2D$). We then have

$$T_1(x) = \frac{D}{v_{\rm D}^2} \left(1 - e^{-v_{\rm D} x / D} \right) e^{v_{\rm D} L / D} - \frac{x}{v_{\rm D}} \quad .$$

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 $\ell = D/|v_{\rm D}|$ and the time scale $\tau = D/v_{\rm D}^2$. 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 $\sigma = {\rm sgn}(v_{\rm D})$. 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 $D/|v_{\rm D}|$. This grows exponentially with $|v_{\rm D}|$. 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

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

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

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.

(2) Consider a continuum model of a polymer, where the position $\boldsymbol{R}(s) = \big(a/\sqrt{d}\big)\,\boldsymbol{W}(s)$, where $\boldsymbol{W}(s) = \{W_1(s), \ldots, W_d(s)\}$ is a d-dimensional Wiener process, with $s \in [0, N]$, where N is the length of the polymer in units of the persistence length a. The density, in units of mass per persistence length, is

$$\rho(\boldsymbol{r}) = \int\limits_0^N ds\,\delta\big(\boldsymbol{r} - \boldsymbol{R}(s)\big) \quad .$$

Show that the structure factor $S(\boldsymbol{k}) = N^{-1}\big\langle\big|\hat{\rho}(\boldsymbol{k})\big|^2\big\rangle$, where $\hat{\rho}(\boldsymbol{k})$ is the Fourier transform of the density, is of the Debye form,

$$S(\boldsymbol{k}) = 2\,(R_0/a)^2\,f(k^2R_0^2/2d) \quad ,$$

where $f(x) = \big(e^{-x} - 1 + x\big)/x^2$.

Solution:

The Fourier transform of $\rho(\boldsymbol{r})$ is $\hat{\rho}(\boldsymbol{k}) = \int\limits_0^N ds\,e^{-i\boldsymbol{k}\cdot\boldsymbol{R}(s)}$, and therefore the structure factor is

$$\begin{aligned}
S(\boldsymbol{k}) &= \frac{1}{N}\int\limits_0^N ds \int\limits_0^N ds'\,\big\langle e^{i\boldsymbol{k}\cdot(\boldsymbol{R}(s') - \boldsymbol{R}(s))}\big\rangle \\
&= \frac{1}{N}\int\limits_0^N ds \int\limits_0^N ds'\,\exp\bigg\{-\frac{k^\alpha k^\beta a^2}{2d}\Big\langle\big(W^\alpha(s) - W^\alpha(s')\big)\big(W^\beta(s) - W^\beta(s')\big)\Big\rangle\bigg\} \quad .
\end{aligned}$$

Now $\big\langle W^\alpha(s)\,W^\beta(s')\big\rangle = \textsf{min}(s,s')\,\delta^{\alpha\beta}$, hence

$$\begin{aligned}
S(\boldsymbol{k}) &= \frac{1}{N}\int\limits_0^N ds \int\limits_0^N ds'\,\exp\bigg\{-\frac{k^2a^2}{2d}\big(s + s' - 2\,\textsf{min}(s,s')\big)\bigg\} \\
&= \frac{2}{N}\int\limits_0^N ds \int\limits_0^s ds'\,e^{-k^2a^2(s-s')/2d} = \frac{4d}{k^2R_0^2}\int\limits_0^N ds\,\big(1 - e^{-k^2R_0^2\,s/2Nd}\big) \\
&= \frac{4Nd}{k^2R_0^2}\bigg(1 - \frac{2d}{k^2R_0^2}\big(1 - e^{-k^2R_0^2/2d}\big)\bigg) = 2\,(R_0/a)^2\,f\big(k^2R_0^2/2d\big) \quad ,
\end{aligned}$$

where $f(x) = \big(e^{-x} - 1 + x\big)/x^2$.

(3) Verify that the distribution

$$\varPi\big[h(x)\big] = \exp\left\{ - \frac{D}{\varGamma} \int\limits_{-\infty}^{\infty} dx \left(\frac{\partial h}{\partial x}\right)^2 \right\}$$

solves the functional Fokker-Planck equation for the one-dimensional KPZ equation.

Solution:

The functional Fokker-Planck equation for the $d = 1$ KPZ system,

$$\frac{\partial h}{\partial t} = D\,\frac{\partial^2 h}{\partial x^2} + \tfrac{1}{2}\lambda\left(\frac{\partial h}{\partial x}\right)^2 + \eta(x,t)$$

is given in Eqn. 6.106 of the notes:

$$\frac{\partial \varPi\big[h(x),t\big]}{\partial t} = \int\! dy \left(\tfrac{1}{2}\varGamma\,\frac{\delta^2}{\delta h(y)^2} - \frac{\delta}{\delta h(y)}\,J(y)\right)\varPi\big[h(x),t\big] \quad ,$$

where

$$J = D\,\frac{\partial^2 h}{\partial x^2} + \tfrac{1}{2}\lambda\left(\frac{\partial h}{\partial x}\right)^2 \quad .$$

To verify the solution, define

$$W\big[h(x)\big] = \frac{D}{\varGamma}\int\limits_{-\infty}^{\infty} dx \left(\frac{\partial h}{\partial x}\right)^2 \quad ,$$

so $\varPi[h] = e^{-W[h]}$. Taking the functional derivative,

$$\frac{\delta W}{\delta h(y)} = -\frac{D}{\varGamma}\,h''(y) \qquad \Rightarrow \qquad \frac{\delta \varPi}{\delta h(y)} = \frac{D}{\varGamma}\,h''(y)\,\varPi \quad .$$

Thus,

$$\frac{\varGamma}{2}\,\frac{\delta^2 \varPi}{\delta h(y)^2} = D\,\delta''(0)\,\varPi + \frac{2D^2}{\varGamma}\,h''(y)^2\,\varPi \quad .$$

Next, we compute

$$-\frac{\delta}{\delta h(y)}\left\{\Big[D\,h''(y) + \tfrac{1}{2}\lambda\,h'(y)^2\Big]\varPi\right\} = -D\,h''(0)\,\varPi - \lambda\,h'(y)\,\delta'(0)\,\varPi - \Big[D\,h''(y) + \tfrac{1}{2}\lambda\,h'(y)^2\Big]\left(\frac{2D}{\varGamma}\,h''(y)\right)\varPi$$

and adding these results we obtain

$$\begin{aligned}\left\{\frac{\varGamma}{2}\,\frac{\delta^2}{\delta h(y)^2} - \frac{\delta}{\delta h(y)}J(y)\right\}\varPi[h] &= -\frac{D\lambda}{\varGamma}\,h'(y)^2\,h''(y)\,\varPi - \lambda\,h'(y)\,\delta'(0)\,\varPi \\ &= -\frac{d}{dy}\left(\frac{D\lambda}{3\varGamma}\,h'(y)^3 + \lambda\,\delta'(0)\,h(y)\right)\varPi \quad ,\end{aligned}$$

and since the y-dependent term on the RHS is a total derivative, we have[1]

$$\int\limits_{-\infty}^{\infty} dy \left\{ \frac{\Gamma}{2} \frac{\delta^2}{\delta h(y)^2} - \frac{\delta}{\delta h(y)} J(y) \right\} \Pi[h] = 0 \quad ,$$

where $J(y) = D\,h''(y) + \frac{1}{2}\lambda\,h'(y)^2$. This says that $\Pi[h]$ is a solution to the functional Fokker-Planck equation.

We can now see why one dimension is special in this regard. *Mutatis mutandis*, if we apply the same procedure to the case where $W[h] = \frac{D}{\Gamma}\int d^d x\, (\boldsymbol{\nabla} h)^2$, we obtain a term $(\nabla h)^2\, \nabla^2 h$, which is the higher dimensional generalization of $h'(y)^2\, h''(y)$ obtained above. But $(\nabla h)^2\, \nabla^2 h$ is a scalar, in which all the spatial indices are contracted; it is not equal to the (vector) gradient of any function!

Finally, let's see how the above functional Fokker-Planck equation results from the continuum limit of an appropriate discrete model. Consider the coupled SODEs

$$\frac{\partial h_n}{\partial t} = \frac{D}{a^2}\left(h_{n+1} + h_{n-1} - 2\,h_n\right) + \frac{\lambda}{2a^2}\left(h_{n+1} - h_n\right)^2 + a^{-1/2}\,\eta_n(t) \quad ,$$

where $\langle \eta_n(t)\,\eta_{n'}(t')\rangle = \Gamma\,\delta_{nn'}\,\delta(t-t')$. Notice the discrete derivatives in the above expression:

$$\frac{h_{n+1} - h_n}{a} \approx \frac{\partial h}{\partial x} \qquad , \qquad \frac{h_{n+1} + h_{n-1} - 2\,h_n}{a^2} = \frac{1}{a}\left(\frac{h_{n+1} - h_n}{a} - \frac{h_n - h_{n-1}}{a}\right) \approx \frac{\partial^2 h}{\partial x^2} \quad .$$

We saw in §3.4.3 how the multicomponent SDE $du_a = A_a\,dt + \beta_{ab}\,dW_b(t)$ with $\langle dW_a(t)\,dW_b(t)\rangle = \delta_{ab}\,dt$ gives rise to the Fokker-Planck equation $\partial_t P = -\frac{\partial}{\partial u_a}(A_a\,P) + \frac{1}{2}\frac{\partial^2}{\partial u_a\,\partial u_b}\big[(\beta\beta^{\rm t})_{ab}\,P\big]$. In our case, we have $u_a \to h_n$, $\beta_{ab} \to \sqrt{\Gamma/a}\,\delta_{nn'}$, and

$$A_a \to A_n = \frac{D}{a^2}\left(h_{n+1} + h_{n-1} - 2\,h_n\right) + \frac{\lambda}{2a^2}\left(h_{n+1} - h_n\right)^2 \quad .$$

The corresponding Fokker-Planck equation is then

$$\begin{aligned}\frac{\partial P}{\partial t} &= \sum_n \left\{ -\frac{\partial}{\partial h_n}(A_n\,P) + \frac{\Gamma}{2a}\frac{\partial^2 P}{\partial h_n^2} \right\} \\ &= a \sum_n \left\{ -\frac{1}{a}\frac{\partial}{\partial h_n}(A_n\,P) + \frac{\Gamma}{2a^2}\frac{\partial^2 P}{\partial h_n^2} \right\} \quad .\end{aligned}$$

We rewrite the RHS on the second line as we did in order to make contact with the continuum functional Fokker-Planck equation, where $a\sum_n \to \int dy$.

We now seek a stationary solution. We again take $P = e^{-W}$, with

$$W = \frac{D}{\Gamma a}\sum_n (h_{n+1} - h_n)^2 \quad .$$

[1]We could also appeal to the fact that $\delta(y)$ is even and insist that $\delta'(0) = 0$. This is a bit dicey because $\delta(y)$ is really a distribution and not a proper function.

From the chain rule, $\frac{\partial P}{\partial h_n} = -P\,\frac{\partial W}{\partial h_n}$. We now have the following:

$$\frac{\partial W}{\partial h_n} = \frac{2D}{\Gamma a}\,(2h_n - h_{n+1} - h_{n-1}) \qquad , \qquad \frac{\partial A_n}{\partial h_n} = -\frac{2D}{a^2} + \frac{\lambda}{a^2}\,(h_n - h_{n+1}) \quad .$$

We therefore have

$$-\frac{1}{a}\,\frac{\partial}{\partial h_n}(A_n P) = \overbrace{\bigg(\frac{2D}{a^3} - \frac{\lambda}{a^3}\,(h_n - h_{n+1})\bigg)}^{-a^{-1}P\,\partial A_n/\partial h_n} P \; + \\ \overbrace{\bigg(\frac{D}{a^2}\,(h_{n+1} + h_{n-1} - 2\,h_n) + \frac{\lambda}{2a^2}\,(h_{n+1} - h_n)^2\bigg)}^{A_n} \cdot \overbrace{\bigg(-\frac{2D}{\Gamma a^2}\,(h_{n+1} + h_{n-1} - 2h_n)\,P\bigg)}^{-a^{-1}\partial P/\partial h_n}$$

as well as

$$\frac{\partial^2 P}{\partial h_n^2} = \frac{\partial}{\partial h_n}\bigg(-P\,\frac{\partial W}{\partial h_n}\bigg) = -P\,\frac{\partial^2 W}{\partial h_n^2} + P\bigg(\frac{\partial W}{\partial h_n}\bigg)^2$$

so that

$$\frac{\Gamma}{2a^2}\,\frac{\partial^2 P}{\partial h_n^2} = -\frac{2D}{a^3} + \frac{2D^2}{\Gamma a^4}\,(2h_n - h_{n+1} - h_{n-1})^2 P$$

When we add these results in the sum of the multivariable FPE, the two terms on the RHS immediately above cancel with corresponding terms in the expression for $-\frac{1}{a}\,\frac{\partial}{\partial h_n}(A_n P)$. Before canceling, it is good to notice that $-2/a^3$ is the lattice equivalent of $\delta''(0)$. After canceling, we have

$$a\sum_n\bigg\{-\frac{1}{a}\,\frac{\partial}{\partial h_n}(A_n\,P) + \frac{\Gamma}{2a^2}\,\frac{\partial^2 P}{\partial h_n^2}\bigg\} = \lambda\,\frac{1}{a}\sum_n\bigg(\frac{h_{n+1} - h_n}{a}\bigg)\,P \\ -\frac{D\lambda}{\Gamma}\,a\sum_n\bigg(\frac{h_{n+1} - h_n}{a}\bigg)^2\bigg(\frac{h_{n+1} + h_{n-1} - 2h_n}{a^2}\bigg)\,P\,.$$

The first term is identified with $-\lambda\,\delta'(0)\int\!dy\;h'(y)$, with $\delta'(0) = 1/a^2$. This identification is due to our asymmetric definition of the lattice derivative at n as $(h_{n+1} - h_n)/a$. At any rate, the sum $\sum_n(h_{n+1} - h_n)$ vanishes, if we assume the field h_n vanishes at spatial infinity, or periodic boundary conditions are employed. The last term is the lattice version of $(D\lambda/\Gamma)\int\!dy\;h'(y)^2\,h''(y)\,P$, which vanishes because $h'(y)^2\,h''(y) = \frac{1}{3}\big(h'(y)^3\big)'$ is a total derivative. However, it is only a total derivative in the continuum, and not on the lattice, therefore our function $P(\{h_n\})$ is *not* a stationary solution of the many variable Fokker-Planck equation.

(4) Consider the Mullins equation,

$$\frac{\partial h}{\partial t} = -\nu\,\nabla^4 h + \eta\,,$$

where $\nabla^4 = (\boldsymbol{\nabla}^2)^2$.

(a) Use dimensional analysis and linearity to show how the interface width $w(t)$ scales with the parameters and time. For what dimensions does the noise roughen the interface?

(b) Compute the interface width and the two point correlation function in dimensions $d = 1$, $d = 2$, and $d = 3$.

Solution:

(a) We have

$$[\nu] = L^4\,T^{-1} \quad , \quad [\Gamma] = L^d\,H^2\,T^{-1} \quad , \quad [t] = T \quad .$$

The interface width is $w(t) = \big\langle h^2(\boldsymbol{x},t)\big\rangle^{1/2}$, so $[w] = H$, and we conclude

$$w(t) \propto \Gamma^{1/2}\,\nu^{-d/8}\,t^{(4-d)/8} \quad .$$

The interface is rough, *i.e.* its width increases with time, in dimensions $d \le 4$ (we expect a logarithm in $d = 4$ dimensions). Recall that for the Edwards-Williamson model, roughening only occured for $d \le 2$.

(b) Fourier transforming the position variable, the Mullins equation becomes

$$\frac{\partial \hat{h}(\boldsymbol{k},t)}{\partial t} = -\nu k^4\,\hat{h}(\boldsymbol{k},t) + \hat{\eta}(\boldsymbol{k},t) \quad .$$

The Fourier space correlator of the stochastic noise is

$$\big\langle \hat{\eta}(\boldsymbol{k},t)\,\hat{\eta}(-\boldsymbol{k}',t')\big\rangle = (2\pi)^d\,\Gamma\,\delta(\boldsymbol{k}-\boldsymbol{k}')\,\delta(t-t') \quad .$$

Directly integrating the Mullins equation in Fourier space yields

$$\hat{h}(\boldsymbol{k},t) = \hat{h}(\boldsymbol{k},0)\,e^{-\nu k^4 t} + \int\limits_0^t\!ds\;\hat{\eta}(\boldsymbol{k},s)\,e^{-\nu k^4 (t-s)} \quad .$$

Assuming we start from a flat surface with $h(\boldsymbol{x},0) = 0$, we have

$$\begin{aligned}
\big\langle h(\boldsymbol{x},t)\,h(\boldsymbol{x}',t')\big\rangle &= \int\!\frac{d^d\!k}{(2\pi)^d}\int\!\frac{d^d\!k'}{(2\pi)^d}\;e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\boldsymbol{k}'\cdot\boldsymbol{x}')}\int\limits_0^t\!ds\int\limits_0^{t'}\!ds'\;e^{-\nu k^4(t-s)}\,e^{-\nu k'^4(t'-s')}\,(2\pi)^d\,\Gamma\,\delta(\boldsymbol{k}-\boldsymbol{k}')\,\delta(s-s') \\
&= \Gamma\int\!\frac{d^d\!k}{(2\pi)^d}\;e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}\int\limits_0^{t_<}\!ds\;e^{-\nu k^4(t+t'-2s)} \\
&= \frac{\Gamma}{2\nu}\int\!\frac{d^d\!k}{(2\pi)^d}\;e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}\;\frac{1}{k^4}\,\Big\{e^{-\nu k^4|t-t'|} - e^{-\nu k^4(t+t')}\Big\} \quad ,
\end{aligned}$$

where $t_< = \textsf{min}(t,t')$. Thus, if we define $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}'$, we have

$$C(\boldsymbol{r},t,t') = \big\langle h(\boldsymbol{r},t)\,h(0,t')\big\rangle = \frac{\Gamma}{2\nu}\,\frac{\Omega_d}{(2\pi)^d}\int\limits_0^\infty\!dk\;k^{d-5}\,f_d(kr)\,\Big\{e^{-\nu k^4|t-t'|} - e^{-\nu k^4(t+t')}\Big\} \quad ,$$

where

$$f_d(z) = \begin{cases} \cos z & \text{if } d = 1 \\ J_0(z) & \text{if } d = 2 \\ \Gamma(d/2)\,(2/z)^{\frac{d}{2}-1} J_{\frac{d}{2}-1}(z) & \text{if } d > 2 \end{cases}$$

and $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the area of the unit sphere in d dimensions[2]. Note that $f_d(0) = 1$. The integral for $C(\boldsymbol{r}, t, t')$ is convergent in the infrared because the term in curly brackets vanishes as k^4 in the $k \to 0$ limit.

In dimensions $d < 4$ the interface width is given by

$$\begin{aligned} w^2(t) &= \frac{\Gamma}{2\nu}\,\frac{\Omega_d}{(2\pi)^d} \int_0^\infty dk\; k^{d-5}\big(1 - e^{-2\nu k^4 t}\big) \\ &= \frac{\Gamma}{2(4-d)\nu}\,\frac{\Omega_d\,\Gamma(d/4)}{(2\pi)^d}\,\big(2\nu t\big)^{1-\frac{d}{4}} \quad , \end{aligned}$$

which agrees with the scaling analysis in part (a). The two-point correlator $C(\boldsymbol{x} - \boldsymbol{x}', t, t')$ is given by

$$\begin{aligned} C_{d=1}(x - x', t, t') &= \frac{\sqrt{2\pi}\,\Gamma}{4\nu}\,|x - x'|^3 \int_0^\infty du\, \frac{\cos u}{u^{7/2}} \Big[e^{-\zeta u^4} - e^{-Z u^4}\Big] \\ C_{d=2}(\boldsymbol{x} - \boldsymbol{x}', t, t') &= \frac{\pi\Gamma}{2\nu}\,|\boldsymbol{x} - \boldsymbol{x}'|^2 \int_0^\infty du\, \frac{J_0(u)}{u^3} \Big[e^{-\zeta u^4} - e^{-Z u^4}\Big] \\ C_{d=3}(\boldsymbol{x} - \boldsymbol{x}', t, t') &= \frac{\pi\Gamma}{\nu}\,|\boldsymbol{x} - \boldsymbol{x}'| \int_0^\infty du\, \frac{\sin u}{u^3} \Big[e^{-\zeta u^4} - e^{-Z u^4}\Big] \quad , \end{aligned}$$

with

$$\zeta = \frac{\nu\,|t - t'|}{|\boldsymbol{x} - \boldsymbol{x}'|^4} \quad , \quad Z = \frac{\nu\,(t + t')}{|\boldsymbol{x} - \boldsymbol{x}'|^4} \quad .$$

For the equal time correlation functions $\big\langle h(\boldsymbol{x}, t)\, h(\boldsymbol{x}', t)\big\rangle$, set $\zeta = 0$ in the above expressions, and $Z = 2\nu t/|\boldsymbol{x} - \boldsymbol{x}'|^4$.

[2]Note $\Omega_{d=1} = 2$.