Diffusion gradients as forces

- To induce trapping, phenomenologically introduce an attractive drift
$$a(X_t) = -\alpha\Gamma(X_t)\nabla\kappa(X_t), \tag{1}$$
$\alpha > 0$ and Onsager coefficient related by an FDT, $\kappa(x) = 2k_B T\Gamma(X_t)$, to our Langevin equation such that
$$dX_t = a(X_t)\,dt + \sqrt{2\kappa(X_t)} \circ dW_t \tag{2}$$

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- The steady state is $\rho_\infty(x) \propto e^{-\beta\alpha\kappa(x)}$ and the FPE
$$\partial_t p(x,t) = \nabla \cdot \left[\kappa\left(\beta\alpha\nabla\kappa + \nabla\right)\right] p(x,t) = -\mathcal{L}p(x,t) \tag{3}$$

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    - Free energy has a long-wavelength contribution $F(X) \sim U(\phi(X))$, which the diffusivity also depends upon explicitly, $\kappa(X) = \kappa(\phi(X))$
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- Thermodynamically, entering a more confined phase has an entropy reduction - needs to be compensated for

A "convenient" change of variables

- Consider the change of variables, for a second differentiable, time-independent diffusivity field satisfying $\kappa(x) > 0$,[1]

$$x \mapsto X = \int_0^x \frac{dx'}{\sqrt{\kappa(x')}}; \qquad \frac{\partial}{\partial x} \mapsto \frac{1}{\sqrt{\kappa(x)}} \frac{\partial}{\partial X} \tag{4}$$

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- After no short amount of algebra, it can be shown that this results in the generator taking the form $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}'$, where $\mathcal{L}_0 = -\partial_X^2$ and the interaction generator is

$$\mathcal{L}' = -\frac{1}{\sqrt{\kappa}} \left(\partial_X \sqrt{\kappa}\right) \left[\partial_X + \beta\alpha(\partial_X \kappa)\right] - \beta\alpha \left[(\partial_X^2 \kappa) + (\partial_X \kappa)\, \partial_X\right] \tag{5}$$

A Green's function formulation

- Assuming time translation invariance and look for Green's function solutions, $G(X, Y; t)$ (transition from X to Y in time t)
- It is easier to consider the Fourier transformed function, $G(X, Y; \omega)$, whose PDE is $\left(-i\omega + \hat{\mathcal{L}}\right)\hat{G} = \mathbb{1}$, which is formally solved by

$$\hat{G} = \left(-i\omega + \hat{\mathcal{L}}\right)^{-1} \tag{6}$$

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- Might prove to be useful if the diffusivity field is largely homogeneous except for small (both in magnitude and area) fluctuations at e.g. lipid raft domains

Trapping's effect on diffusive behaviour

- Consider the Itô SDE,

$$dX_t = \left[1 - \frac{1}{2}\alpha\beta\kappa(X_t)\right] \nabla\kappa(X_t)\, dt + \sqrt{2\kappa(X_t)}\, dW_t \tag{7}$$

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- Choose the system with periodic BC on $[0, L)$, with diffusivity

$$\kappa(x) = A\left[1 - \sin^{2n}\left(\frac{\pi x}{L}\right)\right] + \varepsilon, \tag{8}$$

- SDE can be non-dimensionalized to the form

$$dY_\tau = n\left[\gamma\left(1 + b - \sin^{2n} Y\right) - 2\right]\sin^{2n-1} Y \cos Y\,d\tau + \sqrt{2\left(1 + b - \sin^{2n} Y\right)}\,dW_\tau \tag{9}$$

Trapping's effect on diffusive behaviour

- Was not able to find any reasonable choice of diffusivity that would amount to any change in the asymptotic MSD scaling
  - Apparent anomalous behaviour from last week seems to have exclusively been a result of the domain
  - Recovered apparent anomalous behaviour when $b \to 0$ – effectively converging towards a CTRW

References

[1] T. Miyazawa and T. Izuyama, Phys. Rev. A **36**, 5791 (1987).

The unperturbed Green's function

- Taking the Fourier transform with respect to space maps $\partial_X \to ik$ and hence $G(k,\omega) = (-i\omega + k^2)^{-1}$, which is the standard heat kernel
- We can transform back to real time/ space by taking a pair of contour integrals,

$$G(k,t) = \Theta(t)e^{-k^2 t}; \qquad G(X,t) = \frac{1}{\sqrt{4\pi t}}\Theta(t)e^{-X^2/4t} \tag{10}$$

Perturbation theory

- We regard κ as the continuum limit of a discrete function. First, we consider the case

$$\kappa(X) = \begin{cases} \kappa_1, & X < Z_1 \\ \kappa_2, & X > Z_1 \end{cases} \tag{11}$$

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- The derivative is zero except for at the transition point (step function), $\kappa'(X) = (\kappa_2 - \kappa_1)\,\delta(X - Z_1)$, and hence the interaction operator takes the form

$$\begin{aligned} \mathcal{L}'(X) = -a_1(X)\delta(X - Z_1)\left[\partial_X + \beta\alpha b_1\delta(X - Z_1)\right] \\ - \beta\alpha b_1\left[\delta'(X - Z_1) + \delta(X - Z_1)\partial_X\right], \end{aligned} \tag{12}$$

where we have defined

$$a_1(X) = \frac{\sqrt{\kappa_2} - \sqrt{\kappa_1}}{\sqrt{\kappa(X)}}, \qquad b_1 = \kappa_2 - \kappa_1 \tag{13}$$