Semi-permeable membranes as domain walls

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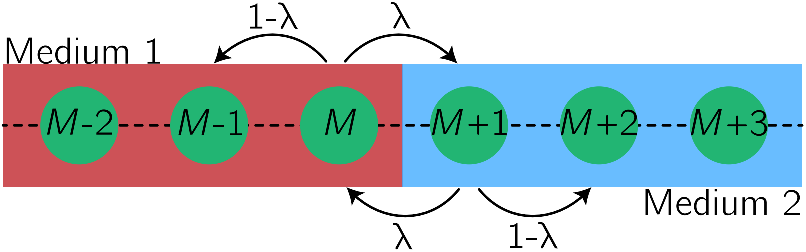
December 23, 2025

Semi-permeable membranes as domain walls

- Consider a 1d lattice of spacing $a > 0$. The lattice is separated by placing a semi-permeable membrane between sites M and $M+1$[1], which can be crossed with probability $\lambda < 1$
- On the left of the membrane consists of a media with temporal step size τ_l and on the right a media with step size τ_r – eventually amounting to varying diffusivities



The master equation

- Let $p_j(t)$ denote the probability of being at site j at time t and $\Delta = \frac{1}{2} - \lambda$. The (global) master equation for the system reads

$$\frac{\partial p_j(t)}{\partial t} = \left[\frac{1}{2}p_{j+1} + \frac{1}{2}p_{j-1} - p_j\right]\left(\frac{1}{\tau_l}\sum_{k=-\infty}^{M}\delta_{j,k} + \frac{1}{\tau_r}\sum_{k=M+1}^{\infty}\delta_{j,k}\right)$$
$$+ \frac{\Delta}{\tau_l}p_M(t)\delta_{j,M-1} + \frac{\Delta}{\tau_r}p_{M+1}(t)\delta_{j,M+2}$$
$$+ \left(\frac{\lambda}{\tau_r} - \frac{1}{2\tau_l}\right)p_{M+1}(t)\delta_{j,M} + \left(\frac{\lambda}{\tau_l} - \frac{1}{2\tau_r}\right)p_M(t)\delta_{j,M+1} \quad (1)$$

The continuum limit

- Consider the discrete-to-continuum mapping, $p_j(t) \to p(x,t)$, $M \to x_b$, $D_i = a^2/2\tau_i$ and $\delta_{j,k} \to a\delta(x-y)$

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- Keep terms to $\mathcal{O}(a^4)$ by enforcing $\kappa_i = \frac{a}{4(2\lambda-1)\tau_i}$ remains finite in the limit $a, \tau_l, \tau_r \to 0$,

$$\begin{aligned}\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\left(D_l\Theta(x_b - x) + D_r\Theta(x - x_b)\right)\frac{\partial p(x,t)}{\partial x}\right] \\ + (4\lambda - 1)\left(D_r - D_l\right)p(x_b,t)\delta'(x - x_b) \\ - \frac{D_r^2}{\kappa_r}\frac{\partial p(x_b,t)}{\partial x}\delta'(x - x_b) \quad (2)\end{aligned}$$

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- When $D_r = D_l$, diffusion becomes homogeneous across membrane and we recover Kay & Giuggioli (2022)[2]
- When $\lambda = 1/2$, $\kappa_r \to \infty$ and the second term remains finite

Moments

- The mean moments of the distribution can be found by integrating with respect to $p(x,t)$. Using Eq. (2), can determine the rate of change of these moments as

$$\frac{d\left\langle x^n(t)\right\rangle}{dt} = \int_{-\infty}^{\infty} x^n \frac{\partial p(x,t)}{\partial t}\, dx \tag{3}$$

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- To first and second order, with $\varsigma = D_r - D_l$,

$$\frac{d\langle x(t)\rangle}{dt} = 2(1-2\lambda)\varsigma p(x_b,t) - \frac{D_r}{\kappa_r}J(x_b,t) \tag{4a}$$

$$\frac{d\langle x^2(t)\rangle}{dt} = 2\left(D_l\mathbb{P}_t(x<x_b) + D_r\mathbb{P}_t(x>x_b)\right) + 4(1-2\lambda)\varsigma x_b p(x_b,t) - \frac{2D_r x_b}{\kappa_r}J(x_b,t) \tag{4b}$$

The case of many domains

- Our interest lies in when there is not just one domain but many. The generalization is straightfoward: membranes are specified by the sequence of 3-tuples $\{(x_i, \lambda_i, D_i)\}$, containing their position, probability of crossing, and diffusivity in the domain to their left, respectively:

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\sum_i \left(D_i \Theta(x_i - x) + D_{i+1}\Theta(x - x_i)\right)\frac{\partial p(x,t)}{\partial x}\right] + \sum_i (4\lambda_i - 1)\left(D_{i+1} - D_i\right) p(x_i,t)\delta'(x - x_i) + \sum_i \frac{D_{i+1}}{\kappa_{i+1}} J_i(x_i,t)\delta'(x - x_i), \quad (5)$$

where $J_i(x,t) := -D_i \partial_x p(x,t)$ is the diffusion-driven probability current in domain i

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  1. Diffusivity is bounded from below by D_0 such that, as $D \to D_0$, the probability density scales as

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  2. Given the diffusivity D in a domain, impose that the mean of the domain size, $r_i = x_i - x_{i-1}$, and hopping rate distributions depend on the diffusivity as D/D_0

References

[1] D. Das and L. Giuggioli, Journal of Statistical Mechanics: Theory and Experiment **2023**, 013201 (2023).

[2] T. Kay and L. Giuggioli, Phys. Rev. Res. **4**, L032039 (2022).

[3] P. Massignan, C. Manzo, J. A. Torreno-Pina, M. F. García-Parajo, M. Lewenstein, and G. J. Lapeyre, Phys. Rev. Lett. **112**, 150603 (2014).

The continuum limit (details)

$$
\begin{aligned}
\frac{\partial p(x,t)}{\partial t} &= \left[D_l \Theta(x_b - x) + D_r \Theta(x - x_b)\right] \frac{\partial^2 p(x,t)}{\partial x^2} \\
&+ a\frac{\Delta}{\tau_l} p(x_b, t)\delta(x - (x_b - a)) + a\frac{\Delta}{\tau_r} p(x_b + a, t)\delta(x - (x_b + 2a)) \\
&+ a\left(\frac{\lambda}{\tau_r} - \frac{1}{2\tau_l}\right) p(x_b + a, t)\delta(x - x_b) \\
&+ a\left(\frac{\lambda}{\tau_l} - \frac{1}{2\tau_r}\right) p(x_b, t)\delta(x - (x_b + a)) \qquad (7)
\end{aligned}
$$

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\frac{\partial p(x,t)}{\partial t} &= \left[D_l \Theta(x_b - x) + D_r \Theta(x - x_b)\right] \frac{\partial^2 p(x,t)}{\partial x^2} \\
&\quad + a^2 \left(2\lambda - \frac{1}{2}\right) p(x_b,t) \delta'(x - x_b) \left(\frac{1}{\tau_r} - \frac{1}{\tau_l}\right) \\
&\quad + \frac{a^2}{2} \left(\frac{1}{\tau_r} - \frac{1}{\tau_l}\right) \frac{\partial p(x_b,t)}{\partial x} \delta(x - x_b) \\
&\quad + \frac{a^3}{4} \left(\frac{1}{\tau_r} - \frac{1}{\tau_l}\right) \left[\frac{\partial p(x_b,t)}{\partial x} \delta(x - x_b) - p(x_b,t)\delta''(x - x_b)\right] \\
&\quad - \frac{a^3}{\tau_r} (2\lambda - 1) \frac{\partial p(x_b,t)}{\partial x} \delta'(x - x_b) + \mathcal{O}(a^4)
\end{aligned} \tag{8}
$$

- The fourth term vanishes since only $\kappa_i = \frac{a}{4(2\lambda-1)\tau_i}$ for $\lambda \neq 1/2$ and $D_i = a^2/2\tau_i$ remain finite in the $a, \tau_l, \tau_r \to 0$ limits