

Mean first passage time of active particles

The SDE

The SDEs governing the dynamics of the particle are

$$\frac{d}{dt} \vec{r}(t) = \vec{\xi}(t) + v_0(r) \vec{p}(t) \quad (1)$$

$$\frac{d}{dt} \vec{p}(t) = \vec{\eta}(t) \times \vec{p}(t), \quad (2)$$

with $\langle \vec{\xi}(t) \vec{\xi}(t') \rangle = 2D_t \delta(t - t') \mathbb{1}$. Averaging out the orientational degrees of freedom results in a course grained equation for the position:

$$\frac{d}{dt} \vec{r}(t) = \vec{\xi}(t) + \vec{\chi}(t). \quad (3)$$

The noise due to the course graining of the equation is approximately Gaussian with exponential time correlations, $\langle \vec{\chi}(t) \vec{\chi}(t') \rangle = \frac{1}{3} v_0(r)^2 e^{-2D_r |t-t'|} \mathbb{1} = \frac{1}{6D_r \tau} v_0(r)^2 e^{-|t-t'|/\tau} \mathbb{1}$ with $\tau = \frac{1}{2D_r}$.

The Fokker Planck Equation

Equation 3 has colored noise, but an approximate FPE can be obtained using Fox's method:

$$\partial_t P(\vec{r}, t) = D_t \nabla^2 P(\vec{r}, t) + \frac{1}{6D_r} \vec{\nabla} \cdot [v_0(r) \vec{\nabla} (v_0(r) P(\vec{r}, t))] \quad (4)$$

$$= -\frac{1}{6D_r} \vec{\nabla} \cdot [(\vec{\nabla} v_0(r)) v_0(r) P(\vec{r}, t)] + \nabla^2 \left[\left(D_t + \frac{v_0(r)^2}{6D_r} \right) P(\vec{r}, t) \right]. \quad (5)$$

Terms of order $\frac{1}{D_r^2}$ and higher are neglected.

The adjoint of the FP operator is

$$L^\dagger = \frac{1}{6D_r} v_0(r) v_0'(r) \hat{r} \cdot \vec{\nabla} + \left(D_t + \frac{v_0(r)^2}{6D_r} \right) \nabla^2, \quad (6)$$

with $\vec{\nabla} v_0(r) = \hat{r} v_0'(r)$.

The mean first passage time

The mean first passage time ($\tau(r)$) is governed by the adjoint of the FP operator:

$$\frac{1}{6D_r} v_0(r) v_0'(r) \hat{r} \cdot \vec{\nabla} \tau(r) + \left(D_t + \frac{v_0(r)^2}{6D_r} \right) \nabla^2 \tau(r) = -1, \quad (7)$$

with boundary conditions

$$\tau(a) = 0 \quad \text{and} \quad \hat{r} \cdot \vec{\nabla} \tau(r) \Big|_{r=R} = \partial_r \tau(r) \Big|_{r=R} = 0, \quad (8)$$

where a is the radius of the inner, absorbing shell, and R is the radius of the outer, reflecting shell. Using the gradient and divergence in spherical coordinates eq. 7 becomes

$$-1 = \frac{1}{6D_r} v_0(r) v_0'(r) \frac{\partial}{\partial r} \tau(r) + \left(D_t + \frac{v_0(r)^2}{6D_r} \right) r^{-2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \tau(r) \right) \quad (9)$$

$$= \left[\frac{1}{6D_r} v_0(r) v_0'(r) + \frac{2}{r} \left(D_t + \frac{v_0(r)^2}{6D_r} \right) \right] \frac{\partial}{\partial r} \tau(r) + \left(D_t + \frac{v_0(r)^2}{6D_r} \right) \frac{\partial^2}{\partial r^2} \tau(r). \quad (10)$$

The derivatives with respect to θ and ϕ are zero. Equation 9 can be written as

$$f(r) \frac{\partial}{\partial r} \tau(r) + \frac{\partial^2}{\partial r^2} \tau(r) = -g(r), \quad (11)$$

with $f(r) = \frac{v_0(r) v_0'(r)}{6D_r D_r + v_0(r)^2} + 2r^{-1}$ and $g(r) = \frac{6D_r}{6D_r D_t + v_0(r)^2}$. Equation 11 can be written as a full derivative,

$$\frac{\partial}{\partial r} \left(\exp \left[\int_b^r dx f(x) \right] \frac{\partial}{\partial r} \tau(r) \right) = -g(r) \exp \left[\int_b^r dx f(x) \right]. \quad (12)$$

Integrating both sides from r to R and using the boundary condition $\partial_r \tau(r) \Big|_{r=R} = 0$ gives

$$\frac{\partial}{\partial r} \tau(r) = \int_r^R dy g(y) \exp \left[\int_r^y dx f(x) \right], \quad (13)$$

and integrating from a to r gives the equation for $\tau(r)$:

$$\tau(r) = \int_a^r dz \int_z^R dy g(y) \exp \left[\int_z^y dx f(x) \right]. \quad (14)$$

Using the definition of $f(r)$ the exponent can be calculated.

$$\int_z^y dx f(x) = \int_z^y dr \frac{v_0(r) v_0'(r)}{6D_r D_r + v_0(r)^2} + 2r^{-1} \quad (15)$$

$$= \frac{1}{2} \int_{v_0(z)}^{v_0(y)} d[v_0(r)^2] \frac{1}{6D_r D_r + v_0(r)^2} + 2 \int_z^y dr \frac{1}{r} \quad (16)$$

$$= \frac{1}{2} \ln \left(\frac{6D_r D_r + v_0(y)^2}{6D_r D_r + v_0(z)^2} \right) + 2 \ln \left(\frac{y}{z} \right) \quad (17)$$

$$\exp \left[\int_z^y dx f(x) \right] = \frac{y^2}{z^2} \sqrt{\frac{6D_r D_r + v_0(y)^2}{6D_r D_r + v_0(z)^2}} \quad (18)$$

Plugging this in equation 14 gives

$$\tau(r) = \int_a^r dz \int_z^R dy \frac{6D_r}{6D_r D_t + v_0(y)^2} \frac{y^2}{z^2} \sqrt{\frac{6D_r D_r + v_0(y)^2}{6D_r D_r + v_0(z)^2}} \quad (19)$$

$$= \int_a^r dz z^{-2} \left(D_r + \frac{v_0(z)^2}{6D_r} \right)^{-\frac{1}{2}} \int_z^R dy y^2 \left(D_r + \frac{v_0(y)^2}{6D_r} \right)^{-\frac{1}{2}} \quad (20)$$