Mean first passage time of active particles

The SDE

The SDEs governing the dynamics of the particle are

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

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

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:

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

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:

$$\begin{aligned}\partial_t P(\vec{r},t) &= D_t\nabla^2 P(\vec{r},t) + \frac{1}{6D_r}\vec{\nabla}\cdot\left[v_0(r)\vec{\nabla}\left(v_0(r)P(\vec{r},t)\right)\right] &(4)\\ &= -\frac{1}{6D_r}\vec{\nabla}\cdot\left[\left(\vec{\nabla}v_0(r)\right)v_0(r)P(\vec{r},t)\right] + \nabla^2\left[\left(D_t + \frac{v_0(r)^2}{6D_r}\right)P(\vec{r},t)\right]. &(5)\end{aligned}$$

Terms of order $\frac{1}{D_r^2}$ and higher are neglected.
The adjoint of the FP operator is

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

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:

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

with boundary conditions

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

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

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

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

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

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

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,

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

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

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

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

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

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

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

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

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

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

Plugging this in equation 14 gives

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

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