

APPENDIX B: DIFFUSION IN A HARMONIC WELL

We consider a particles diffusing within an isotropic elastic cage of stiffness k , centered at the origin $\vec{R}_{ctr} = \vec{0}$. The cage corresponds to a potential well $U = (k/2)R^2$ and produces a binding force $F^{(ela)}(\vec{R}) = -k\vec{R}$, so that

$$\vec{F}^{(tot)} = \vec{F}^{(rnd)} + \vec{F}^{(fri)} + \vec{F}^{(ela)}. \quad (\text{B1})$$

The equation of motion can be written in the form

$$\left[\alpha \frac{d}{dt} + k \right] \vec{R}(t) = \vec{F}^{(rnd)}(t). \quad (\text{B2})$$

The response (Greens-) function $G(t)$ of this linear system is the special solution of the above equation for a δ -like driving force pulse:

$$\left[\alpha \frac{d}{dt} + k \right] G(t) = \delta(t - 0). \quad (\text{B3})$$

It is given by

$$G(t) = \frac{1}{\alpha} \theta(t - 0) e^{-(k/\alpha)t}, \quad (\text{B4})$$

where $\theta(t)$ is the Heavyside step function. The trajectory resulting from a general random force $\vec{F}^{(rnd)}(t)$ is then the convolution $\vec{R}(t) = G(t) \otimes \vec{F}^{(rnd)}(t)$, or

$$\vec{R}(t) = \frac{1}{\alpha} \int_{-\infty}^t dt' e^{-(k/\alpha)(t-t')} \vec{F}^{(rnd)}(t'). \quad (\text{B5})$$

To determine the statistical properties of the particle trajectory, we consider the correlator

$$c(\tau) = \langle \vec{R}(\tau) \vec{R}(0) \rangle = \int_{-\infty}^{\tau} dt_1 \int_{-\infty}^0 dt_2 e^{-(k/\alpha)(\tau-t_1-t_2)} \cdot \langle \vec{F}^{(rnd)}(t_1) \vec{F}^{(rnd)}(t_2) \rangle / \alpha^2 \quad (\text{B6})$$

In order to proceed, we assume that the random force is isotropic white noise on the time scale considered here:

$$\langle F_i^{(rnd)}(t) F_j^{(rnd)}(t') \rangle = \delta_{ij} \Gamma \delta(t_1 - t_2), \quad (\text{B7})$$

where Γ is the spectral power density of the noise in each spatial dimension. If the actual random force fluctuations have a variance $\overline{F^2}$ and a small, but finite correlation time τ_1 , the effective noise density is $\Gamma = 2\overline{F^2}\tau_1$ (comp. Appendix). The vectorial autocorrelation then reads

$$\langle \vec{F}^{(rnd)}(t_1) \vec{F}^{(rnd)}(t_2) \rangle = 2\Gamma \delta(t_1 - t_2). \quad (\text{B8})$$

Inserting this into Eq.(B6) yields for the spatial correlator

$$\langle \vec{R}(\tau) \vec{R}(0) \rangle = \frac{\Gamma}{k\alpha} e^{-(k/\alpha)\tau}. \quad (\text{B9})$$

Its value at zero lag time $c(0) = \langle R^2 \rangle = \frac{\Gamma}{k\alpha}$ describes the variance of the spatial fluctuations relative to the origin of the coordinate system. The MSD can be easily computed from the above correlator, using the relation

$$\begin{aligned} \overline{\Delta R^2}(\tau) &= \langle (\vec{R}(\tau) - \vec{R}(0))^2 \rangle \\ &= 2 \left(\langle R^2 \rangle - \langle \vec{R}(\tau) \vec{R}(0) \rangle \right) \\ &= \frac{2\Gamma}{k\alpha} (1 - e^{-(k/\alpha)\tau}). \end{aligned} \quad (\text{B10})$$

APPENDIX C: ANGULAR CORRELATIONS AND MSD

Since the close relation between directionality and diffusivity is an important point here, we will next derive an explicit relation between the turning angle distributions and the MSD curves. Following the arguments in Ref.(.), we first consider for this purpose a simple random walk model with angular correlations:

Assume the two-dimensional position \vec{R}_n of a particle at time step n is the sum of random displacements, $\vec{R}_n = \sum_{m=1}^n \Delta \vec{R}_m$. For simplicity, let the length λ of each step be constant. When the absolute angular direction of step n is denoted by θ_n , the displacement vector can be written as $\Delta \vec{R}_m = \lambda(\cos \theta_m, \sin \theta_m)$. The turning angle ϕ_n between successive steps $n-1$ and n is defined as $\phi_n = \theta_n - \theta_{n-1}$ and is supposed to obey a given probability distribution $P(\phi_n)$.

A dimensionless parameter γ is introduced as the average cosine of the turning angle:

$$\gamma = \langle \cos \phi_n \rangle = \int_{-\pi}^{+\pi} d\phi P(\phi) \cos \phi. \quad (\text{C1})$$

If the particle is moving always in the same direction (perfect angular correlation, $P(\phi) \propto \delta(\phi - 0)$), we have $\gamma = 1$. If it jumps back and forth (perfect angular anticorrelation, $P(\phi) \propto \delta(\phi \pm \pi)$), one obtains $\gamma = -1$. Without correlations ($P(\phi) = \text{const}$) the parameter yields $\gamma = 0$. Since successive turning angles are statistically independent, it is straight forward to show that for larger 'lag times' $s > 1$, the average cosine of the turning angle satisfies

$$\langle \cos(\theta_n - \theta_{n-s}) \rangle = \gamma^s. \quad (\text{C2})$$

The MSD of the correlated walker can now be evaluated as follows:

$$\begin{aligned} \overline{R_s^2} &= \left\langle \sum_{m=1}^s \Delta \vec{R}_m \sum_{n=1}^s \Delta \vec{R}_n \right\rangle \\ &= \sum_{k=1}^s \langle \Delta \vec{R}_k^2 \rangle + 2 \sum_{m=1}^s \sum_{n>m}^s \langle \Delta \vec{R}_m \cdot \Delta \vec{R}_n \rangle \\ &= s\lambda^2 + 2\lambda^2 \sum_{m=1}^s \sum_{n>m}^s \langle \cos(\phi_n - \phi_m) \rangle. \end{aligned} \quad (\text{C3})$$