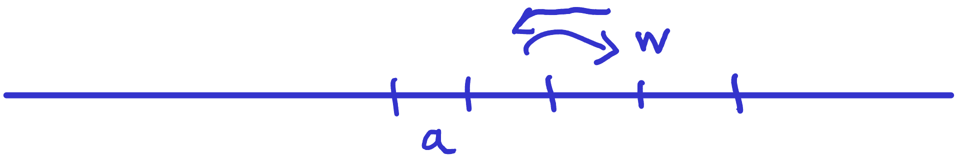
# PHYS 320/420: Lecture 5

MSD: $\langle \Delta_i^2 \rangle_t = a^2\left(\langle i^2\rangle_t - 2 i_0 \langle i \rangle_t + i_0^2\right)$

$\Delta_i = a(i - i_0)$




$\Omega_{ij}$ = trans. rate $j \to i$ $\quad (i \neq j)$

$$\frac{d\langle i^n\rangle_t}{dt} = \sum_j \sum_{i\neq j} (i^n - j^n)\,\Omega_{ij}\,P_j$$

$$\Omega = \begin{pmatrix} -w & w & & & \\ w & -2w & w & & \\ & w & -2w & w & \\ & & & \ddots & \end{pmatrix}$$

$\sum_i P_i(t) = 1$

$\frac{d}{dt}\sum_i P_i(t) = 0$

$\Rightarrow n=1$: $\quad \frac{d\langle i \rangle_t}{dt} = w P_1(t) - w P_N(t)$

$n=2$: $\quad \frac{d\langle i^2\rangle_t}{dt} = 2w\sum_{j=2}^{N-1} P_j(t) + 3w P_1(t) + (1-2N) w P_N(t)$

assume $N$ is large ($a$ small) &
molecule is far from walls

$$P_1(t) \approx 0 \qquad P_N(t) \approx 0$$

$$\Rightarrow 1 = \sum_{j=1}^{N} P_j(t) \cong \sum_{j=2}^{N-1} P_j(t)$$

$$\Rightarrow \frac{d\langle i\rangle_t}{dt} = 0 , \qquad \frac{d\langle i^2\rangle_t}{dt} = 2w$$

no bias toward left or right

initial condition: all particles in our ensemble start $i_0$ at $t=0$:

$$\langle i\rangle_0 = i_0 \qquad \langle i^2\rangle_0 = i_0^2$$

$$\langle i\rangle_t = i_0 \qquad \langle i^2\rangle_t = 2wt + i_0^2$$

$$\langle \Delta_i^2\rangle_t = 2wa^2t \qquad \text{MSD}$$

$$\equiv 2Dt$$

$D = wa^2$ diffusion constant

units: $\frac{\text{length}^2}{\text{time}}$

this result is for 1 dimension ($\hat{x}$) but by symmetry you would get same answer for other axes

$$\vec{r} = a\,(i, j, k) \qquad \langle \Delta_j^2 \rangle_t = 2Dt$$

$$\vec{r}_0 = a\,(i_0, j_0, k_0) \qquad \langle \Delta_k^2 \rangle_t = 2Dt$$

$$\Delta_j = a\,(j - j_0)$$

$$\Delta_k = a\,(k - k_0)$$

3 D MSD: $\langle (\vec{r} - \vec{r}_0)^2 \rangle_t$

$$= \langle a^2 (i - i_0)^2 + a^2 (j - j_0)^2 + a^2 (k - k_0)^2 \rangle$$

$$= 6Dt$$

rough timescale for diffusion to cover a distance $L$ in one dim:

$$\text{MSD} \sim L^2 = 2Dt \Rightarrow t \sim \frac{L^2}{2D}$$

Survey of diffusion coeff. scales in biology:

Stokes law: sphere of radius $R$ in a liquid of viscosity $\eta$ at temp. $T$

$$w a^2 = D = \frac{k_B T}{6\pi\eta R}$$

$k_B = 1.38 \times 10^{-23} \frac{J}{K}$

$T = 298\ K$

$\eta = 0.89 \times 10^{-3}$ Pa·s for water

$R = 1\,nm$

$D = 245\ \mu m^2/s$