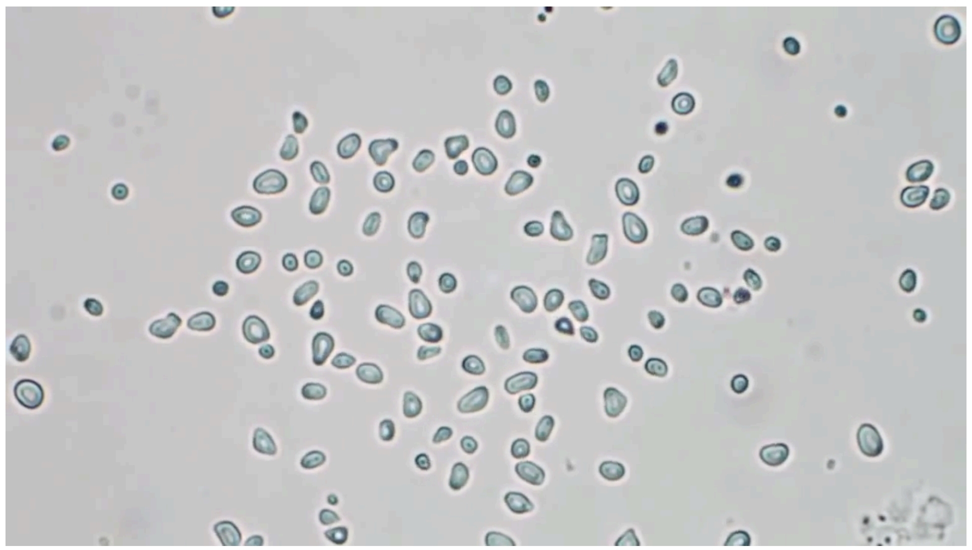
MAE 545: Lecture 17 (4/10)

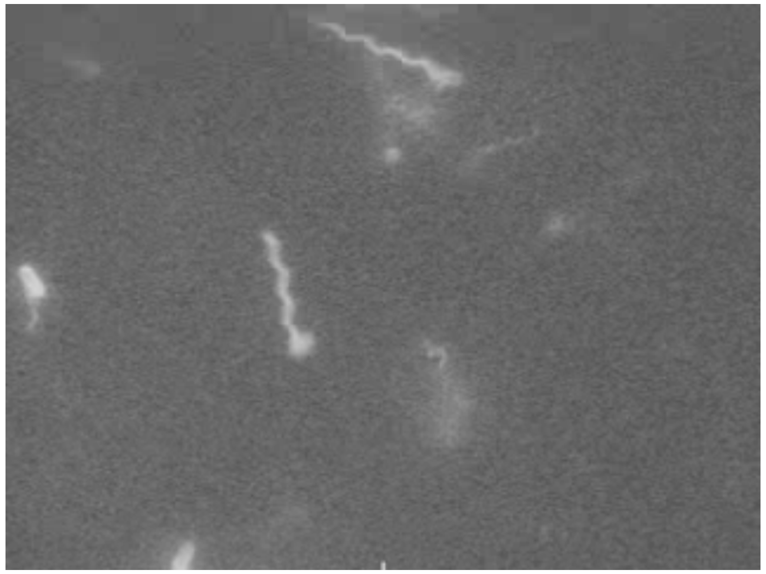
Random walks

Random walks

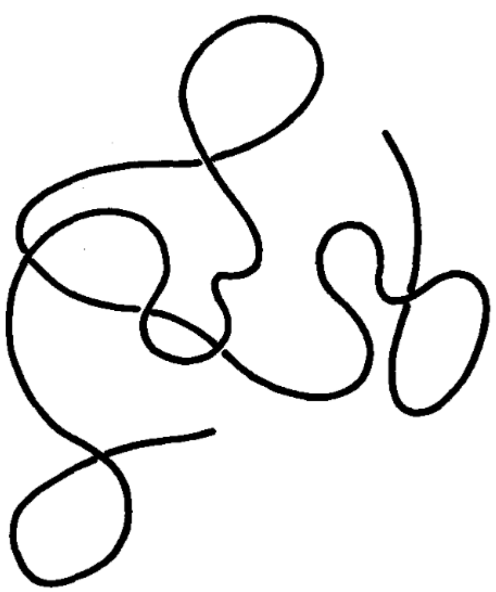
Brownian motion



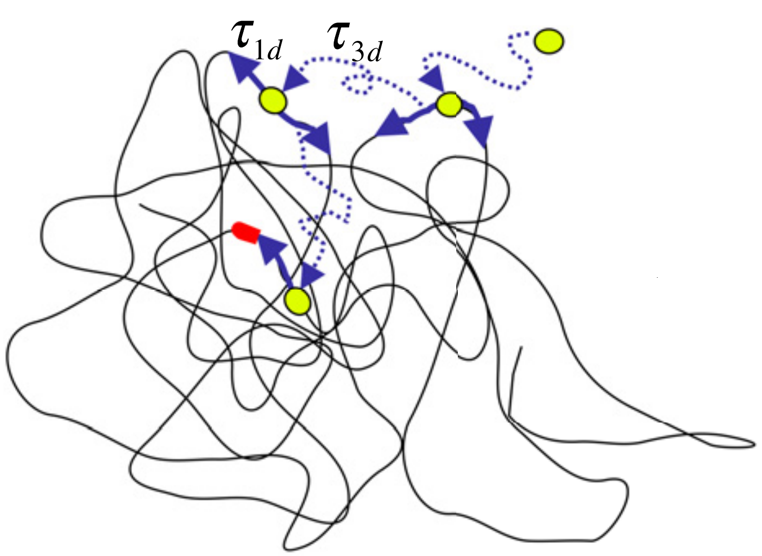
Swimming of E. coli



Polymer random coils

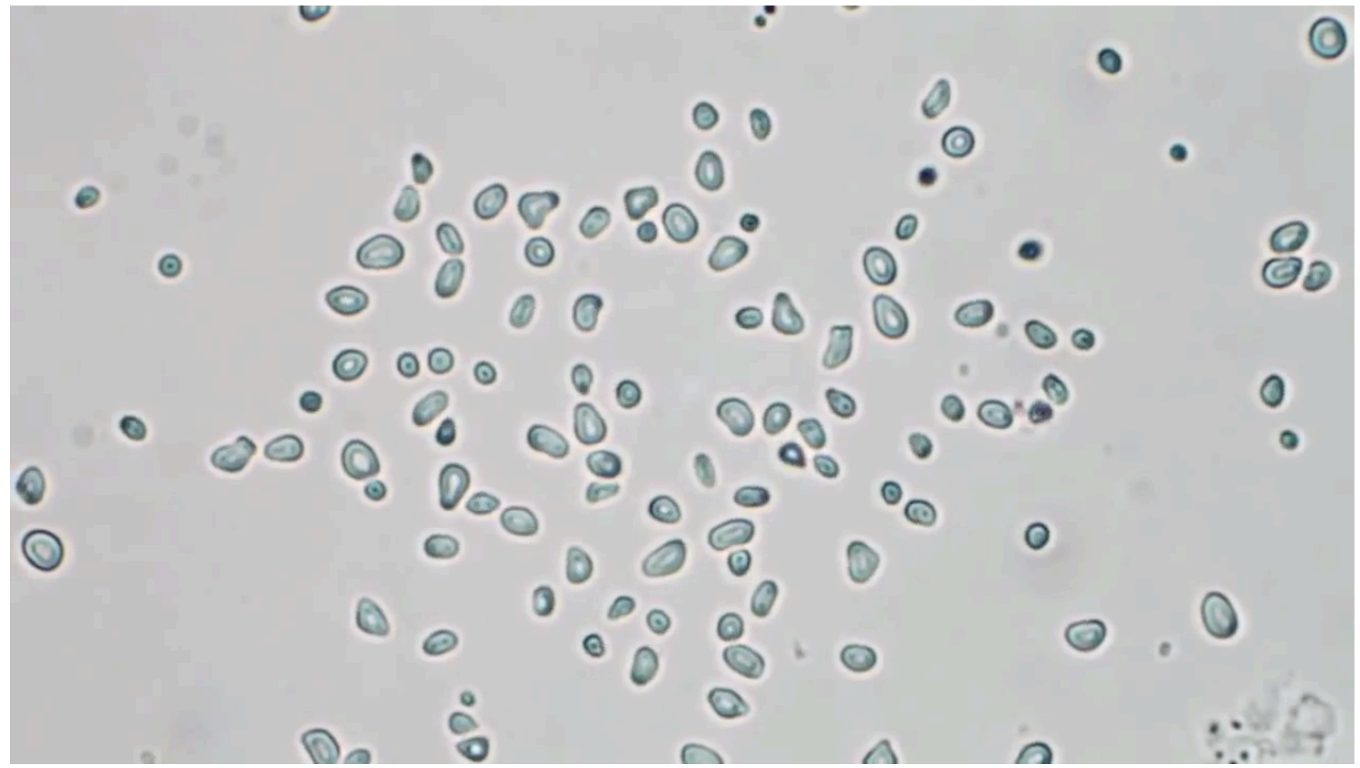


Protein search for a binding site on DNA



Brownian motion of small particles

1827 Robert Brown: observed irregular motion of small pollen grains suspended in water

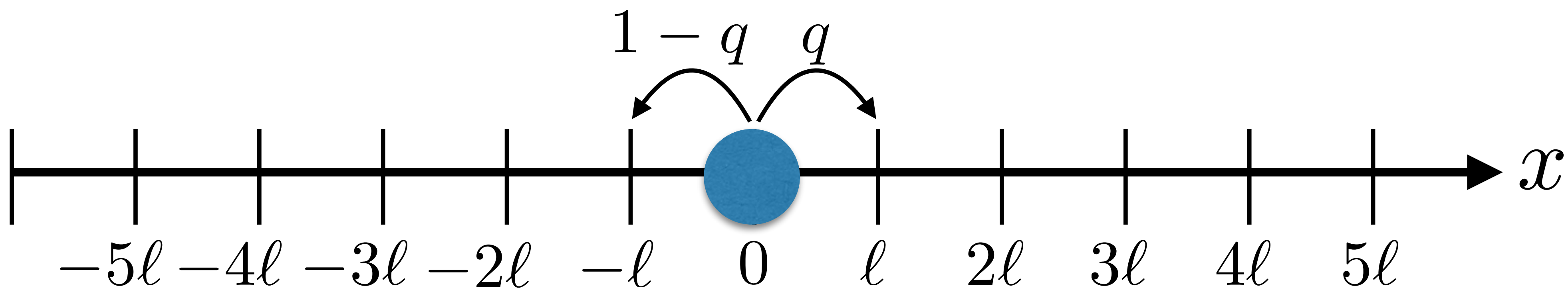


$| \approx 10 \mu m$

https://www.youtube.com/watch?v=R5t-oA796to

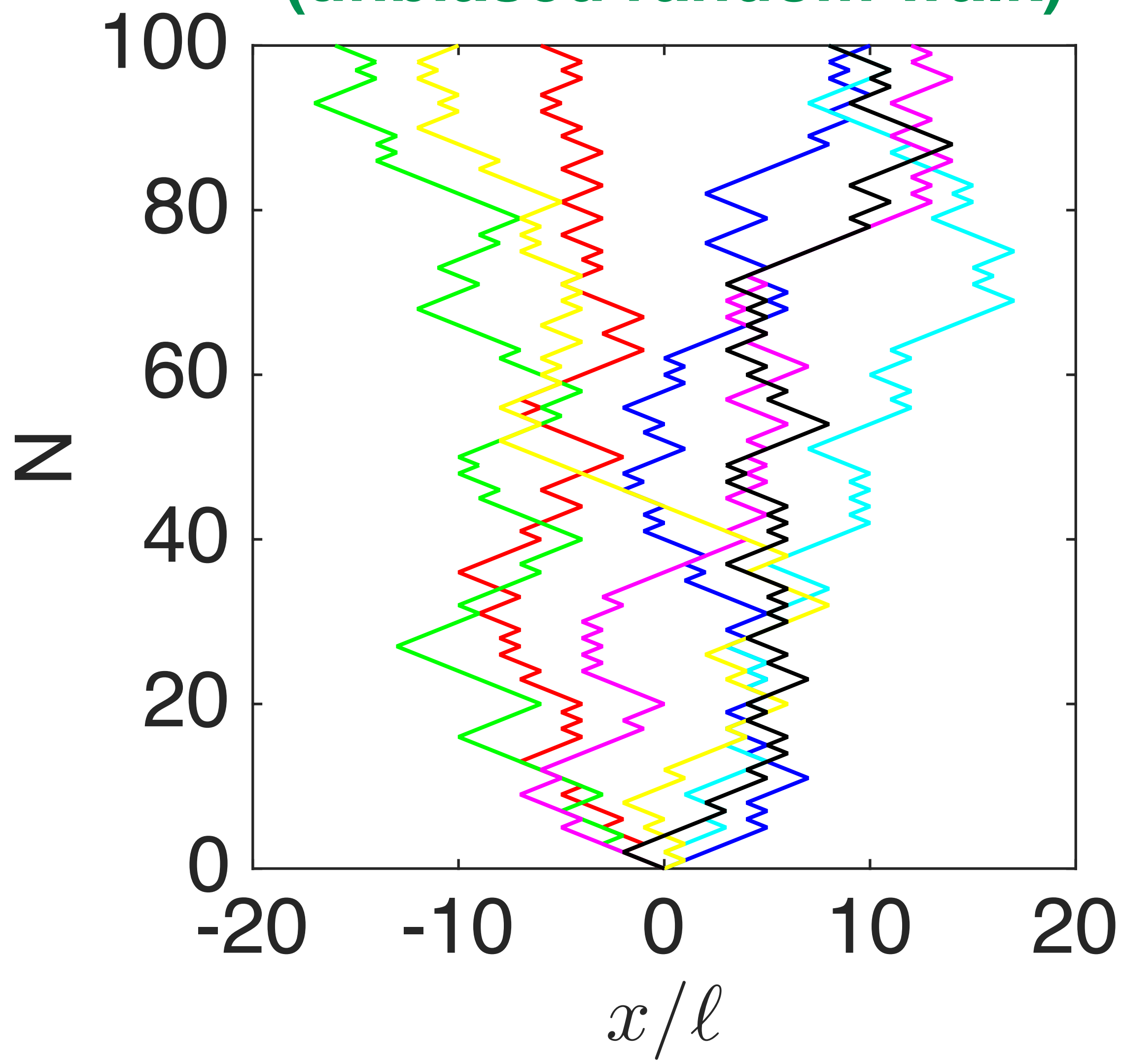
1905-06 Albert Einstein, Marian Smoluchowski: microscopic description of Brownian motion and relation to diffusion equation

Random walk on a 1D lattice

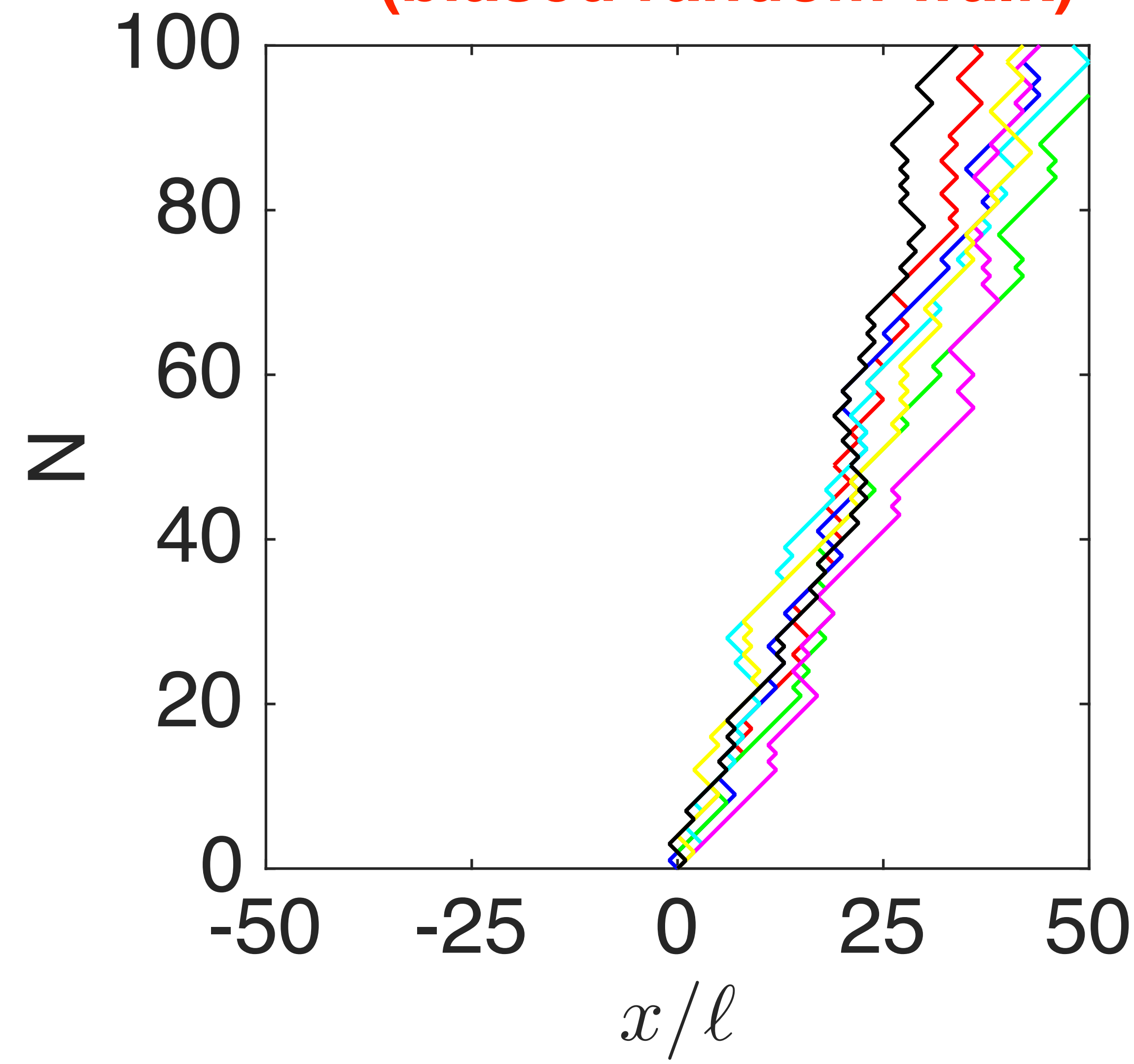


At each step particle jumps to the right with probability q and to the left with probability 1-q.

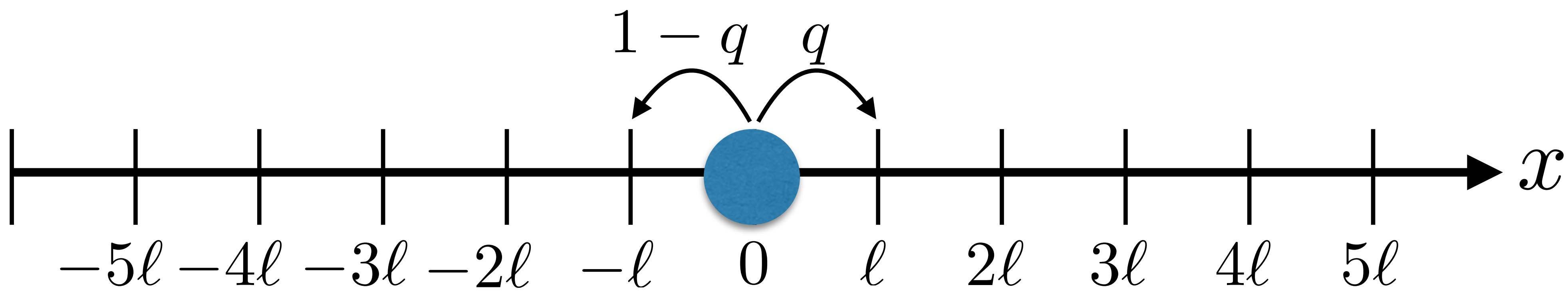
sample trajectories for q=1/2 (unbiased random walk)



sample trajectories for q=2/3 (biased random walk)



Random walk on a 1D lattice



At each step particle jumps to the right with probability q and to the left with probability 1-q.

What is the probability *p(x,N)* that we find particle at position *x* after *N* jumps?

Probability that particle makes *k* jumps to the right and *N-k* jumps to the left obeys the binomial distribution

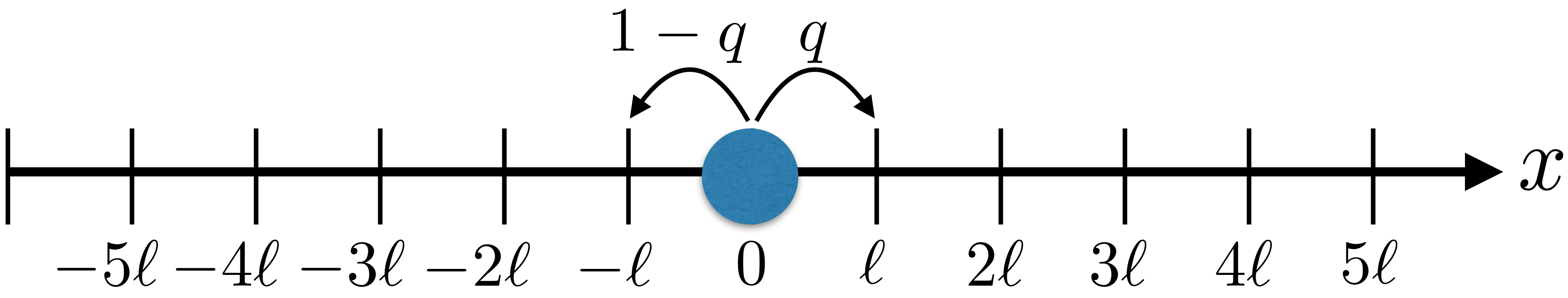
$$\boxed{p(k,N) = \binom{N}{k} q^k (1-q)^{N-k}}$$

Relation between *k* and particle position *x*:

$$x = k\ell - (N-k)\ell = (2k-N)\ell$$

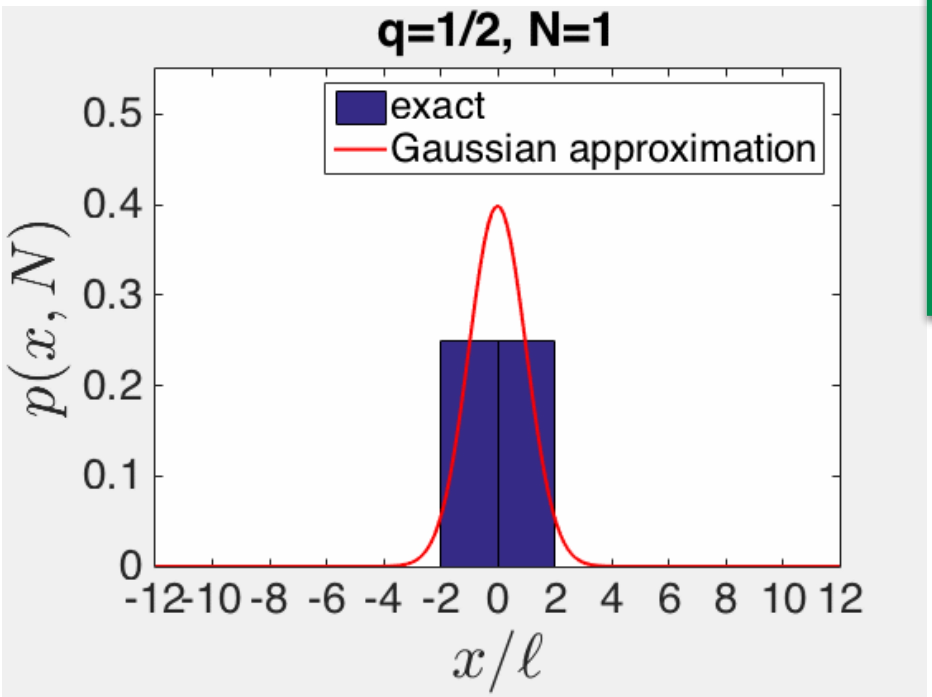
$$k = \frac{1}{2}\left(N + \frac{x}{\ell}\right)$$

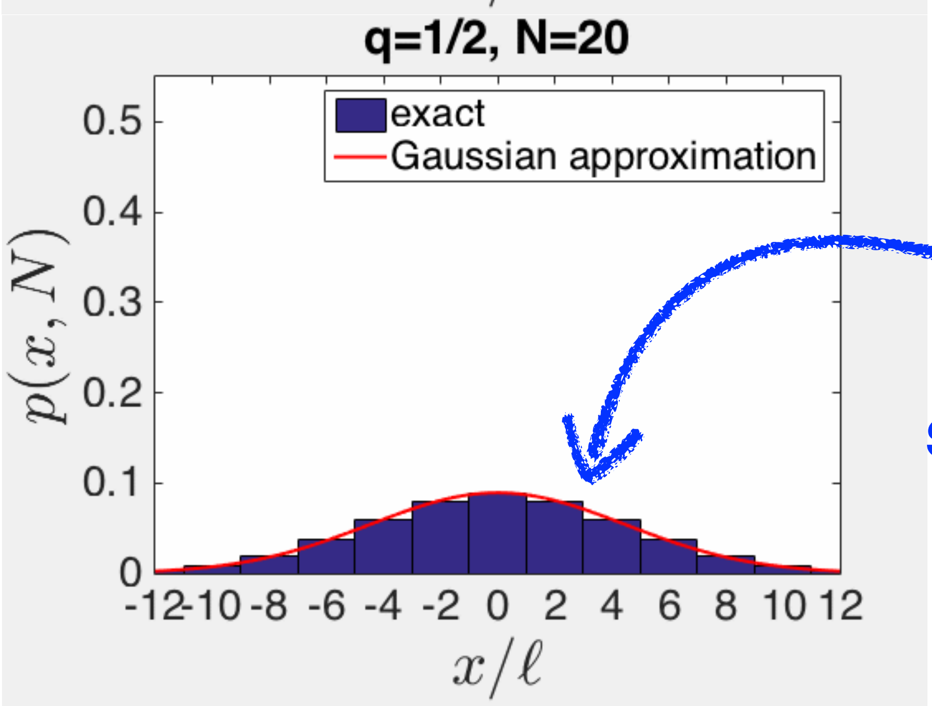
Random walk on a 1D lattice



unbiased random walk

biased random walk

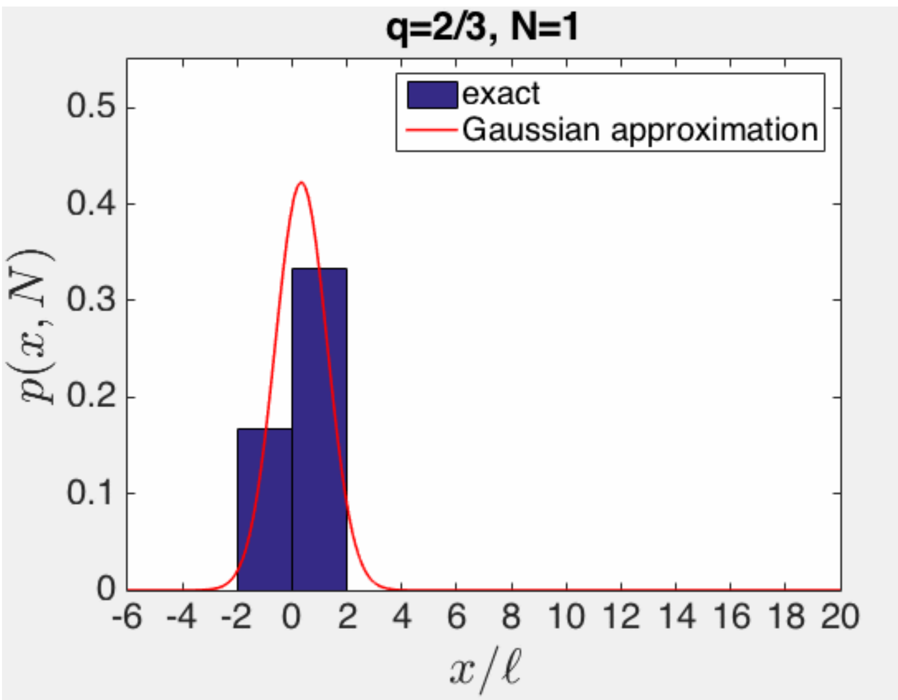


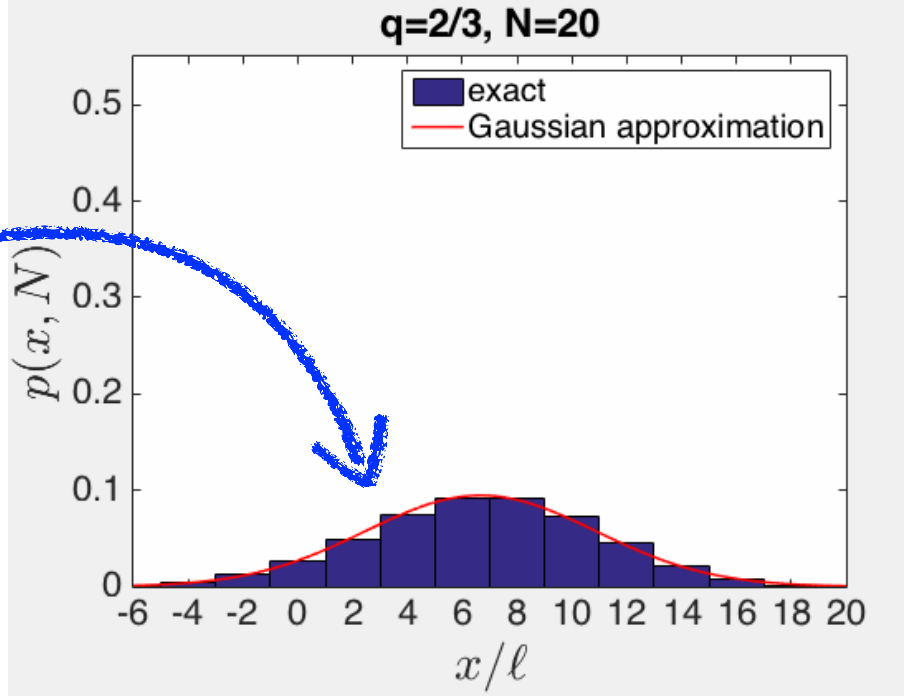


$$p(k, N) = \binom{N}{k} q^k (1-q)^{N-k}$$

$$k = \frac{1}{2}\left(N + \frac{x}{\ell}\right)$$

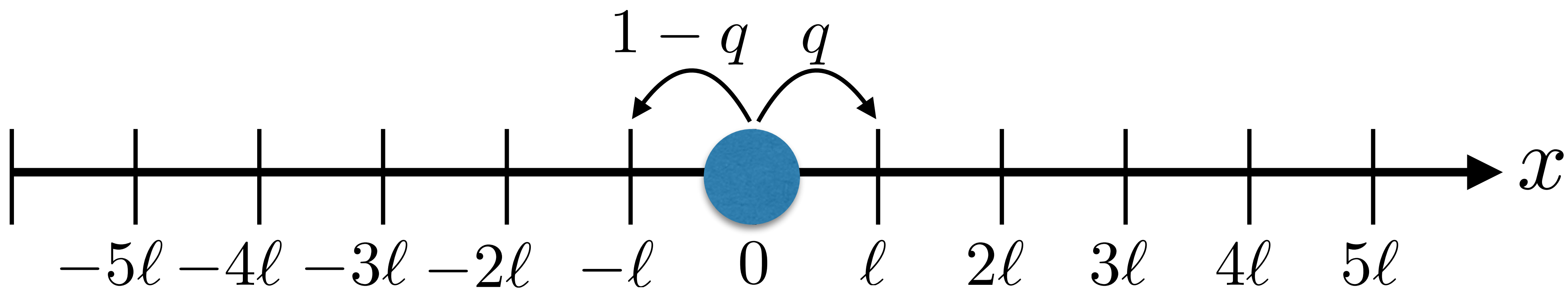
Note: exact discrete distribution has been made continuous by replacing discrete peaks with boxes whose area corresponds to the same probability.





after several steps the probability distribution spreads out and becomes approximately Gaussian

Gaussian approximation for p(x,N)



Position *x* after *N* jumps can be expressed as the sum of individual jumps $x_i \in \{-\ell, \ell\}$.

$$x = \sum_{i=1}^{N} x_i$$

Mean value averaged over all possible random walks

$$\langle x \rangle = \sum_{i=1}^{N} \langle x_i \rangle = N \langle x_1 \rangle = N \left(q\ell - (1-q)\ell \right)$$

$$\boxed{\langle x \rangle = N\ell \left(2q - 1 \right)}$$

Variance averaged over all possible random walks

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = N\sigma_1^2 = N \left(\langle x_1^2 \rangle - \langle x_1 \rangle^2 \right)$$

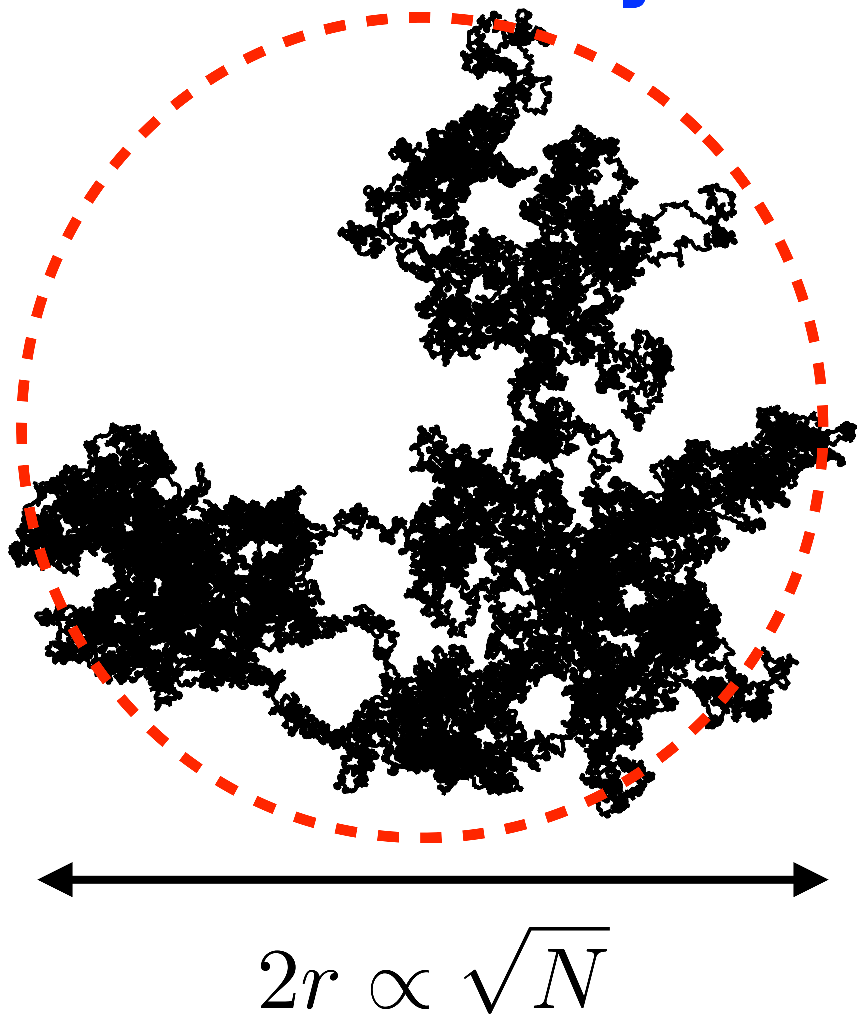
$$\sigma^2 = N \left(q\ell^2 + (1-q)\ell^2 - \langle x_1 \rangle^2 \right)$$

$$\boxed{\sigma^2 = 4N\ell^2 q(1-q)}$$

According to the central limit theorem p(x,N) approaches Gaussian distribution for large N:

$$\boxed{p(x,N) \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\langle x \rangle)^2/(2\sigma^2)}}$$

Number of distinct sites visited by unbiased random walks



Total number of sites inside explored region after *N* steps

1D $N_{\text{tot}} \propto \sqrt{N}$

2D $N_{\text{tot}} \propto N$

3D $N_{\text{tot}} \propto N\sqrt{N}$

In 1D and 2D every site gets visited after a long time

In 3D some sites are never visited even after a very long time!

Shizuo Kakutani: "A drunk man will find his way home, but a drunk bird may get lost forever."

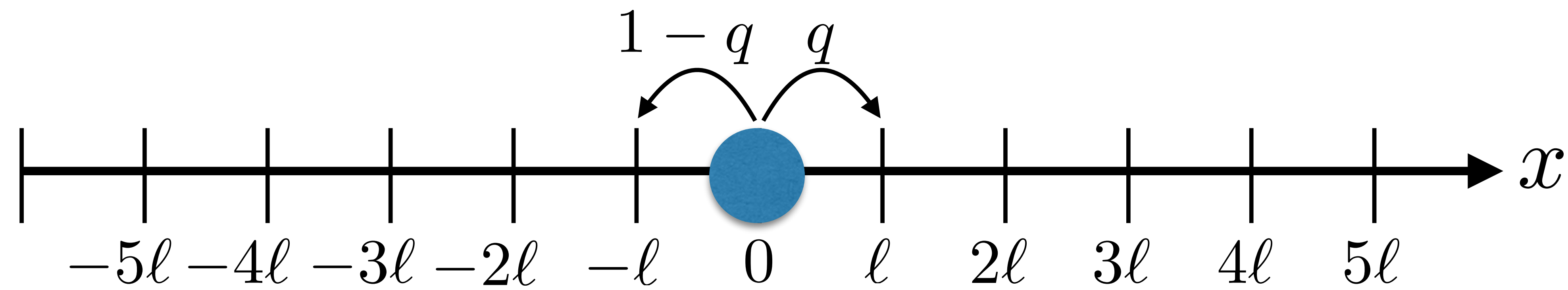
Number of distinct visited sites after *N* steps

1D $N_{\text{vis}} \approx \sqrt{8N/\pi}$

2D $N_{\text{vis}} \approx \pi N/\ln(8N)$

3D $N_{\text{vis}} \approx 0.66N$

Master equation



Master equation provides recursive relation for the evolution of probability distribution, where $\Pi(x,y)$ describes probability for a jump from *y* to *x*.

$$p(x, N+1) = \sum_y \Pi(x,y) p(y,N)$$

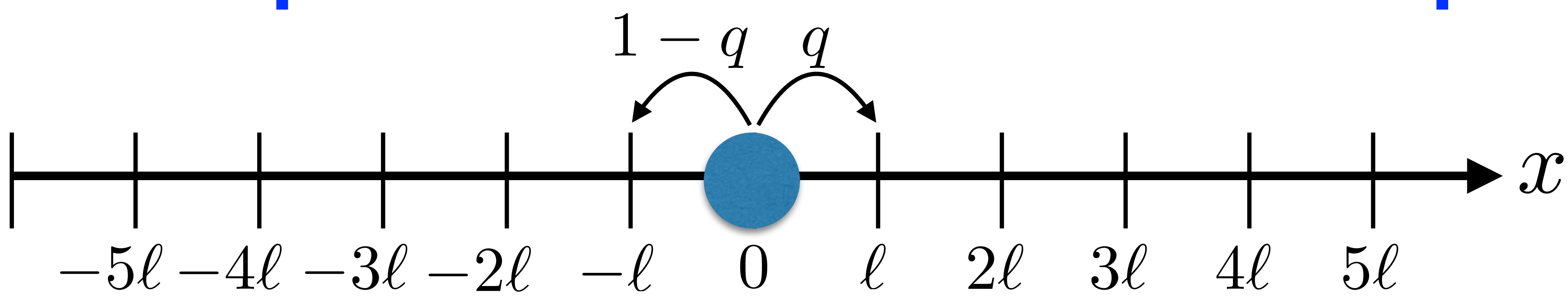
For our example the master equation reads:

$$p(x, N+1) = q\, p(x-\ell, N) + (1-q)\, p(x+\ell, N)$$

Initial condition: $p(x,0) = \delta(x)$

Probability distribution *p*(*x*,*N*) can be easily obtained numerically by iteratively advancing the master equation.

Master equation and Fokker-Planck equation



Assume that jumps occur in regular small time intervals: Δt

Master equation:

$$\boxed{p(x, t+\Delta t) = q\, p(x-\ell, t) + (1-q)\, p(x+\ell, t)}$$

In the limit of small jumps and small time intervals, we can Taylor expand the master equation to derive an approximate drift-diffusion equation:

$$p + \Delta t \frac{\partial p}{\partial t} = q \left(p - \ell \frac{\partial p}{\partial x} + \frac{1}{2} \ell^2 \frac{\partial^2 p}{\partial x^2} \right) + (1-q) \left(p + \ell \frac{\partial p}{\partial x} + \frac{1}{2} \ell^2 \frac{\partial^2 p}{\partial x^2} \right)$$

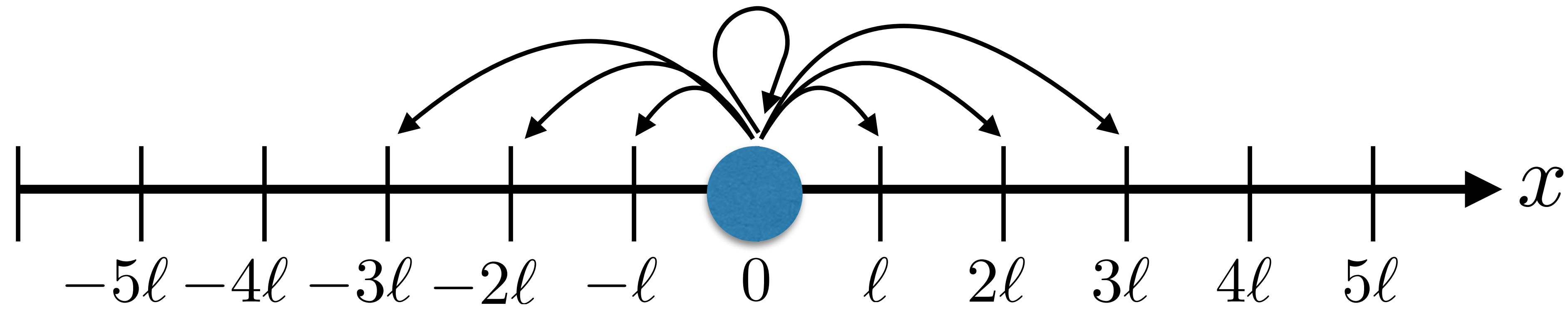
Fokker-Planck equation:

$$\boxed{\frac{\partial p}{\partial t} = -v \frac{\partial p}{\partial x} + D \frac{\partial^2 p}{\partial x^2}}$$

drift velocity $v = (2q-1)\dfrac{\ell}{\Delta t}$

diffusion coefficient $D = \dfrac{\ell^2}{2\Delta t}$

Fokker-Planck equation



In general the probability distribution Π of jump lengths *s* can depend on the particle position *x*

$$\Pi(s|x)$$

Generalized master equation:

$$p(x, t+\Delta t) = \sum_s \Pi(s|x-s)\, p(x-s, t)$$

Again Taylor expand the master equation above to derive the Fokker-Planck equation:

$$\boxed{\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big[v(x)p(x,t)\Big] + \frac{\partial^2}{\partial x^2}\Big[D(x)p(x,t)\Big]}$$

drift velocity
(external fluid flow, external potential)

$$v(x) = \sum_s \frac{s}{\Delta t}\Pi(s|x) = \frac{\langle s(x)\rangle}{\Delta t}$$

diffusion coefficient
(e.g. position dependent temperature)

$$D(x) = \sum_s \frac{s^2}{2\Delta t}\Pi(s|x) = \frac{\langle s^2(x)\rangle}{2\Delta t}$$

Lévy flights

Probability of jump lengths in *D* dimensions

$$\boxed{\Pi(\vec{s}) = \begin{cases} C|\vec{s}|^{-\alpha}, & |\vec{s}| > s_0 \\ 0, & |\vec{s}| < s_0 \end{cases}}$$

Normalization condition

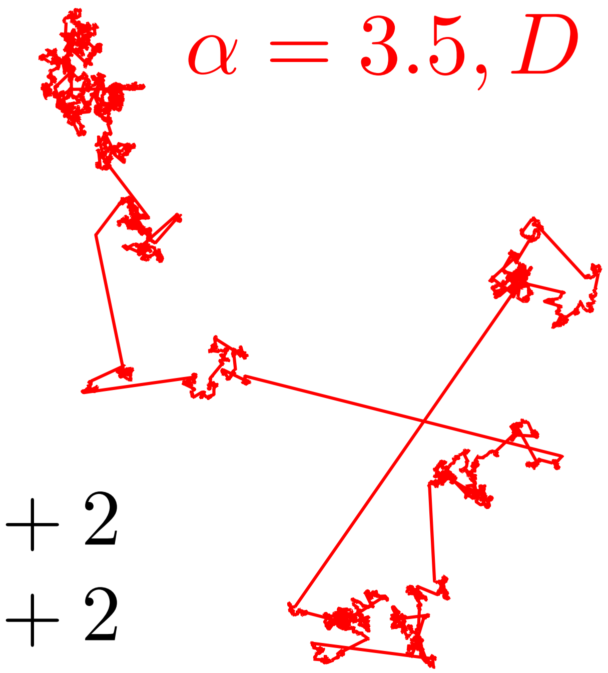
$$\int d^D\vec{s}\,\Pi(\vec{s}) = 1 \longrightarrow \alpha > D$$

Moments of distribution

$$\langle \vec{s} \rangle = 0 \qquad \langle \vec{s}^{\,2} \rangle = \begin{cases} A_D s_0^2, & \alpha > D+2 \\ \infty, & \alpha < D+2 \end{cases}$$

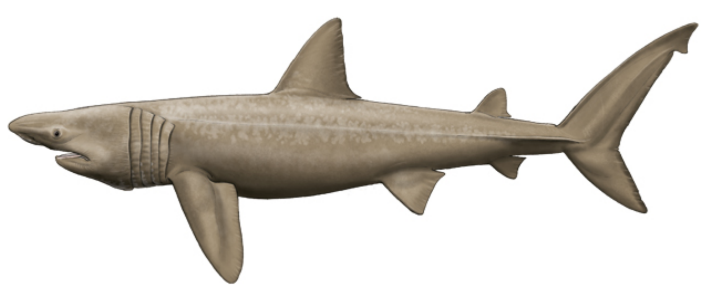
Lévy flight trajectory

$\alpha = 3.5, D = 2$



2D random walk trajectory

Lévy flights are better strategy than random walk for finding prey that is scarce



D. W. Sims *et al.*
Nature **451**, 1098-1102 (2008)

Probability current

Fokker-Planck equation

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big[v(x)p(x,t)\Big] + \frac{\partial^2}{\partial x^2}\Big[D(x)p(x,t)\Big]$$

Conservation law of probability (no particles created/removed)

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}$$

Probability current:

$$\boxed{J(x,t) = v(x)p(x,t) - \frac{\partial}{\partial x}\Big[D(x)p(x,t)\Big]}$$

Note that for the steady state distribution, where $\partial p^*(x,t)/\partial t \equiv 0$ the steady state current is constant and independent of *x*

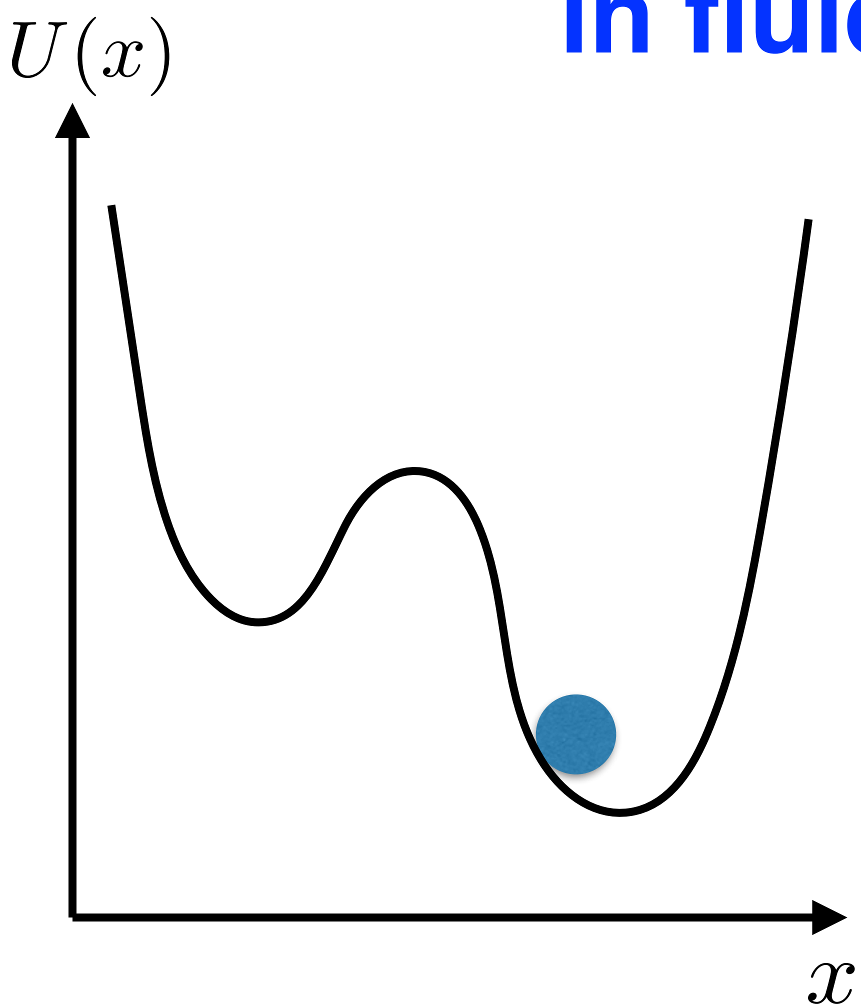
$$J^* \equiv v(x)p^*(x) - \frac{\partial}{\partial x}\Big[D(x)p^*(x)\Big] = \text{const}$$

Equilibrium probability distribution:

If we don't create/remove particles at boundaries then *J=0** $\longrightarrow$

$$\boxed{p^*(x) \propto \frac{1}{D(x)} \exp\left[\int_{-\infty}^{x} dy \frac{v(y)}{D(y)}\right]}$$

Spherical particle suspended in fluid in external potential



Newton's law:

$$m\frac{\partial^2 x}{\partial t^2} = -\lambda v(x) - \frac{\partial U(x)}{\partial x} + F_r$$

fluid drag | external potential force | random Brownian force

For simplicity assume overdamped regime: $\frac{\partial^2 x}{\partial t^2} \approx 0$

Drift velocity averaged over time $\langle v(x)\rangle = -\frac{1}{\lambda}\frac{\partial U(x)}{\partial x}$

R	particle radius
η	fluid viscosity
$\lambda = 6\pi\eta R$	Stokes drag coefficient
k_B	Boltzmann constant
T	temperature
D	diffusion constant

Equilibrium probability distribution

$$p^*(x) = Ce^{-U(x)/\lambda D} = Ce^{-U(x)/k_B T}$$

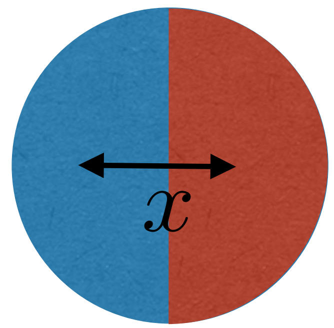
(see previous slide) (equilibrium physics)

Einstein - Stokes equation

$$\boxed{D = \frac{k_B T}{\lambda} = \frac{k_B T}{6\pi\eta R}}$$

Translational and rotational diffusion for particles suspended in liquid

Translational diffusion



$$\langle x^2 \rangle = 2D_T t$$

Stokes viscous drag: $\lambda_T = 6\pi\eta R$

Einstein - Stokes relation

$$\boxed{D_T = \frac{k_B T}{6\pi\eta R}}$$

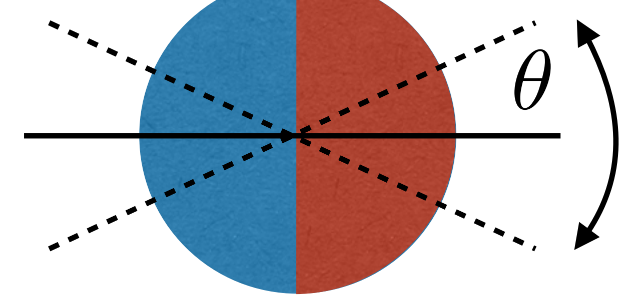
Time to move one body length in water at room temperature

$$\langle x^2 \rangle \sim R^2 \longrightarrow t \sim \frac{3\pi\eta R^3}{k_B T}$$

$$R \sim 1\mu\text{m} \longrightarrow t \sim 1\text{s}$$

$$R \sim 1\text{mm} \longrightarrow t \sim 100\,\text{years}$$

Rotational diffusion



$$\langle \theta^2 \rangle = 2D_R t$$

Stokes viscous drag: $\lambda_R = 8\pi\eta R^3$

Einstein - Stokes relation

$$\boxed{D_R = \frac{k_B T}{8\pi\eta R^3}}$$

Time to rotate by 90⁰ in water at room temperature

$$\langle \theta^2 \rangle \sim 1 \longrightarrow t \sim \frac{4\pi\eta R^3}{k_B T}$$

Boltzmann constant $k_B = 1.38 \times 10^{-23}\text{J/K}$

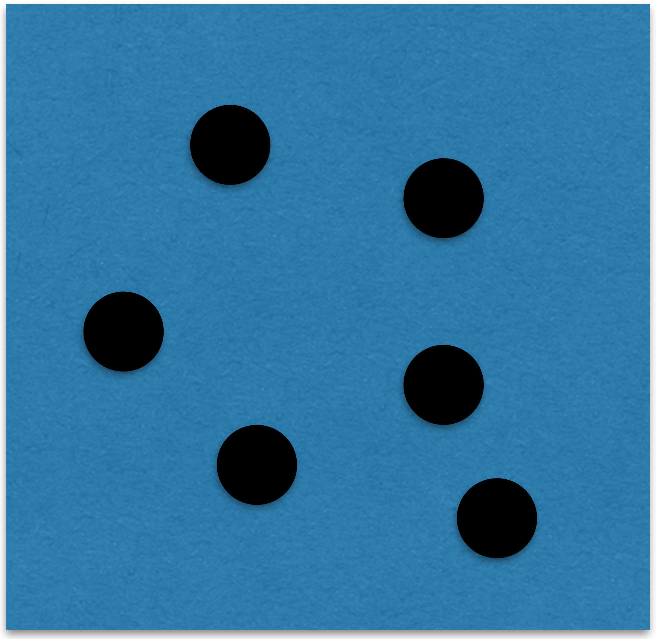
water viscosity $\eta \approx 10^{-3}\text{kg}\,\text{m}^{-1}\text{s}^{-1}$

room temperature $T = 300\text{K}$

Fick's laws

Adolf Fick 1855

N noninteracting Brownian particles



Local concentration of particles

$$c(x,t) = Np(x,t)$$

Fick's laws are equivalent to Fokker-Plank equation

First Fick's law

Flux of particles

$$\boxed{J = vc - D\frac{\partial c}{\partial x}}$$

Second Fick's law

Diffusion of particles

$$\boxed{\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} = -\frac{\partial}{\partial x}\left[vc\right] + \frac{\partial}{\partial x}\left[D\frac{\partial c}{\partial x}\right]}$$

Generalization to higher dimensions

$$\vec{J} = c\vec{v} - D\vec{\nabla}c$$

$$\frac{\partial c}{\partial t} = -\vec{\nabla}J = -\vec{\nabla}\cdot(c\vec{v}) + \vec{\nabla}\cdot(D\vec{\nabla}c)$$

Further reading