Modelling of Complex Systems

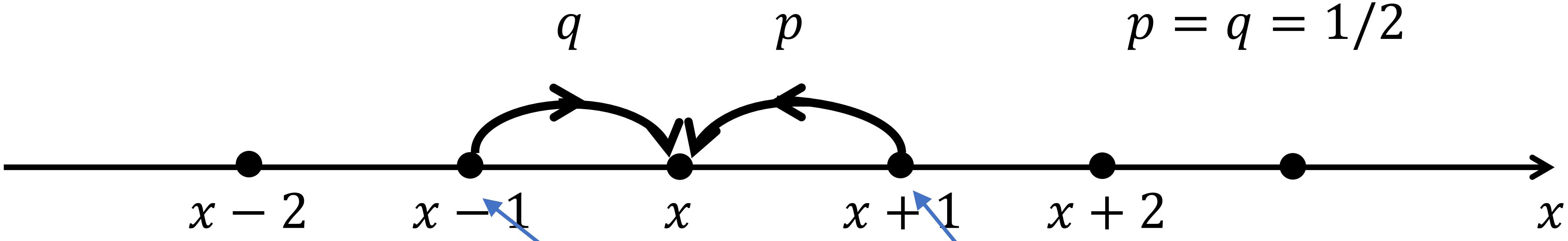
One-dimensional Random Walks

Master equation approach

Random walks and diffusion

Master Equation

We consider random walks of a particle on a 1D-lattice with symmetric jumps



We introduce $P(x,t)$ as the probability that at time t the particle stay at a point x. Let us find a relation between $P(x,t)$ and $P(x,t+1)$.

The **master equation** is:

$$P(x,t+1) = \frac{1}{2}P(x-1,t) + \frac{1}{2}P(x+1,t)$$

Using the initial condition $P(x,t=0) = \delta_{x,0}$, we can find sequentially one by one $P(x,t=1), P(x,2), \ldots$. For example,

$$P(x,1) = \frac{1}{2}P(x-1,0) + \frac{1}{2}P(x+1,0) = \frac{1}{2}\delta_{x-1,0} + \frac{1}{2}\delta_{x+1,0} = \frac{1}{2}\delta_{x,1} + \frac{1}{2}\delta_{x,-1}$$

We want to find the distribution function $P(x,t)$ over x at $t \gg 1$.
Let us assume that $P(x,t)$ varies slowly in time and space.
Then we can use the Taylor expansion:

$$P(x, t + \Delta t) = P(x,t) + \frac{\partial P(x,t)}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 P(x,t)}{\partial t^2}(\Delta t)^2 + \cdots$$

$$P(x + \Delta x, t) = P(x,t) + \frac{\partial P(x,t)}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 P(x,t)}{\partial x^2}(\Delta x)^2 + \cdots$$

where $\Delta t = \pm 1, \Delta x = \pm 1$. Substituting this Taylor expansion into the master equation, we get

$$\cancel{P(x,t)} + \frac{\partial P(x,t)}{\partial t} + \cancel{\frac{1}{2}\frac{\partial^2 P(x,t)}{\partial t^2}}$$

$$= \cancel{\frac{1}{2}P(x,t)} - \cancel{\frac{1}{2}\frac{\partial P(x,t)}{\partial x}} + \frac{1}{4}\frac{\partial^2 P(x,t)}{\partial x^2} + \cancel{\frac{1}{2}P(x,t)} + \cancel{\frac{1}{2}\frac{\partial P(x,t)}{\partial x}} + \frac{1}{4}\frac{\partial^2 P(x,t)}{\partial x^2}$$

Assuming that $\frac{\partial^2 P(x,t)}{\partial t^2} \ll \frac{\partial^2 P(x,t)}{\partial x^2}$, we obtain

$$\frac{\partial P(x,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 P(x,t)}{\partial x^2}$$

It is the well-known **diffusion equation** in a one-dimensional lattice.

In the general case

$$\frac{\partial P(x,t)}{\partial t} = D\,\frac{\partial^2 P(x,t)}{\partial x^2}$$

where D is the diffusion coefficient. In a regular lattice $D = 1/2$.

The general solution of the diffusion equation in one dimension is

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$

$P(x,t)$ represents the density of particles at point x at time t.

This means that random walks are the stochastic process responsible for diffusion.

Fick's laws of diffusion

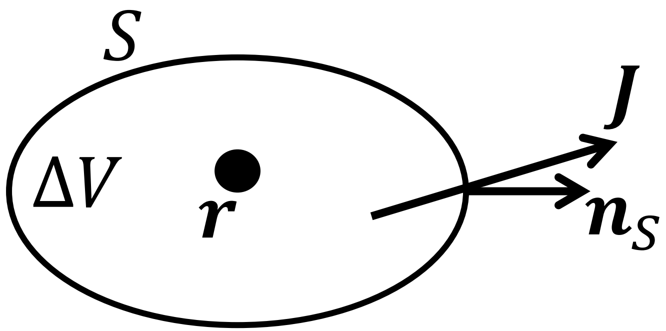
The diffusion equation is a consequence of the particle conservation.

Particles do not appear nor disappear. They only move from one region into another.

Let $\rho(\boldsymbol{r}, t)$ be the density of particles at point $\boldsymbol{r}$.

Fick's first law of diffusion says that the flow of particles $\boldsymbol{J}$ is proportional to the gradient of density: $\boldsymbol{J} = -D\boldsymbol{\nabla}\rho$.

Now let us consider a region of a small volume ΔV around a point $\boldsymbol{r}$. This volume is surrounded by a surface S, $\boldsymbol{n}_S$ is the unit vector normal to the surface.



Then, the number of particles in the *small* region ΔV is $\rho(\boldsymbol{r}, t)\Delta V$.

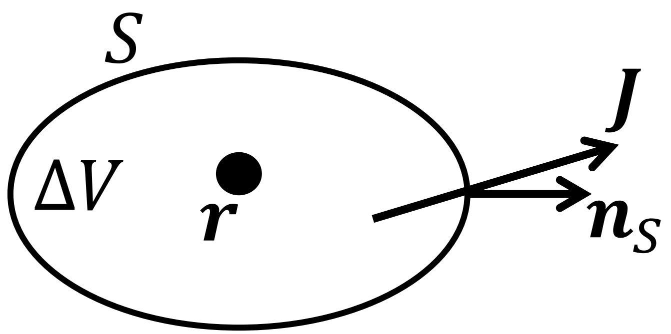
During the time interval Δt this number of particles changes by

$$\delta\rho\Delta V = [\rho(\boldsymbol{r}, t + \Delta t) - \rho(\boldsymbol{r}, t)]\Delta V = \frac{\partial\rho}{\partial t}\Delta t\Delta V$$

This change is due to the flux of particles through the surface S.

The number of particles that leave this region during time interval Δt is

$$\Delta t \oint_S \boldsymbol{J} \cdot \boldsymbol{n}_S \, dS$$



According to the particle conservation law, we have

$$\frac{\partial\rho}{\partial t}\Delta t\Delta V = -\Delta t \oint_S \boldsymbol{J} \cdot \boldsymbol{n}_S \, dS$$

Sign (-1) is because particles leaving ΔV leads to decrease of nº of particles.

The Divergence Theorem tells us that

$$\oint_S \boldsymbol{F}\cdot\boldsymbol{n}_S\,dS = \int_V \boldsymbol{\nabla}\cdot\boldsymbol{F}\,dV \qquad \left(\boldsymbol{\nabla}\cdot\boldsymbol{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right)$$

Therefore,

$$\frac{\partial \rho}{\partial t}\Delta t\Delta V = -\Delta t\oint_S \boldsymbol{J}\cdot\boldsymbol{n}_S\,dS = -\Delta t\int_{\Delta V} \boldsymbol{\nabla}\cdot\boldsymbol{J}dV \approx -\Delta t\Delta V\,\boldsymbol{\nabla}\cdot\boldsymbol{J}$$

$$\Longrightarrow \quad \frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{J}$$

Replacing $\boldsymbol{J} = -D\boldsymbol{\nabla}\rho$ into this equation we get the diffusion equation (also known as Fick's second law of diffusion):

$$\frac{\partial \rho}{\partial t} = D\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\rho$$

$$\Longrightarrow \quad \frac{\partial \rho}{\partial t} = D\Delta\rho$$