

Let the function describing the density of particles be $\rho(x, y, z, t)$. The density per unit volume per unit time is then proportional to the probability to find a particle given by equation $P(x, y, z, t)$. Thus, ρ and P obey the same equation. We find this equation by focusing on an individual walker. We also assume that the walker is confined to a cubic lattice making steps along the edges of the lattice.

The probability to find the walker at the site (i, j, k) at time n is $P(i, j, k, n)$. The walker has six neighboring nodes that it can arrive from to the site (i, j, k) each of which have a $1/6$ chance to make a step into the (i, j, k) node.

Therefore, the following equation is derived:

$$P(i, j, k, n) = \frac{1}{6} [P(i+1, j, k, n-1) + P(i-1, j, k, n-1) + P(i, j+1, k, n-1) + P(i, j-1, k, n-1) + P(i, j, k+1, n-1) + P(i, j, k-1, n-1)]$$

Rearranging the equation, we get:

$$\begin{aligned} & P(i, j, k, n) - P(i, j, k, n-1) \\ &= \frac{1}{6} \{ [P(i+1, j, k, n-1) - P(i, j, k, n-1)] + [P(i-1, j, k, n-1) - P(i, j, k, n-1)] \\ &+ [P(i, j+1, k, n-1) - P(i, j, k, n-1)] + [P(i, j-1, k, n-1) - P(i, j, k, n-1)] \\ &+ [P(i, j, k+1, n-1) - P(i, j, k, n-1)] + [P(i, j, k-1, n-1) - P(i, j, k, n-1)] \} \end{aligned}$$

We then notice that the equation is in the form of a second order symmetric derivative, and, upon taking the limit, we arrive to the diffusion equation.

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