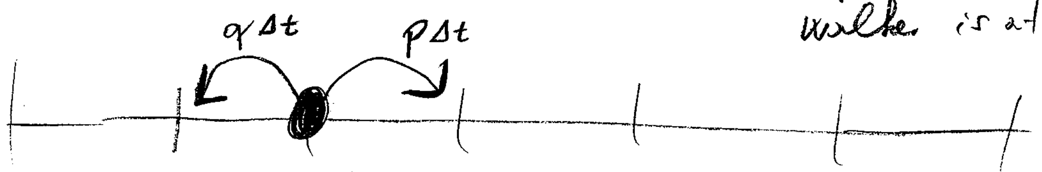
Random Walk and Diffusion

$P(i,t)$: probability that the walker is at site i at time t



$$\underbrace{(1-p\Delta t)(1-q\Delta t)}_{\text{prob. of "staying"}} \overset{o(\Delta t)}{\approx} 1 - p\Delta t - q\Delta t$$

(only up to $o(\Delta t)$ needed once $\Delta t \to 0$ limit is taken)

$$P(i, t+\Delta t) = P(i,t)\left(1 - p\Delta t - q\Delta t + o(\Delta t)^2\right)$$
$$P(i-1,t)\, p\Delta t + P(i+1,t)\, q\Delta t$$

$$P(i, t+\Delta t) - P(i,t) = P(i,t)(p+q)\Delta t + P(i-1,t)\,p\Delta t + P(i+1,t)\,q\Delta t + o(\Delta t)^2$$

$\Delta t \to 0$

$$\boxed{\frac{\partial P(i,t)}{\partial t} = P(i+1,t)\,q + P(i-1,t)\,p - P(i)(p+q)}$$

"master equation"

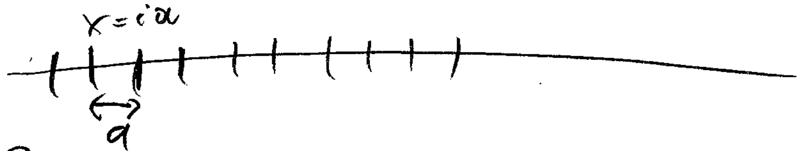
$$p = D + \varepsilon/2$$
$$q = D - \varepsilon/2$$

($\varepsilon \neq 0$: biased RW)

$$\frac{\partial P}{\partial t} = P(i+1,t)\left(D - \frac{\varepsilon}{2}\right) + P(i-1,t)\left(D + \frac{\varepsilon}{2}\right) - P(i,t)\,2D$$
$$= D\left[P(i+1,t) + P(i-1,t) - 2P(i,t)\right] - \frac{\varepsilon}{2}\left[P(i+1,t) - P(i-1,t)\right]$$

Continuum limit:

$$ai \to x$$
$$a(i \pm 1) \to x \pm a$$



$P(i,t) \to P(x,t)$

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

$$\frac{\partial P}{\partial t} = D\left[\frac{\partial^2 P}{\partial x^2} a^2\right] - \frac{\varepsilon}{2}\left[2a\frac{\partial P}{\partial x}\right]$$

$$\frac{\partial P}{\partial t} = D a^2 \frac{\partial^2 P}{\partial x^2} - \varepsilon a \frac{\partial P}{\partial x}$$

$Da^2 \to D$

$\varepsilon a \to \varepsilon$

$$\boxed{\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} - \varepsilon\frac{\partial P}{\partial x}}$$ biased diffusion equation

unbiased $$\boxed{\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}}$$ [or $\frac{\partial P}{\partial t} = D\nabla^2 P$ for $P(\vec{x},t)$ in higher dimensions]

diffusion equation

initial cond.: $P(x,0) = \delta(x)$

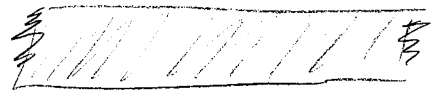
$$\int_{-\infty}^{+\infty} P(x,t)\,dx = 1 \quad \forall t$$

(probability is conserved)

Note:

if there are sources or sinks $\rho(\bar{x})$

$$\partial_t \rho + \bar{\nabla}\cdot \bar{J} = 0 \quad (S(\bar{x}))$$



Gradient driven flows

(other applications of gradient-driven flows)

continuity equation

$$\bar{J} = -D\,\bar{\nabla}\rho(\bar{x})$$

$$\partial_t \rho - D\bar{\nabla}^2\rho = 0$$

$$\boxed{\partial_t \rho = D\bar{\nabla}^2\rho} \rightarrow \rho(\bar{x},t)$$

Solution of the diffusion eq.

$$\partial_t P(x,t) = D\nabla^2 P$$

1d:

$$\tilde{P}(k,t) = \int dx\, P(x,t)\, e^{-ikx}$$

$$P(x,t) = \frac{1}{2\pi}\int dk\, \tilde{P}(k,t)\, e^{ikx}$$

$$\tilde{P}(k,0) = \int dx\, \delta(x)\, e^{-ikx} = 1$$

$$\boxed{\partial_t \tilde{P}(k,t) = -Dk^2\tilde{P}(k,t)}$$

$$\tilde{P}(k,0) \equiv 1 \quad (\forall k)$$

$$\tilde{P}(k,t) = C_k\, e^{-Dk^2 t} \Rightarrow C_k = 1 \quad (\forall k)$$

$$P(x,t) = \frac{1}{2\pi}\int dk\, \tilde{P}(k,t)\, e^{ikx} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\, e^{-Dk^2t + ikx}$$

$$-Dk^2t + ikx = -Dt\left[k^2 - \frac{ikx}{Dt}\right] = -Dt\left[\left(k - \frac{ix}{2Dt}\right)^2 + \frac{x^2}{4(Dt)^2}\right]$$

$$= -Dt\left(k - \frac{ix}{2Dt}\right)^2 - \frac{x^2}{4Dt}$$

("completed square")

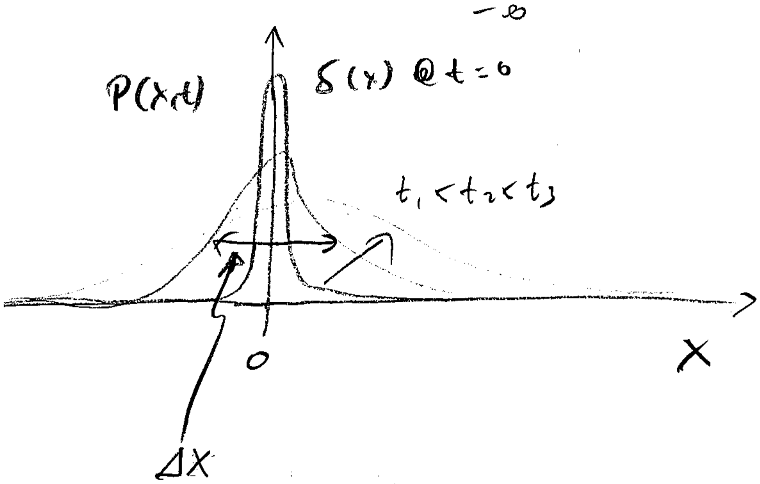
$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} dk \; e^{-Dt\left(k-\frac{ix}{2Dt}\right)^2} e^{-\frac{x^2}{4Dt}} = \frac{1}{2\pi} e^{-\frac{x^2}{4Dt}} \int_{-\infty}^{+\infty} dk \; e^{-Dt\left(k-\frac{ix}{2Dt}\right)}$$

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

$$\boxed{P(x,t) = \frac{1}{\sqrt{2\pi(2Dt)}} e^{-\frac{x^2}{2(2Dt)}}} \qquad P(x,0) = \delta(x)$$

$$\langle X(t)\rangle = \int_{-\infty}^{+\infty} P(x,t)\,x\,dx = 0$$

$$\langle x^2\rangle = \int_{-\infty}^{+\infty} P(x,t)\,x^2\,dx = 2Dt$$



$$\boxed{\langle x^2\rangle = 2Dt}$$

$$\langle(\Delta x)^2\rangle = \langle(x-\langle x\rangle)^2\rangle = \\ = \langle x^2\rangle - \langle x\rangle^2$$

diffusive spread: $\sqrt{\langle(\Delta x)^2\rangle} = \sqrt{2Dt} \sim t^{1/2}$