Notes on Diffusion for modeling workshop

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$\langle v_x^2 \rangle = kT/m$

One dimensional random walk:

1) Particle moves $\pm v_x dt - \delta \to$ distance
2) $P(\text{Direction}) = 0.5$. Assume Markovian process
3) Assume dilute solution $\to$ particles don't interact

$x_i(n) \to$ position of i^{th} particle after n steps

$x_i(n) = x_i(n-1) \pm \delta$

Mean displacement:

$$\langle x(n) \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i(n)$$

$$= \frac{1}{N}\sum_{i=1}^{N}\left[x_i(n-1) \underbrace{\pm \delta}_{\text{becomes } 0}\right]$$

$$= \frac{1}{N}\sum_{i=1}^{N} x_i(n-1) = \langle x(n-1) \rangle$$

Thus, mean position of particles does not change.

$$x_i^2(n) = x_i^2(n-1) \pm 2x_i(n-1)\delta + \delta^2$$

$$\langle x^2(n) \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i^2(n) = \frac{1}{N}\sum_{i=1}^{N}\left[x_i^2(n-1) \overbrace{\pm 2x_i(n-1)\delta}^{0} + \delta^2\right]$$

$$= \frac{1}{N}\sum_{i=1}^{N}\left[x^2(n-1)\right] + \delta^2 = \langle x^2(n-1) \rangle + \delta^2$$

$\langle x^2(0) \rangle = 0$; $\langle x^2(1) \rangle = \langle x^2(0) \rangle + \delta^2$

$\langle x^2(2) \rangle = \langle x^2(0) \rangle + 2\delta^2 \ldots.$

Thus, $\langle x^2(n) \rangle = n\delta^2 = \frac{t}{\tau}\delta^2 = 2Dt$ where $D = \frac{\delta^2}{2\tau}$

n is basically t/τ

$\Rightarrow \sqrt{\langle x^2 \rangle} = \sqrt{2Dt}$

For k dimensions, $r_1, r_2 \ldots r_k$

$r^2 = \sum_{i=1}^{k} r_i^2 \qquad \langle r^2 \rangle = \sum_{i=1}^{k} 2Dt$

$\Rightarrow \langle r^2 \rangle = 2kDt$

$(n-k)$ steps $\leftarrow 0 \rightarrow$ k steps

Binomial Dist. Prob of stepping right

$$P(k;n,p) = \frac{n!}{k!\,(n-k)!}\, p^k q^{n-k}$$

Distance travelled in 'n' steps:

$$x(n) = \left[k - (n-k)\right]\delta = (2k-n)\delta$$

$\langle x(n) \rangle = (2\langle k \rangle - n)\delta$

Since binomial, $k = np$ — thus, $\langle x(n) \rangle = 0$

msd:

$$\langle x^2(n) \rangle = \left(4\langle k^2 \rangle - 4\langle k \rangle n + n^2\right)\delta^2$$

$$\langle k^2 \rangle = (np)^2 + npq$$

thus,

$$\langle x^2(n) \rangle = n\delta^2$$

When n and $np >> 0$

$$P(k)\,dk = \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-(k-\mu)^2/2\sigma^2} dk$$

Subst.

$x = (2k - n)\delta$, $dx = 2\delta\, dk$,

$p = q = 1/2$, $t = n/\tau$, and

$D = \delta^2/2\tau$

and we get

$$P(x)\,dx = \frac{1}{(4\pi Dt)^{1/2}} e^{-x^2/4Dt} dx$$

$$\sigma_x = (2Dt)^{1/2}$$