Lecture 3

General solution to the random walk problem [Markov]

Consider $\vec{R} = \sum_{i=1}^{N} \vec{r}_i$ ← single-step displacement

$\vec{R}$ ↑ part. position after N displacements

Define $\underbrace{\tau_i \, d\vec{r}_i}_{\text{prob. that the displacement is in } (\vec{r}_i, \vec{r}_i + d\vec{r}_i) \text{ interval}}$

τ_i ← prob. density

For example, in 3D one has:

$$\tau_i(x_i, y_i, z_i)\, dx_i dy_i dz_i$$

We're interested in $\underbrace{W_N(\vec{R})d\vec{R}}_{\text{prob. that the particle position lies in } (\vec{R}, \vec{R}+d\vec{R})}$

Consider a very general problem (following Markov):

let $\vec{\varphi}_j = (\varphi_j^1, \ldots, \varphi_j^n)$ $j = 1 \ldots N$ be N n-dim vectors. Each vector component is a function of S coordinates: $\varphi_j^k = \varphi_j^k(q_j^1 \ldots q_j^S)$

$$j = 1 \ldots N, \quad k = 1 \ldots n$$

Further, $\tau_j(q_j^1 \ldots q_j^s)\, dq_j^1 \ldots dq_j^s =$

$$= \underbrace{\tau_j(\vec{q}_j)}_{\text{prob. density for } \vec{q}_j} d\vec{q}_j$$

Let $\vec{\Phi} = \sum_{j=1}^{N} \vec{\varphi}_j$

$\vec{\Phi} = (\varphi^1, \ldots, \varphi^n)$ n-dim vector

What is the prob. that

(**) $-\frac{d\vec{\Phi}_0}{2} + \vec{\Phi}_0 \leq \vec{\Phi} \leq \vec{\Phi}_0 + \frac{d\vec{\Phi}_0}{2}$? $\Rightarrow W_N(\vec{\Phi}_0)\underbrace{d\vec{\Phi}_0}_{d\varphi_0^1 \ldots d\varphi_0^n}$

$\uparrow$ user-defined value

Clearly, $$W_N(\vec{\Phi}_0)\, d\vec{\Phi}_0 = \underbrace{\int \ldots \int}_{\substack{Ns \text{ integrals} \\ \text{(restricted)}}} \prod_{j=1}^{N} \{\tau_j(\vec{q}_j)\underbrace{d\vec{q}_j}_{dq_j^1 \ldots dq_j^s}\}$$

However, we need to restrict the integrals s.t. (**) is satisfied:

introduce

$$\Delta(\vec{q}_1, \ldots, \vec{q}_N) = \begin{cases} 1 & \vec{\Phi}_0 - \frac{d\vec{\Phi}_0}{2} \leq \vec{\Phi} < \vec{\Phi}_0 + \frac{d\vec{\Phi}_0}{2}, \\ 0 & \text{otherwise} \end{cases}$$

$\uparrow$ s-dim vector

So, $$W_N(\vec{\Phi}_0)\, d\vec{\Phi}_0 = \underbrace{\int \ldots \int}_{\substack{Ns \text{ integrals} \\ \text{(unrestricted)}}} \Delta(\vec{q}_1 \ldots \vec{q}_N) \prod_{j=1}^{N} \{\tau_j(\vec{q}_j)\, d\vec{q}_j\}$$

Fortunately, Δ can be written out explicitly (!)

Consider

$$\delta_k = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin(\alpha_k p_k)}{p_k} e^{i p_k \gamma_k} dp_k \qquad k = 1 \dots n$$

$\uparrow$ Dirichlet $\int$

In fact, $\delta_k = \begin{cases} 1 & -\alpha_k < \gamma_k < \alpha_k \\ 0 & \text{otherwise} \end{cases}$

Now, use $\begin{cases} \alpha_k = \dfrac{d\varphi_0^k}{2} \\ \gamma_k = \sum_{j=1}^{N} \varphi_j^k - \varphi_0^k \end{cases} \quad k = 1 \dots n$

Then

$$\delta_k = \begin{cases} 1 & \varphi_0^k - \dfrac{d\varphi_0^k}{2} < \sum_{j=1}^{N} \varphi_j^k < \varphi_0^k + \dfrac{d\varphi_0^k}{2} \\ 0 & \text{otherwise} \end{cases}$$

Finally, $\Delta = \prod_{k=1}^{n} \delta_k$.

Consequently,

$$W_N(\vec{\varphi}_0) d\vec{\varphi}_0 = \frac{1}{\pi^n} \underbrace{\int \dots \int}_{n \int\text{'s over } \vec{p}} \overbrace{\int \dots \int}^{N\text{s } \int\text{'s over } \vec{\varphi}_1 \dots \vec{\varphi}_N} \left\{ \prod_{j=1}^{N} \tau_j(\vec{\varphi}_j) d\vec{\varphi}_j \right\} \times$$

$$\times \left\{ \prod_{k=1}^{n} \frac{\sin\left(\frac{d\varphi_0^k}{2} p_k\right)}{p_k} \right\} e^{i\left[\sum_{k=1}^{n} \sum_{j=1}^{N} \varphi_j^k p_k - \sum_{k=1}^{n} \varphi_0^k p_k\right]} \times$$

$$\times \, dp_1 \dots dp_n .$$

Now, write

$$A_N(\vec{p}) = \prod_{j=1}^{N} \Big\{ \underbrace{\int \dots \int}_{s\text{ integrals}} d\vec{\varphi}_j \, e^{i\vec{p}\cdot\vec{\varphi}_j} \tau_j(\vec{\varphi}_j) \Big\}$$

$$\frac{\sin\left(\frac{d\varphi_0^k}{2} p_k\right)}{p_k} \approx \frac{d\varphi_0^k}{2}.$$

Then

$$W_N(\vec{\Phi}_0)\,d\vec{\Phi}_0 = \frac{\overbrace{d\vec{\Phi}_0}^{d\varphi_0^1 \dots d\varphi_0^n}}{2^n \pi^n} \underbrace{\int \dots \int}_{n\ \int\text{'s over } \vec{p}} e^{-i\overbrace{\vec{p}\cdot\vec{\Phi}_0}^{\sum_{k=1}^{n} p_k \varphi_0^k}} A_N(\vec{p})\,d\vec{p}.$$

So, $$W_N(\vec{\Phi}_0) = \frac{1}{(2\pi)^n} \int \dots \int e^{-i\vec{p}\cdot\vec{\Phi}_0} \underbrace{A_N(\vec{p})}_{\substack{n\text{-dim FT of} \\ W_N(\vec{\Phi}_0)}} d\vec{p}$$

If $\tau_j(\vec{\varphi}_j)$ are indep. of j,

$$A_N(\vec{p}) = \Big[\underset{\substack{\uparrow \\ s\text{-dim} \int}}{\int} e^{i\vec{p}\cdot\vec{\varphi}} \tau(\vec{\varphi})\,d\vec{\varphi} \Big]^N.$$

Now consider 3D random walks:

$$W_N(\vec{R}) = \frac{1}{(2\pi)^3} \underbrace{\int_{-\infty}^{\infty} d\vec{p}}_{3D \int} \, e^{-i\vec{p}\cdot\vec{R}} A_N(\vec{p}),$$

($n = s$ here)
$\quad = 3$

$$A_N(\vec{p}) = \prod_{j=1}^{N} \underbrace{\int_{-\infty}^{\infty} d\vec{r}_j}_{3D \int} \, e^{i\vec{p}\cdot\vec{r}_j} \underbrace{\tau_j(\vec{r}_j)}_{\text{prob. density for displacement } \vec{r}_j}$$

Special cases / examples

1. Gaussian distr'n for $\vec{r}_j$:

$$\tau_j = \left(\sqrt{\frac{3}{2\pi \ell_j^2}}\right)^3 e^{-\frac{3|\vec{r}_j|^2}{2\ell_j^2}} \qquad j = 1, \ldots, N$$

note that $\ell_{j,x}^2 = \ell_{j,y}^2 = \ell_{j,z}^2 = \frac{\ell_j^2}{3}$

$[\ell_{j,x}^2 + \ell_{j,y}^2 + \ell_{j,z}^2 = \ell_j^2]$ by isotropy

Then $A_N(\vec{p}) = e^{-|\vec{p}|^2 \frac{\sum_{j=1}^{N} \ell_j^2}{6}} = e^{-\frac{N\langle \ell^2 \rangle |\vec{p}|^2}{6}}$,

where $\langle \ell^2 \rangle = \frac{1}{N} \sum_{j=1}^{N} \ell_j^2$.

Finally, $W_N(\vec{R}) = \left(\sqrt{\frac{3}{2\pi N \langle \ell^2 \rangle}}\right)^3 e^{-\frac{3|\vec{R}|^2}{2N\langle \ell^2 \rangle}}$.

Exact solution for $\forall N$.

(2.) $\vec{r}_j$ of fixed length, random directions:

$$\tau_j = \frac{1}{4\pi \ell_j^2}\,\delta(|\vec{r}_j| - \ell_j) \qquad j = 1, \dots, N$$

Indeed, $\int d\Omega\, r^2 dr \,\frac{1}{4\pi\ell^2}\,\delta(r-\ell) = \underline{\underline{1}}.$

Then
$$A_N(\vec{p}) = \prod_{j=1}^{N} \frac{1}{4\pi\ell_j^2} \int_{-\infty}^{\infty} d\vec{r}_j\, e^{i\vec{p}\vec{r}_j}\,\delta(\underbrace{|\vec{r}_j|}_{\equiv r_j} - \ell_j) =$$

$$= \prod_{j=1}^{N} \frac{1}{4\pi\ell_j^2} \int_0^{\infty} r_j^2 dr_j \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\varphi \,\times$$
$$\times\, e^{i|\vec{p}| r_j \cos\theta}\,\delta(r_j - \ell_j) \;=$$

$$\left[\int_{-1}^{1} dx\, e^{i|\vec{p}|r_j x} = \frac{1}{i|\vec{p}|r_j}\left[e^{i|\vec{p}|r_j} - e^{-i|\vec{p}|r_j}\right] = \frac{2\sin(|\vec{p}|r_j)}{|\vec{p}|r_j}\right]$$

$$= \prod_{j=1}^{N} \frac{1}{\ell_j^2}\int_0^{\infty} r_j^2 dr_j\, \frac{\sin(|\vec{p}|r_j)}{|\vec{p}|r_j}\,\delta(r_j - \ell_j) =$$

$$= \underline{\underline{\prod_{j=1}^{N} \frac{\sin(|\vec{p}|\ell_j)}{|\vec{p}|\ell_j}}}\,.$$

Finally,
$$W_N(\vec{R}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} d\vec{p}\, e^{-i\vec{p}\cdot\vec{R}} \,\times$$
$$\times \prod_{j=1}^{N} \frac{\sin(|\vec{p}|\ell_j)}{\underbrace{|\vec{p}|}_{\equiv p}\ell_j} \;\boxed{=}$$

$$\boxed{=}\ \frac{1}{(2\pi)^3}\int_0^\infty p^2 dp \int_{-1}^{1} dx \int_0^{2\pi} d\varphi \; e^{-ip|\vec{R}|x} \times$$

$$\times \prod_{j=1}^{N} \frac{\sin(p\ell_j)}{p\ell_j} =$$

$$= \frac{1}{2\pi^2 |\vec{R}|}\int_0^\infty p\,dp\, \sin(p|\vec{R}|) \prod_{j=1}^{N} \frac{\sin(p\ell_j)}{p\ell_j} .$$

↑ Rayleigh's solution

If $\ell_j = \ell$, $\forall j = 1, \dots, N$:

$$W_N(\vec{R}) = \frac{1}{2\pi^2|\vec{R}|}\int_0^\infty p\,dp\,\sin(p|\vec{R}|)\left[\frac{\sin(p\ell)}{p\ell}\right]^N .$$

Possible to solve for finite N, but easier to look at the $N \gg 1$ limit:

$$\lim_{N\to\infty}\left(\frac{\sin(p\ell)}{p\ell}\right)^N = \lim_{N\to\infty}\left(1 - \frac{p^2\ell^2}{3!} + \dots\right)^N =$$

$$= e^{-\frac{Np^2\ell^2}{6}} .$$

So, $W(\vec{R})$ (↑ in the $N\to\infty$ limit) $= \frac{1}{2\pi^2|\vec{R}|}\int_0^\infty p\,dp\,\sin(p|\vec{R}|)\, e^{-\frac{Np^2\ell^2}{6}} =$

$$= \left(\sqrt{\frac{3}{2\pi N\ell^2}}\right)^3 e^{-\frac{3|\vec{R}|^2}{2N\ell^2}} \quad (**)$$

, just like the Gaussian chain above.

Indeed, more generally, if

$$\tau_j(\vec{r}_j) = \overset{\swarrow \text{ indep. of } j}{\tau}(\underbrace{|\vec{r}_j|}_{r_j}) \qquad j=1,\dots,N$$

$$A_N(\vec{p}) = \Big[\underbrace{\int d\vec{r}\, \tau(r)\, e^{i\vec{p}\cdot\vec{r}}}_{\parallel} \Big]^N \Rightarrow$$

$$\int_0^\infty r^2 dr \int_{-1}^{1} dx \int_0^{2\pi} d\varphi\, e^{i|\vec{p}|rx}\, \tau(r) =$$

$$= 4\pi \int_0^\infty dr\, r^2 \tau(r)\, \frac{\sin(|\vec{p}|r)}{|\vec{p}|r} .$$

$$\Rightarrow \lim_{N\to\infty} A_N(\vec{p}) = \lim_{N\to\infty} \Big[4\pi \int_0^\infty dr\, r^2 \tau(r) \big(1 - \tfrac{1}{3!} |\vec{p}|^2 r^2 + \dots\big) \Big]^N =$$

$$= \lim_{N\to\infty} \Big[1 - \tfrac{1}{6} |\vec{p}|^2 \langle r^2 \rangle + \dots \Big]^N = e^{-\frac{N|\vec{p}|^2 \langle r^2\rangle}{6}}$$

Finally,

$$W(\vec{R}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d\vec{p}\, e^{-i\vec{p}\cdot\vec{R} - N|\vec{p}|^2\langle r^2\rangle/6} =$$

$$= \left(\sqrt{\frac{3}{2\pi N \langle r^2 \rangle}} \right)^3 e^{-\frac{3|\vec{R}|^2}{2N\langle r^2\rangle}}$$

generalization of (**) above