

University of Washington
Department of Chemistry
Chemistry 553
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Lecture 2: The Characteristic Function and the Biased Random Flight

Text Reading: Chandrasekhar, Ch. 1.1

A. Biased Random Walk: The Characteristic Function

- The Fourier transform of the probability is also called a characteristic function in the theory of stochastic processes. Call the characteristic function $\psi(s,t)$. Then the distribution function and characteristic functions form a Fourier pair:

$$\psi(s,t) = \int_{-\infty}^{+\infty} f(x,t) e^{isx} dx; \quad \text{and} \quad f(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi(s,t) e^{-isx} ds \quad (2.1)$$

- The utility of the characteristic function lies in the fact that its logarithm can be expressed as a Taylor expansion around $s=0$, and the first few elements of this expansion are familiar features of a distribution. The expansion also converges rapidly so we need not evaluate usually more than the first few terms.
- Here we can use the characteristic function to obtain the distribution function for a biased one dimensional random walk.
- Assume x varies randomly in time and its distribution in time is described by the function $f(x,t)$. We define the expectation value of x $\langle x \rangle$ and the variance of x : $D(x)$:

$$\langle x \rangle = \int_{-\infty}^{+\infty} xf(x,t)dx; \quad \text{and} \quad D(x) = \int_{-\infty}^{+\infty} (x - \langle x \rangle)^2 f(x,t)dx \quad (2.2)$$

- Consider the Taylor expansion of $\ln\psi(s)$ around $s=0$...

$$\ln \psi(s) = \ln \psi(0) + s \left. \frac{d \ln \psi}{ds} \right|_{s=0} + \frac{s^2}{2} \left. \frac{d^2 \ln \psi}{ds^2} \right|_{s=0} + \dots \quad (2.3)$$

- Recall $\psi(s,t) = \int_{-\infty}^{+\infty} f(x,t) e^{isx} dx$. Then

$$\frac{d \ln \psi}{ds} = \frac{1}{\psi(s)} \frac{d\psi}{ds} = \frac{1}{\psi(s)} \frac{d}{ds} \int_{-\infty}^{+\infty} f(x,t) e^{isx} dx = \frac{i}{\psi(s)} \int_{-\infty}^{+\infty} xf(x,t) e^{isx} dx \quad (2.4)$$

$$\therefore \left. \frac{d \ln \psi}{ds} \right|_{s=0} = \frac{i}{\psi(0)} \int_{-\infty}^{+\infty} xf(x,t) dx = i \langle x \rangle$$

- Similarly:

$$\left. \frac{d^2 \ln \psi}{ds^2} \right|_{s=0} = -D(x) \quad (2.5)$$

- Then

$$\ln \psi(s, t) = is \langle x \rangle - \frac{s^2}{2} D(x) + \dots \quad (2.6)$$

- Define a variable ℓ that randomly varies between +1 or -1 such that the probability of ℓ at any time t being +1 or -1 is $f(1)=p$ and $f(-1)=q$ and $p+q=1$. Define the discrete FT;

$$\psi(s) = \sum_{\ell=\pm 1} f(\ell) e^{i\ell s} = p e^{is} + q e^{-is} \quad (2.7)$$

- It can be shown that $\langle \ell \rangle = p - q$ and $D(\ell) = 4pq$ so that

$$\ln \psi(s) \approx is(p - q) - \frac{s^2}{2} (4pq) \quad (2.8)$$

- Assume N random processes occur with identical statistics as shown in equation 2.7. Note that the definition of ℓ changes for N jumps. ℓ is now the displacement or total number of jumps to the right or left of the starting point after N jumps. As such $|\ell|$ can be much greater than 1! Designate the characteristic function for N such processes

$$\psi_N(s) = \left(\sum_{\ell=\pm 1} f(\ell) e^{i\ell s} \right)^N = (p e^{is} + q e^{-is})^N \quad (2.9)$$

- It can be shown that

$$\ln \psi_N(s) \approx isN \langle x \rangle - \frac{s^2 N}{2} D(x) = isN(p - q) - \frac{s^2 N}{2} (4pq) \quad (2.10)$$

- The distribution function for N such systems jumping randomly as described in equation (2.1) is

$$f(\ell, N) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi_N(s) e^{-is\ell} ds = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp \left[isN \langle \ell \rangle - \frac{s^2 N}{2} D(\ell) \right] e^{-is\ell} ds \quad (2.11)$$

- Making the substitution $u = i(\ell - \langle \ell \rangle)$ and evaluating the integral, equation (2.11) becomes:

$$f(\ell, N) = \frac{1}{2\pi} \sqrt{\frac{2}{D(\ell)}} e^{u^2/2D(\ell)} = \frac{1}{\sqrt{8\pi Npq}} \exp \left[-\frac{(\ell - N(p - q))^2}{8Npq} \right] \quad (2.12)$$

- Equation (2.12) has f as a function of a discrete variable ℓ , which is the excess number of jumps to the right or left after N jumps. We can obtain an expression for f as a function of a continuous variable x . Designate the length of the unit jump δ . Then $x = \ell \delta$.
- Now $f(x, N) dx$ is the probability of the net displacement occurring between x and $x+dx$. Similarly $f(\ell, N) d\ell$ is the probability of a net displacement occurring between ℓ and $\ell + d\ell$. Both of these functions express the same thing using different distance metrics. So they can be equated:

$$f(x, N) dx = f(\ell, N) d\ell = f(\ell, N) \frac{dx}{\delta} \quad (2.13)$$

$$\begin{aligned}
\therefore f(x, N) &= \frac{f(\ell, N)}{\delta} = \frac{1}{\delta \sqrt{8\pi Npq}} \exp\left[-\frac{(\ell - N(p - q))^2}{8Npq}\right] \\
&= \frac{1}{\sqrt{8\pi\delta^2 Npq}} \exp\left[-\frac{(x - \delta N(p - q))^2}{8\delta^2 Npq}\right]
\end{aligned} \tag{2.14}$$

- Note for $p=q=1/2$ we obtain the unbiased random walk result:

$$f(x, N) = \frac{1}{\sqrt{2\pi\delta^2 N}} \exp\left[-\frac{x^2}{2\delta^2 N}\right] \tag{2.15}$$

for which $\langle x^2 \rangle = D(x) = \delta^2 N$. This result is the hallmark of an unbiased random flight process. We will apply this relationship in the next lecture.