PHY 341/641
Thermodynamics and Statistical Physics

Lecture 10

Probability concepts (Chapter 3 in STP)

A. Binomial distribution (continued)
B. Central Limit theorem
C. Poisson distribution and others

Comment on HW problem:

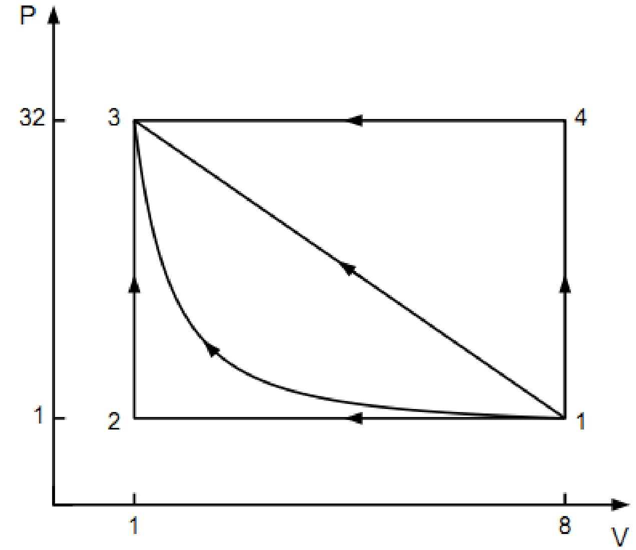


Figure 2.17: Illustration of various thermodynamic processes discussed in Problem 2.56. of the pressure P and the volume V are Pa and m^3, respectively.

For analyzing work $W_{1\to3}$ (along straight line):

$$P = P(V) = P_1 + \frac{P_3 - P_1}{V_3 - V_1}\left(V - V_1\right) \quad \text{for } V_3 \le V \le V_1$$

$$W_{1\to3} = -\int_{V_1}^{V_3} P(V)dV = -\int_{V_1}^{V_3}\left(P_1 + \frac{P_3 - P_1}{V_3 - V_1}\left(V - V_1\right)\right)dV$$

Binomial distribution (review) –

Assume each elemental event has 2 possible outcomes (for example H with probability p and T with probability q=1-p). $P_N(n)$ gives the probability distribution for N elemental events having n instances of H.

$$P_N(n) = \frac{N!}{n!(N-n)!} p^n q^{N-n}$$

Average value:

$$\langle n \rangle = pN$$

Variance:

$$\langle n^2 \rangle - \langle n \rangle^2 \equiv \sigma^2 = Npq$$

$$P_{N\to\infty}(n) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(n-\langle n \rangle)^2/2\sigma^2}$$

Check :

$$\langle n \rangle = \int_{-\infty}^{\infty} n P_{\infty}(n)\,dn = \int_{-\infty}^{\infty} n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left(n-\langle n \rangle\right)^2/2\sigma^2}\,dn$$

$$\sigma^2 = \langle n^2 \rangle - \langle n \rangle^2 = \int_{-\infty}^{\infty} n^2 \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left(n-\langle n \rangle\right)^2/2\sigma^2}\,dn - \langle n \rangle^2$$

More general importance of Gaussian probability distribution – "central limit theorem"

One-dimensional random walk

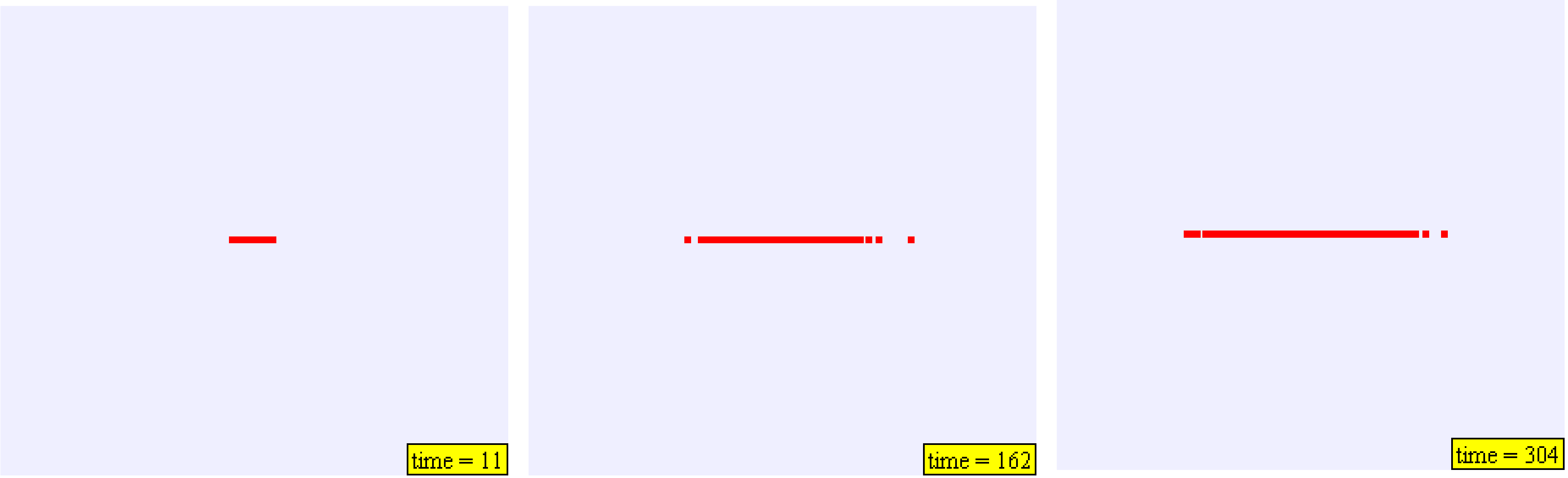
- It is possible to describe a version of a random walk process as a binomial distribution. If each step has a fixed length s, then an elementary event is a step to the right with probability p or a step to the left with probability q. The probability of n steps to the right is then the binomial distribution.

$$P_N(n) = \frac{N!}{n!(N-n)!} p^n q^{N-n}$$

$$P_{N\to\infty}(n) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left(n-\langle n\rangle\right)^2/2\sigma^2}$$

Example of random walk:

stp_RandomWalk2D.jar



One-dimensional fixed step walk, continued

For N total steps and n steps to the right with probability $P_N(n)$, displacement is

$$x=ns-(N-n)s=(2n-N)s$$

$$\langle x\rangle=(2\langle n\rangle-N)s=(2p-1)Ns$$

$$\langle x^2\rangle-\langle x\rangle^2 =4pqNs^2$$

Generalization – one-dimensional variable step (s_i) walk

(derivations following *Fundamentals of statistical and thermal physics* by F. Reif (1965))

$$x = \sum_{i=1}^{N} s_i$$

Let $w(s_i)ds_i$ denote the probability that i^{th} displacement is between s_i and $s_i + ds_i$

The probability distribution for displacement x is

$$P(x)dx = \iiint \ldots \iint ds_1 ds_2 \ldots ds_N w(s_1) w(s_2) \cdots w(s_N)$$

where $x < \sum_{i=1}^{N} s_i < x + dx$

$$P(x)dx = \iiint \ldots \iint ds_1 ds_2 \ldots ds_N w(s_1) w(s_2) \cdots w(s_N) \left[\delta\left(x - \sum_{i=1}^{N} s_i \right) \right] dx$$

Evaluation :

$$\delta(u) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{iku} \qquad \delta(x - \sum s_i) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik\left(\sum s_i - x\right)}$$

$$\text{Let } Q(k) \equiv \int_{-\infty}^{\infty} ds e^{iks} w(s)$$

$$P(x)dx = \iiint \ldots \iint ds_1 ds_2 \ldots ds_N w(s_1) w(s_2) \cdots w(s_N) \left[\delta\left(x - \sum_{i=1}^{N} s_i \right) \right] dx$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \left(Q(k)\right)^N e^{-ikx} dx$$

Evaluation in the limit of $N \to \infty$

$$P(x)dx = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\left(Q(k)\right)^N e^{-ikx}dx$$

$$Q(k) \equiv \int_{-\infty}^{\infty} ds e^{iks} w(s) \approx \int_{-\infty}^{\infty} ds\left(1 + iks - \tfrac{1}{2}k^2 s^2 \cdots\right) w(s) \approx 1 + ik\langle s\rangle - \tfrac{1}{2}k^2\langle s^2\rangle$$

$$\ln\left(Q(k)\right)^N = N\ln\left(Q(k)\right) \approx N\ln\left(1 + ik\langle s\rangle - \tfrac{1}{2}k^2\langle s^2\rangle\right)$$

Assuming $k\langle s\rangle << 1$:

$$N\ln\left(Q(k)\right) \approx N\left(ik\langle s\rangle - \tfrac{1}{2}k^2\left(\langle s^2\rangle - \langle s\rangle^2\right)\right) \equiv N\left(ik\langle s\rangle - \tfrac{1}{2}k^2\langle \Delta s^2\rangle\right)$$

Let $\sigma^2 = N\langle \Delta s^2\rangle$ $\qquad\qquad$ $\langle x\rangle = N\langle s\rangle$

$$\Rightarrow P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\left(x - \langle x\rangle\right)^2}{2\sigma^2}}$$

Poisson probability distribution –

Approximation to binomial distribution for small p

$$P_N(n) = \frac{N!}{n!(N-n)!} p^n q^{N-n}$$

Assume $\quad N >> n \qquad\qquad p << 1$

$$\frac{N!}{n!(N-n)!} \approx \frac{N^n}{n!}$$

$$\ln q^{N-n} = (N-n)\ln(1-p) \approx -(N-n)p \approx -Np$$

$$P_N(n) \approx \frac{N^n}{n!} p^n e^{-Np} = \frac{\langle n \rangle^n}{n!} e^{-\langle n \rangle}$$

Check : $\quad \langle n \rangle = \sum_{n=0}^{\infty} n \frac{\langle n \rangle^n}{n!} e^{-\langle n \rangle} = \langle n \rangle$

Other probability distributions:

Continuous distributions $p(x) \equiv$ probability distribution

$$\int_{-\infty}^{\infty} p(x)dx = 1$$

Probability for x in given range: $P(a \le x \le b) = \int_a^b p(x)dx$

Average value of any function for $f(x)$: $\langle f \rangle = \int_{-\infty}^{\infty} f(x)\,p(x)dx$

Example:

$$p(x) = \frac{1}{\pi}\frac{\gamma}{(x-a)^2 + \gamma^2}$$