

# Physics 463: Statistical Mechanics and Thermodynamics

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# 1 Intro to statistical methods

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- Goal: Study systems consist of many particles (magnitude of moles) that interact with each other.
- Stat Mech bridges the gap between the Macroscopic and Microscopic Description of a system.

Macroscopic Description  $> \mu\text{m}$ :

- Temperature, Pressure, Volume Entropy, etc.

Microscopic Description  $\text{\AA}$ :

## Worksheet

- (1) Avogadro's number:  $N_A = 6.022 \times 10^{23}$  e.g. in 12g of carbon-12, there are  $N_A$  atoms!  
 1 mole of air : 22.4 L at 273 K, 1 atm.  
 e.g. Say a room is 5m x 5m x 8m = 200 m<sup>3</sup> =  $200 \times 10^3$  L, how many moles of air are in the room?  
 $\sim 10000 N_A$

- (2)  $k_B = 1.38 \times 10^{-23}$  J/K  
 Physical Meaning:  $k_B T$  will roughly gives us the energy in one atom

- (3) On a number line with 1 and  $+\infty$ , where is  $N_A$ ?  
 In mathematics, we would place  $N_A$  closer to 1, but in physics we would place it closer to  $+\infty$  because this number is huge in the context of physics.

- (4) In the physics convention, we use  $\theta$  as the polar angle and  $\phi$  as the azimuthal angle. So a volume element in a sphere is

$$r^2 \sin \theta dr d\theta d\phi$$

Thus the volume of a sphere is

$$V = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \int_0^R r^2 \sin \theta dr d\theta d\phi = \frac{4}{3} \pi R^3$$

- (5) The ideal gas law comes in two forms:

$$PV = N k_B T$$

$$PV = nRT$$

where  $n = \frac{N}{N_A}$ , and  $N$  is the number of particles in the system.

- (6) The container with gas confined to half a container at  $t = 0$  releases the gas to fill the whole container at  $t > 0$ . What is the change in entropy?

The equation for the change in entropy is

$$dS = \frac{dQ}{T}$$

but this doesn't tell us much...

**Basic Statistical Concepts** : “statistical ensemble”

Example: Fair coin toss (50/50)  $N$  times. The expected value of heads is  $N/2$ . Repeating this many times gives a Gaussian distribution centered at  $N/2$ .

**Random walk in 1D** Starting at  $x = 0$ , we have a probability  $p$  to move one unit to the right and probability  $(1 - p) = q$  to move left.

For a ‘trajectory’

- $n_L$ : # of steps left
- $n_R$ : # of steps right
- $N = n_L + n_R$
- Displacement:  $x = n_R - n_L$

Each step is independent: “no memory”, “Markovian/Markov process”

The probability of a specific trajectory is

$$p \cdot p \cdots p \cdot q \cdots q = p^{n_R} q^{n_L}$$

How many ways this  $(n_R, n_L)$  can be arranged?

$$\binom{N}{n_R} = \frac{N!}{n_R! n_L!}$$

So the probability of taking  $n_R$  steps to the right is

$$W_N(n_R) = \frac{N!}{n_R! n_L!} p^{n_R} q^{n_L}$$

## Finishing the Random Walk

$$W_N(n_R) = \frac{N!}{n_R!n_L!} p^{n_R} q^{n_L}$$

is indeed the “Binomial distribution”.

The mean displacement (or expected value) is

$$\bar{m} = \bar{n}_R - \bar{n}_L = pN - qN = N(p - q)$$

How do we define variance/dispersion?

$$\begin{aligned} \overline{(\Delta n_R)^2} &= \overline{(n_R - \bar{n}_R)^2} = \overline{n_R^2 - 2n_R\bar{n}_R + \bar{n}_R^2} \\ &= \overline{n_R^2} - 2\bar{n}_R^2 + \bar{n}_R^2 \\ &= \overline{n_R^2} - \bar{n}_R^2 = Npq \end{aligned}$$

So the deviation or width is roughly  $\sim \sqrt{Npq}$

For large  $N$ , the distribution can be approximated a continuous:

$$\left. \frac{dW(n_R)}{dn_R} \right|_{\bar{n}_R} = 0$$

or equivalently

$$\left. \frac{d \ln W(n_R)}{dn_R} \right|_{\bar{n}_R} = 0$$

And using

$$n_R \equiv \bar{n}_R + \xi$$

where  $\xi$  is the deviation from the mean.

So now we can Taylor expand  $\ln W$ :

$$\ln W(n_R) = \ln W(\bar{n}_R) + \cancel{\left. \frac{d \ln W(n_R)}{dn_R} \right|_{\bar{n}_R} (n_R - \bar{n}_R)} + \frac{1}{2} B_z \xi^2 + \dots$$

where

$$W(n_R) \equiv W_{max} e^{-\frac{1}{2} B_z \xi^2}, \quad B_z = \frac{1}{Npq}$$

This yields the Gaussian distribution approximation.

$$P(m) = W(n_R) = (2\pi Npq)^{-1/2} e^{-\frac{[m - N(p-q)]^2}{8Npq}}$$

## Worksheet

1. If a coin is flipped 400 times, what's the probability of getting 215 heads?

$$N = 215 + 185 = 400, \quad p = 0.5, \quad q = 0.5, \quad m = 215 - 185 = 30$$

Plugging in the numbers gives  $P(30) = 1.295\%$