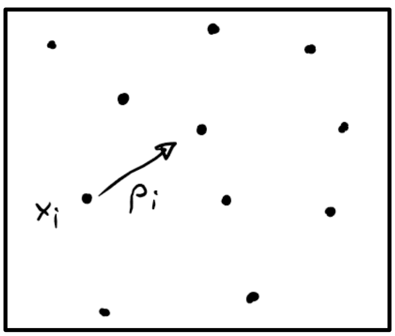
Lecture 1 – Probability & multiplicity

KEY CONCEPT: Microscopic vs. macroscopic states

- Microscopic state (or "microstate") = complete description of each particle or configuration in a system
- Macroscopic state (or "macrostate") = description of a system in terms of a few (e.g. 2) properties

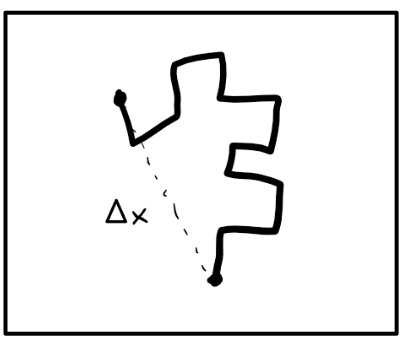
Ex: gas molecules in a box



Microstate = set $\{x_i, p_i\}$ of all positions and momentum of all particles in the system

Macrostate = gas pressure p (for example)

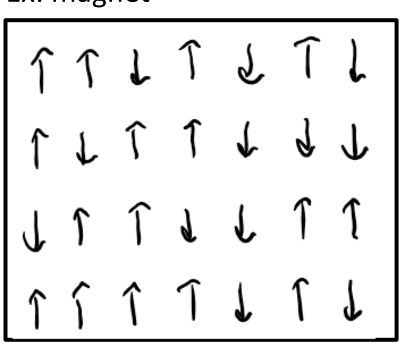
Ex: polymer



Microstate = configuration of every segment of the polymer

Macrostate = end-to-end extension Δx

Ex: magnet



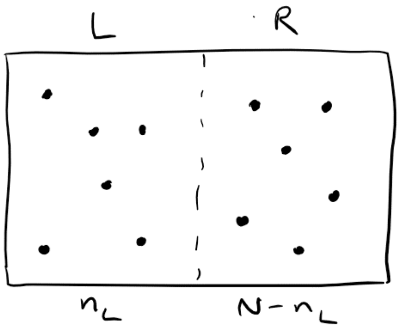
Microstate = configuration of every spin in the magnet

Macrostate = average magnetization M of the magnet

In general there are many more microstates than macrostates.

Note that the definition of microstate/macrostate is not rigid; it will depend on the system and the question being asked.

Ex: Imagine N identical particles in a box split in equal halves



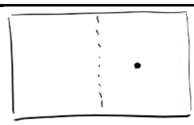
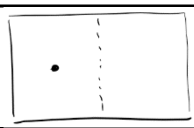
Define macrostate & microstate as:

Macrostate = number of particles in left half, n_L

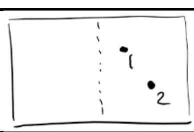
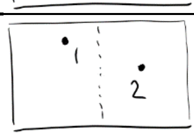
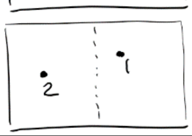
Microstate = configuration of all N particles (i.e. a list of L/R state of each particle: LRRL…RL)

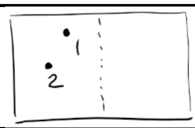
KEY CONCEPT: The <u>multiplicity</u> $\Omega(n_L, N)$ – How many microstates (configurations of N particles) give the same macrostate (n_L particles in left half)?

For $N = 1$

Microstate	Multiplicity $\Omega(n_L, N)$	Macrostate n_L
	1	0
	1	1
Total	2^1	2

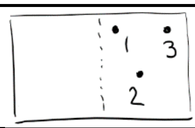
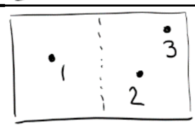
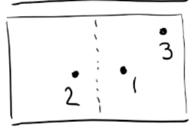
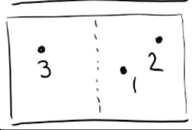
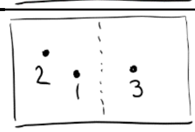
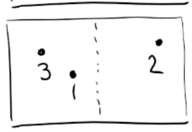
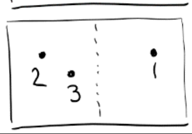
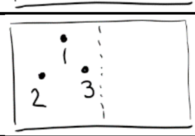
For $N = 2$

Microstate	Multiplicity $\Omega(n_L, N)$	Macrostate n_L
	1	0
 	2	1

	1	2
Total	$2^2 = 4$	2+1 = 3

Question 1: Complete table for *N* = 3

For N = 3

Microstate	Multiplicity $\Omega(n_L, N)$	Macrostate n_L
	1	0
  	3	1
  	3	2
	1	3
Total	$2^3 = 8$	3+1 = 4

These are called <u>statistical ensembles</u>

- Measurement repeated many times to get every possible configuration or microstate

Question 2: What is the total number of microstates and macrostates for arbitrary *N*?

Following the pattern:
Total number of microstates = 2^N
Total number of macrostates = $N+1$ Huge difference for large N

There are $\Omega(n_L, N)$ ways of configuring N particles so that n_L are to the left half
How do we get $\Omega(n_L, N)$ in general for arbitrary N?

- Take N slots, representing N particles
- Distribute n_L particles to the L, $N - n_L$ to the R
- Like so:

L	R	R	L		R	L
1	2	3	4	…	$N-1$	N

N choices for 1st L particles
$N-1$ choices for 2nd L particle
$N-2$ choices for 3rd L particle
⋮
$N - n_L + 1$ choices for the n_Lth L particle

So, $N(N-1)(N-2)\cdots(N-n_L+1)$ total choices

This actually overcounts the multiplicity. In the above example, we can interchange slots #1, #4, and #N to give the exact same configuration, so we need to divide this number by all the ways to interchange the L particles. For n_L particles there are $n_L!$ identical ways to arrange them.

(In the example above, the 3 particles #1, #4, #N can be rearranged into the following ways: 14N, 1N4, 41N, 4N1, N14, N41, or 6 = 3x2x1 = 3! ways)

Therefore

$$\Omega(n_L, N) = \frac{N(N-1)(N-2)\cdots(N-n_L+1)}{n_L!} = \frac{N!}{n_L!(N-n_L)!} \equiv \binom{N}{n_L} \qquad \text{“}N\text{ choose }n_L\text{”}$$

This is called the <u>binomial coefficient</u>

Comes from the binomial identity:

$$(p+q)^N = \sum_{n=0}^{N} \binom{N}{n} p^n q^{N-n}$$

Note that, setting $p = q = 1$, $2^N = \sum_{n_L=0}^{N} \Omega(n_L, N)$, as expected.

KEY CONCEPT: The fundamental assumption – in a closed or isolated system (not interacting with surroundings) each microstate in system is equally likely:

$$\text{Prob. of 1 particular microstate} = \frac{1}{2^N}$$

(Same as saying each particle has a prob. ½ of being to the left. For N particles, prob. is $\frac{1}{2^N}$)

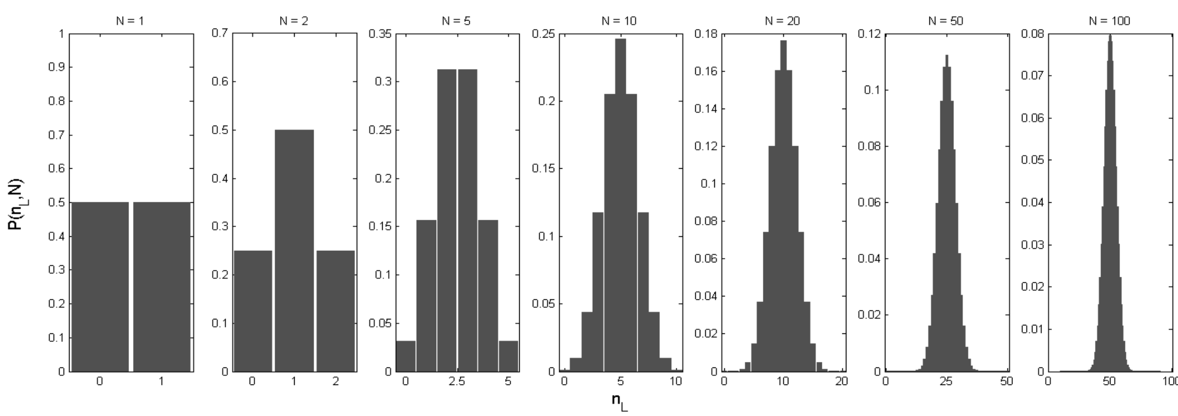
Although each microstate is equally likely, some macrostates are more likely than others (ex: $N = 3$, $n_L = 1$ is 3x more likely then $N = 3$, $n_L = 0$)

Prob. that n_L out of N particles are to the left =

$$P(n_L, N) = \frac{\Omega(n_L, N)}{\Omega(0,N) + \Omega(1,N) + \cdots \Omega(N,N)}$$
$$= \frac{\Omega(n_L, N)}{2^N} = \frac{N!}{n_L!(N-n_L)!}\left(\frac{1}{2}\right)^N$$

This is an example of the binomial distribution

What does $P(n_L, N)$ look like?



$P(n_L, N)$ is peaked at $n_L = N/2$, gets sharper as $N >> 1$

Therefore, the most likely macrostate is with ½ the particles in L, ½ in R, because most microstates have $n_L = N/2$.

Properties of probabilities

Normalization:

$$\text{Prob. of being in any one macrostate} = \sum_{n_L=0}^{N} P(n_L, N) = 1$$

Check using binomial identity, setting $p = q = 1/2$:

$$\left(\frac{1}{2}+\frac{1}{2}\right)^N = \sum_{n_L=0}^{N} \frac{N!}{n_L!(N-n_L)!}\left(\frac{1}{2}\right)^{n_L}\left(\frac{1}{2}\right)^{N-n_L} = \sum_{n_L=0}^{N} \frac{N!}{n_L!(N-n_L)!}\left(\frac{1}{2}\right)^N$$

$$1 = \sum_{n_L=0}^{N} P(n_L, N)$$

Expectation (or mean) values:

For some function $f(n_L)$: $\langle f(n_L)\rangle = \sum_{n_L=0}^{N} f(n_L)P(n_L, N)$

$$\langle n_L\rangle = \sum_{n_L=0}^{N} n_L P(n_L, N), \quad \text{and} \quad \langle n_L{}^2\rangle = \sum_{n_L=0}^{N} n_L{}^2 P(n_L, N), \text{ etc.}$$

What is $\langle n_L\rangle$ for $P(n_L, N)$ we derived?

$$\langle n_L\rangle = \sum_{n_L=0}^{N} n_L \frac{N!}{n_L!(N-n_L)!}\left(\frac{1}{2}\right)^N = \left(\frac{1}{2}\right)^N N \sum_{n_L=1}^{N} \frac{(N-1)!}{(n_L-1)!(N-n_L)!}, \qquad \text{let } n = n_L - 1$$

$$= \left(\frac{1}{2}\right)^N N \underbrace{\sum_{n=0}^{N-1} \frac{(N-1)!}{n!(N-n-1)!}}_{2^{N-1}} = \frac{N}{2} \qquad \text{as expected}$$

Note: Here is an alternate method of deriving this result using a math trick (we'll use this type of trick many times over the semester):

Consider the binomial identity $(p+q)^N = \sum_{n=0}^{N} \binom{N}{n_L} p^{n_L} q^{N-n_L}$.

Since $\left(p\frac{\partial}{\partial p}\right)p^{n_L} = n_L p^{n_L}$ it follows that

$$\sum_{n=0}^{N} \binom{N}{n_L} n_L p^{n_L} q^{N-n_L} = p\frac{\partial}{\partial p}\sum_{n=0}^{N} \binom{N}{n_L} p^{n_L} q^{N-n_L} = p\frac{\partial}{\partial p}(p+q)^N$$

$$= Np(p+q)^{N-1}$$

Setting $p = q = 1/2$:

$$\langle n_L \rangle = \sum_{n=0}^{N} \binom{N}{n_L} n_L \left(\frac{1}{2}\right)^N = \frac{N}{2}$$

Question 3: Calculate $\langle n_L{}^2 \rangle$

Apply the same operator twice: $\left(p\dfrac{\partial}{\partial p}\right)^2 p^{n_L} = n_L{}^2 p^{n_L}$

$$\sum_{n=0}^{N} \binom{N}{n_L} n_L{}^2 p^{n_L} q^{N-n_L} = \left(p\frac{\partial}{\partial p}\right)^2 \sum_{n=0}^{N} \binom{N}{n_L} p^{n_L} q^{N-n_L} = \left(p\frac{\partial}{\partial p}\right)^2 (p+q)^N$$

$$= p\frac{\partial}{\partial p} Np(p+q)^{N-1} = Np(p+q)^{N-1} + N(N-1)p^2(p+q)^{N-2}$$

Setting $p = q = 1/2$:

$$\langle n_L{}^2 \rangle = \sum_{n=0}^{N} \binom{N}{n_L} n_L{}^2 \left(\frac{1}{2}\right)^N = \frac{N}{2} + \frac{N(N-1)}{4} = \frac{N(N+1)}{4}$$

From these we can determine the variance in n_L:

$$\sigma_{n_L}^2 \equiv \left\langle \left(n_L - \langle n_L \rangle\right)^2 \right\rangle = \langle n_L{}^2 \rangle - 2\langle n_L \rangle \langle n_L \rangle + \langle n_L \rangle^2 = \langle n_L{}^2 \rangle - \langle n_L \rangle^2$$

$$= \frac{N(N+1)}{4} - \frac{N^2}{4} = \frac{N}{4}$$

So the standard deviation, or the half width of the probability $P(n_L, N)$, $\sigma_{n_L} = \sqrt{N}/2$ and the fractional deviation is:

$$\frac{\sigma_{n_L}}{\langle n_L \rangle} = \frac{1}{\sqrt{N}}$$

For a large system $N \sim 10^{20}$, this is 10^{-10}, i.e. the width of the probability distribution is 10^{-10} of the total range of the graph! This is extremely sharp.

In sum:

- The most likely macrostate has $N/2$ particles to the L and $N/2$ particles to the R. This is because there are the most microstates with this number, i.e. $\Omega(n_L, N)$ is maximum.
- When $N >> 1$ any other macrostate is extremely unlikely to occur, due to sharpness of $P(n_L, N)$.
- This applies to all binary systems (see K & K, Chapter 1)