Lecture 4

Microstates, Multiplicity of a macrostate

29.08.2018

Macrostate and microstates

Example

Combinatorics of flipping N fair coins

Suppose $N = 5$

- List the possible configurations of 4H and 1T for a set of 5 coins

Combinatorics of H&T's

List the possible configurations of 4H and 1T for a set of 5 coins

THHHH; HTHHH; HHTHH; HHHTH; HHHHT $\boldsymbol{\Omega(1T) = 5}$

- The state of a system of coins with 4H and 1T is called a **macrostate**
- A *particular* arrangement of 4H and 1T is called a **microstate**
- **Number of microstates with 4H and 1T is called the multiplicity of that macrostate**

$$\boldsymbol{\Omega(1T) = 5}$$

How many possible combinations of tails (T) and heads (H) there are?

Combinatorics of H&T's

List the microstates with 3H and 2T for a set of 5 coins

TTHHH; HTTHH; HHTTH; HHHTT;
THTHH; THHTH; THHHT
HTHTH; HTHHT
HHTHT

$$\Omega(2T) = \frac{5\times 4}{2} = \frac{5!}{2!\,3!} = 10$$

How many possible microstates of H&T are there for a set of 5 coins? $2^5 = 32$ microstates

How many possible macrostates of H&T are there for a set of 5 coins? $T = 0, \cdots 5, \quad hence\ 6$ macrostates

List the possible configurations of H and T for a set of 5 coins

HHHHH $\Omega(0T) = 1$

«THHHH» $\Omega(1T) = 5$

«TTHHH» $\Omega(2T) = 10$

«TTTHH» $\Omega(3T) = 10$

«TTTTH» $\Omega(4T) = 5$

TTTTT $\Omega(5T) = 1$

$$\Omega_t = \sum_{n=0}^{5} \Omega(nT) = 32(= 2^5)$$

Probability of a macrostate

$$\mathrm{P(0T)} = \Omega_t^{-1}\Omega(0T) = \frac{1}{32}$$

$$\mathrm{P(1T)} = \Omega_t^{-1}\Omega(1T) = \frac{5}{32}$$

$$\mathrm{P(2T)} = \Omega_t^{-1}\Omega(2T) = \frac{10}{32}$$

$$\mathrm{P(3T)} = \Omega_t^{-1}\Omega(3T) = \frac{10}{32}$$

$$\mathrm{P(4T)} = \Omega_t^{-1}\Omega(4T) = \frac{5}{32}$$

$$\mathrm{P(5T)} = \Omega_t^{-1}\Omega(5T) = \frac{1}{32}$$

Multiplicity of a macrostate with n tails

Number of microstates with n tails: $\Omega(n) = \frac{N!}{n!(N-n)!}$

Total number of microstates

$$\sum_{n=0}^{N} \Omega(n) = \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!} = 2^N$$

Probability of a **macrostate** with n tails

$$P(n) = \frac{\Omega(n)}{\sum_n \Omega(n)}$$

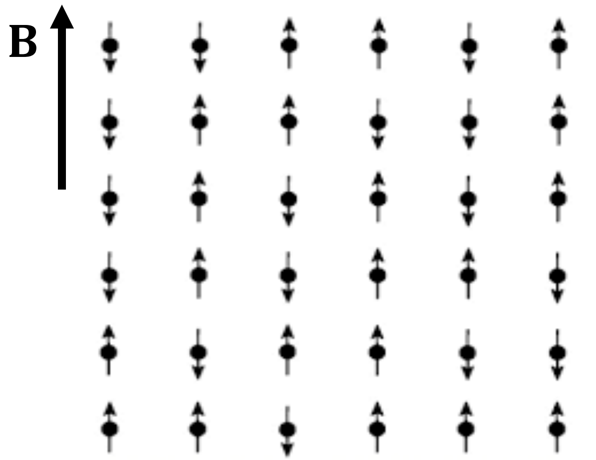
Apply this type of combinatorics to

1. Paramagnetic systems

2. Random walks

3. Thermal vibrations in crystals

Two-state paramagnet model



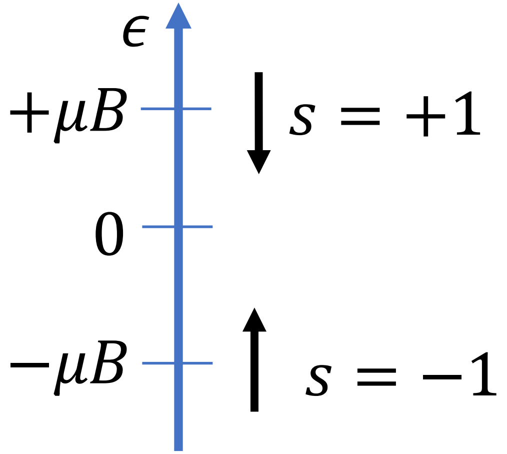
Paramagnetic solid:

- A system of N *independent, localised* particles with spin $s = \pm 1$ in a constant magnetic field $\boldsymbol{B}$
- Energy of a single spin $\epsilon = -s\mu B$
- For N spins , we have $N = N_{\downarrow} + N_{\uparrow}$
- **Net magnetization**

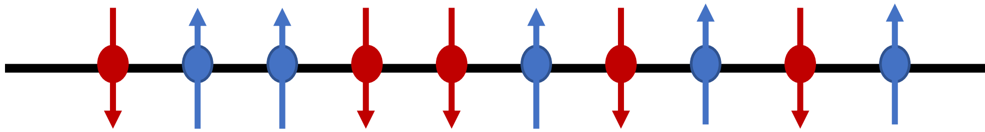
$$\boldsymbol{M} = \boldsymbol{\mu} \sum_{i=1}^{N} \boldsymbol{s_i} = \boldsymbol{\mu}(\boldsymbol{N_{\uparrow}} - \boldsymbol{N_{\downarrow}}) = \boldsymbol{\mu}(\boldsymbol{N} - \boldsymbol{2N_{\uparrow}})$$

- **Average magnetization**

$$\langle \boldsymbol{M} \rangle = \boldsymbol{\mu}(\boldsymbol{N} - \boldsymbol{2}\langle \boldsymbol{N_{\uparrow}} \rangle)$$



Two-state paramagnet model



- Consider a paramagnet with N spins at zero applied field

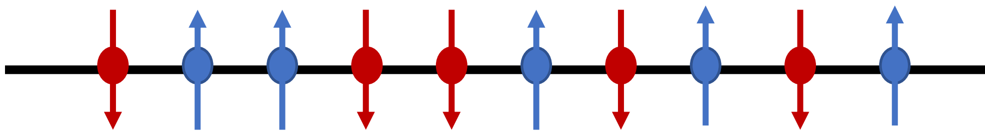
- Spins ↑ or ↓ have the same energy

- Microstate is a particular configuration of spins ↑ and ↓

What is the multiplicity of macrostate with $N_\uparrow$ out of N spins?

$$\boldsymbol{\Omega}(\mathbf{N}, \mathbf{N}_\uparrow) = ?$$

What is the multiplicity of macrostate with $\boldsymbol{N_\uparrow}$ out of $\boldsymbol{N}$ spins?



$$\Omega(N, N_\uparrow) = \frac{N!}{N_\uparrow!\,(N - N_\uparrow)!}$$

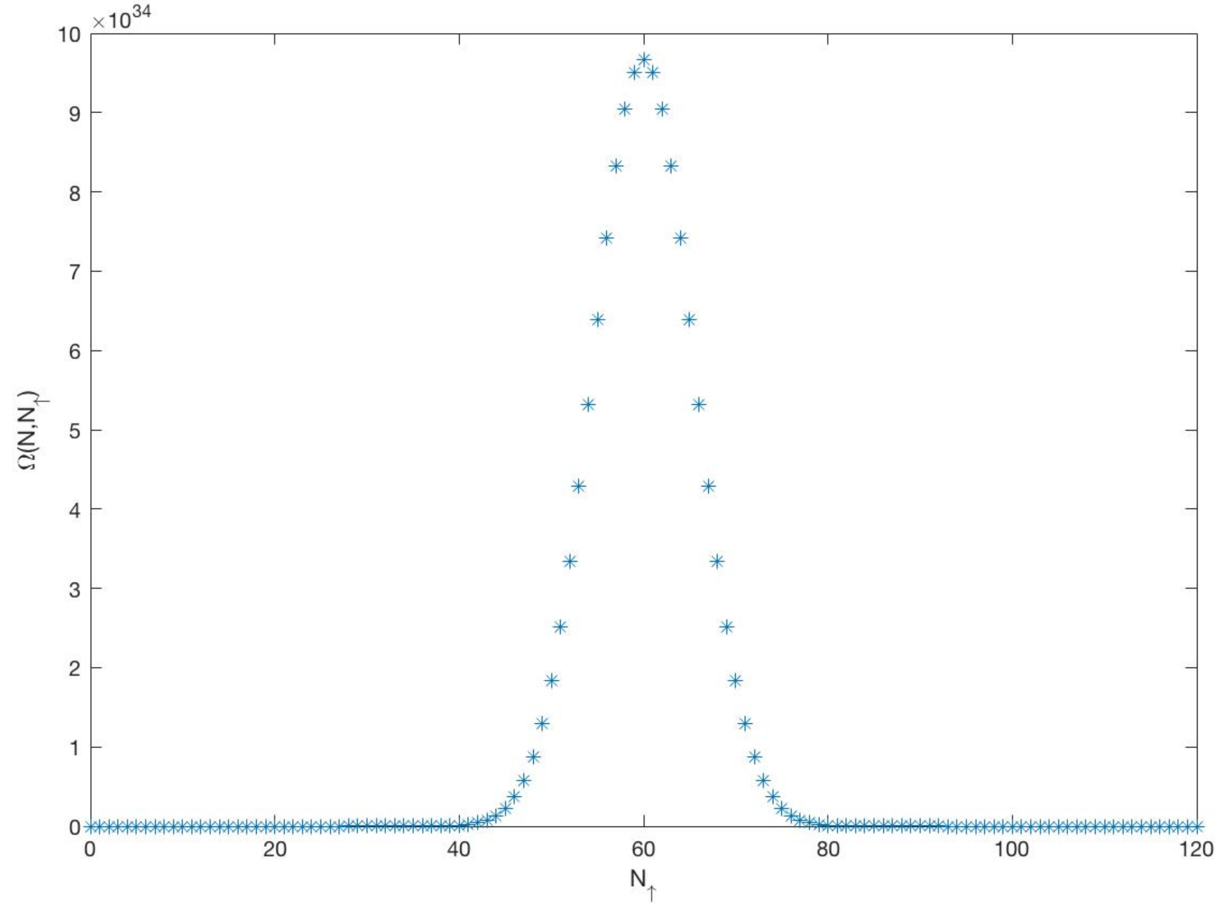
Total number of microstates

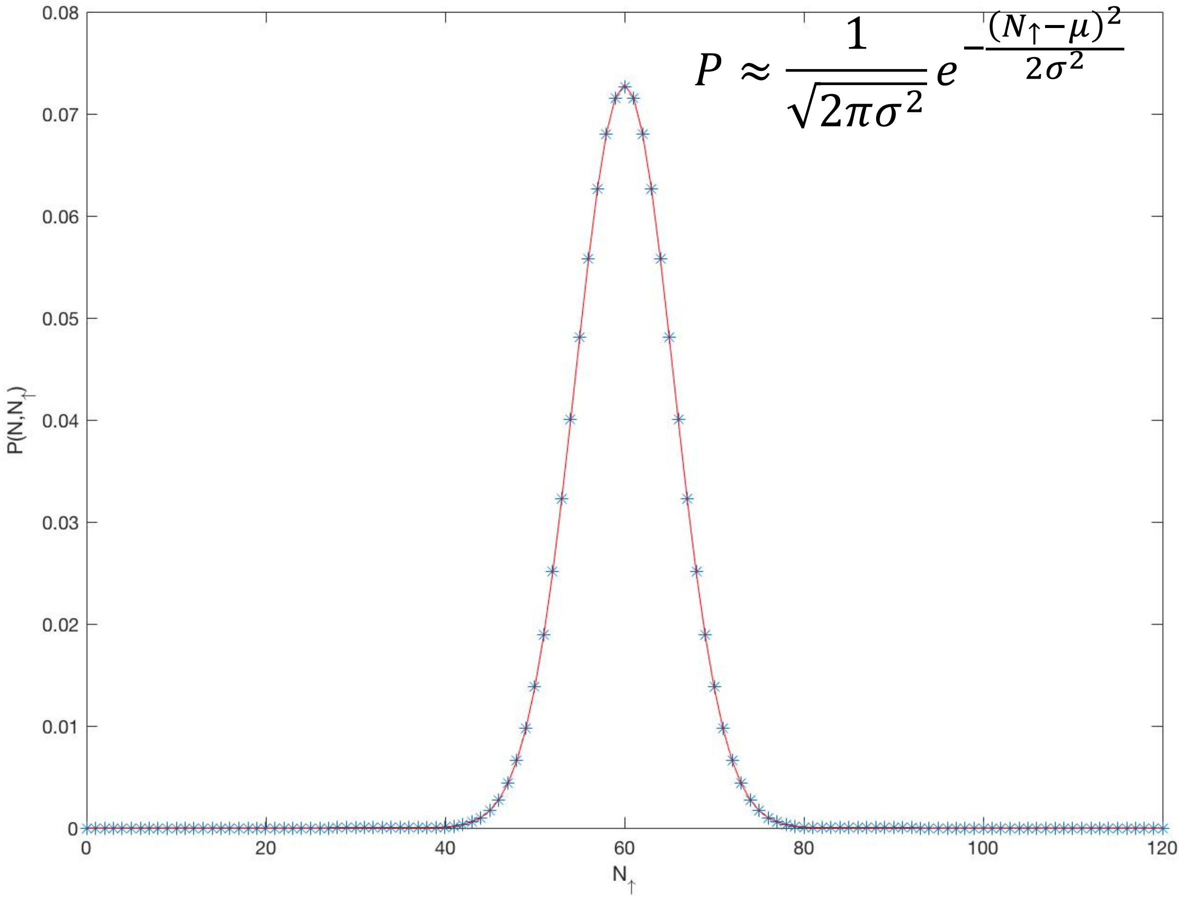
$$\sum_{N_\uparrow=0}^{N} \Omega(N_\uparrow) = \sum_{n=0}^{N} \frac{N!}{N_\uparrow!\,(N - N_\uparrow)!} = 2^N$$

Probability of a **macrostate** with $N_\uparrow$ spins up

$$P(N_\uparrow) = 2^{-N}\Omega(N, N_\uparrow)$$

Multiplicity of a macrostate in a paramagnetic





$$P \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(N_\uparrow - \mu)^2}{2\sigma^2}}$$

Matlab plotting

What is the average number of $N_\uparrow$?

$$\langle N_\uparrow \rangle = \sum_{N_\uparrow=0}^{N} N_\uparrow\, P(N, N_\uparrow) = 2^{-N} \sum_{N_\uparrow=0}^{N} N_\uparrow \frac{N!}{N_\uparrow!\,(N-N_\uparrow)!}$$

Use binomial formula $\sum_{N_\uparrow=0}^{N} \frac{N!}{N_\uparrow!(N-N_\uparrow)!}\, a^{N_\uparrow} b^{N-N_\uparrow} = (a+b)^N$

$$\langle N_\uparrow \rangle = 2^{-N} \left(\sum_{N_\uparrow=0}^{N} N_\uparrow \frac{N!}{N_\uparrow!\,(N-N_\uparrow)!}\, a^{N_\uparrow} b^{N-N_\uparrow} \right)_{a=b=1}$$

What is the average number of $N_\uparrow$?

$$\langle N_\uparrow \rangle = 2^{-N} \left(\sum_{N_\uparrow=0}^{N} N_\uparrow \frac{N!}{N_\uparrow!\,(N-N_\uparrow)!} a^{N_\uparrow} b^{N-N_\uparrow} \right)_{a=b=1}$$

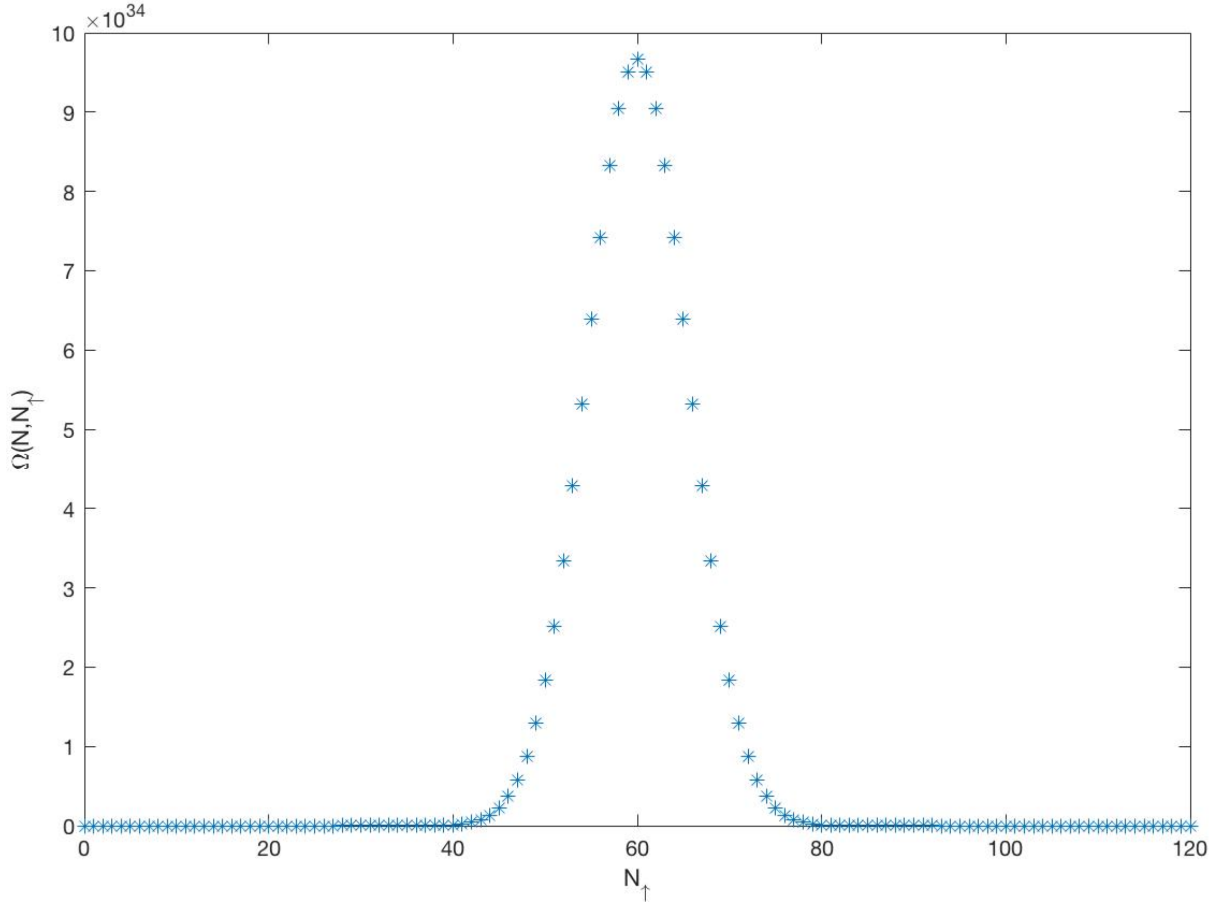
$$\langle N_\uparrow \rangle = 2^{-N} \left(a \frac{d}{da} \sum_{N_\uparrow=0}^{N} \frac{N!}{N_\uparrow!\,(N-N_\uparrow)!} a^{N_\uparrow} b^{N-N_\uparrow} \right)_{a=b=1}$$

What is the average number of $N_\uparrow$?

$$\langle N_\uparrow \rangle = 2^{-N} \left(a \frac{d}{da} \sum_{N_\uparrow = 0}^{N} \frac{N!}{N_\uparrow ! \, (N - N_\uparrow)!} a^{N_\uparrow} b^{N - N_\uparrow} \right)_{a=b=1}$$

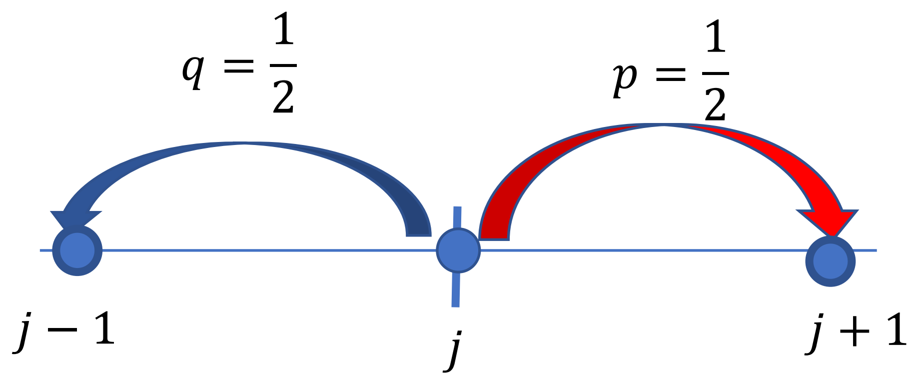
$$\langle N_\uparrow \rangle = \frac{N}{2}$$

Macrostate with $N_\uparrow = \langle N_\uparrow \rangle$ has the largest multiplicity



- $\langle N_\uparrow \rangle = \frac{N}{2}$
- $\langle \boldsymbol{M} \rangle = \boldsymbol{\mu}(\boldsymbol{N} - \boldsymbol{2}\langle \boldsymbol{N}_\uparrow \rangle)$
- $\langle \boldsymbol{M} \rangle = \boldsymbol{0}$
- In the absence of an external magnetic field, spins are **randomly** oriented with a **zero net magnetization**

1D Random walk



- Random motion of a walker along a line
  - Discrete time steps $N = 0,1,2 \cdots$ in units of $\Delta t = 1$
  - Discrete space: lattice index $j = 0, \pm 1, \pm 2 \cdots$ with increments $\Delta x = 1$

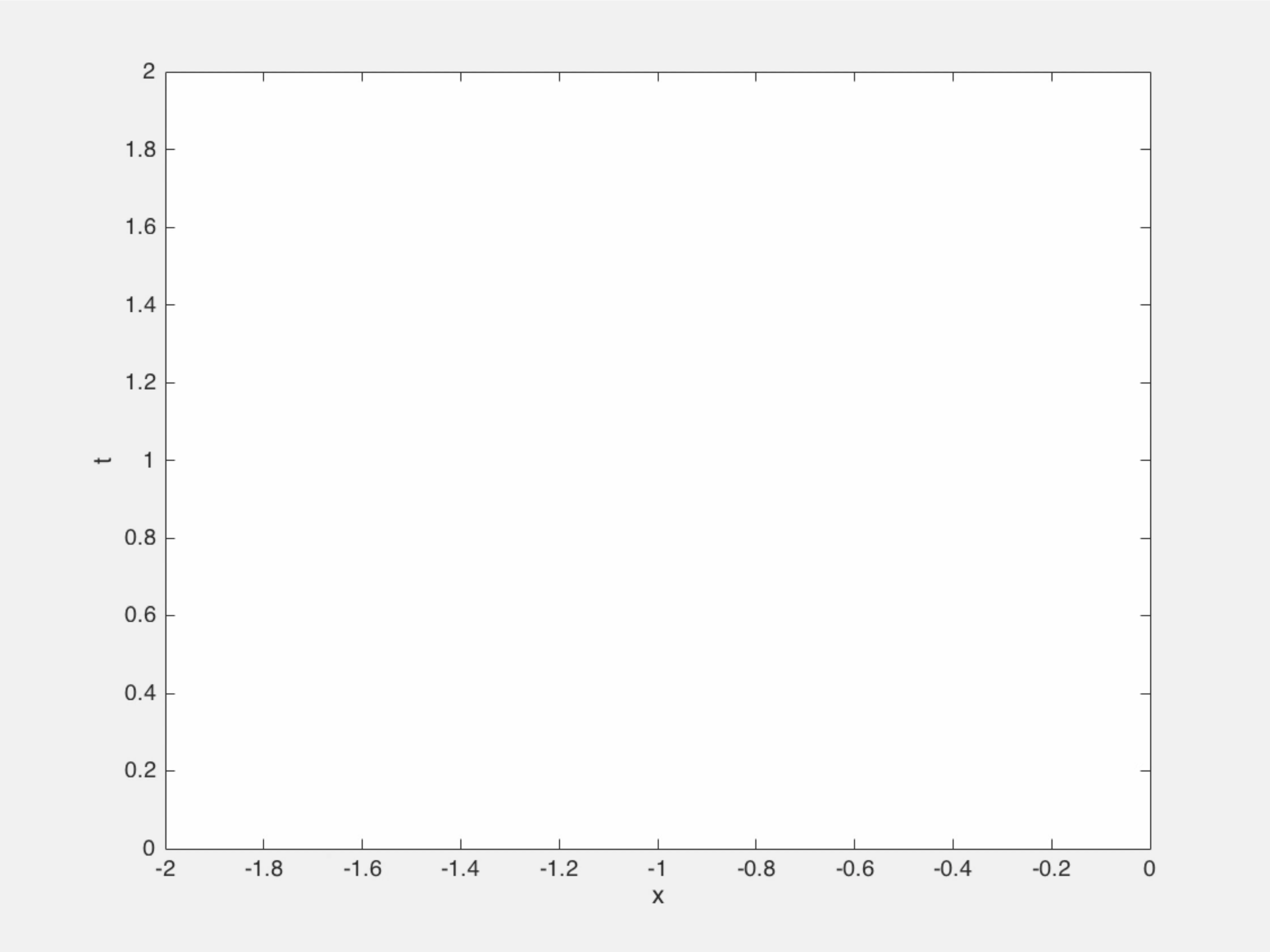
- **At each timestep**, the walker has probability $p = \frac{1}{2}$ to the right $j \to j+1$

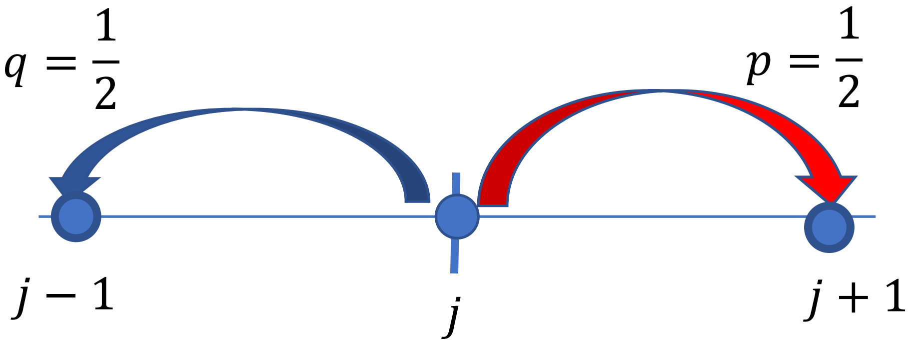
and probability $q = \frac{1}{2}$ to the left $j \to j-1$

- *What is the probability distribution for R steps to the rightN steps, $P(N, R)$?*

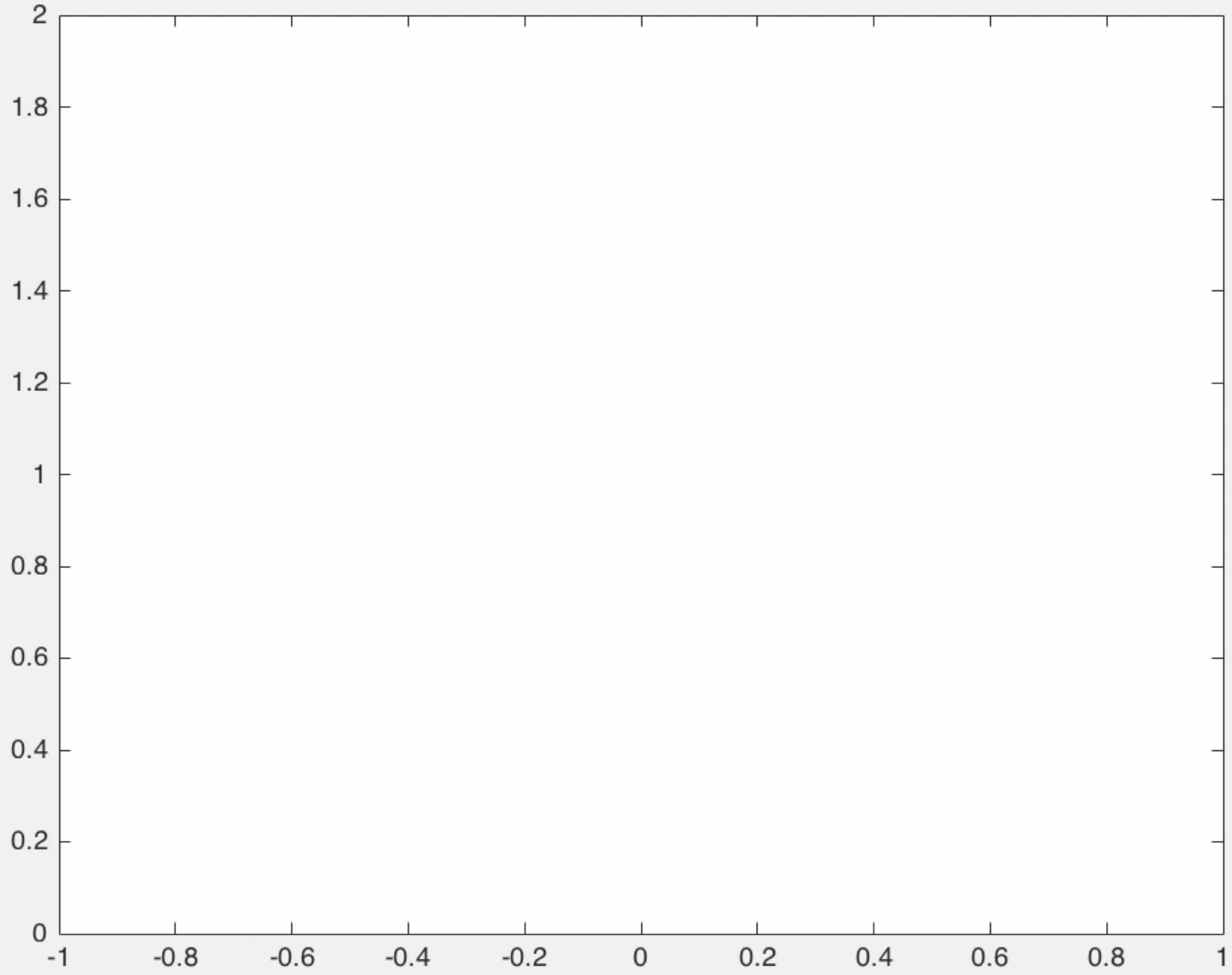
- *What is the mean displacement $\langle S \rangle$ after N steps?*

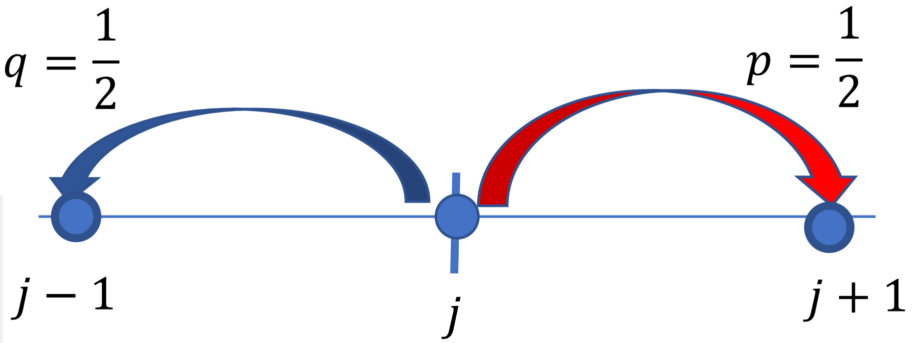
1D Random Walk



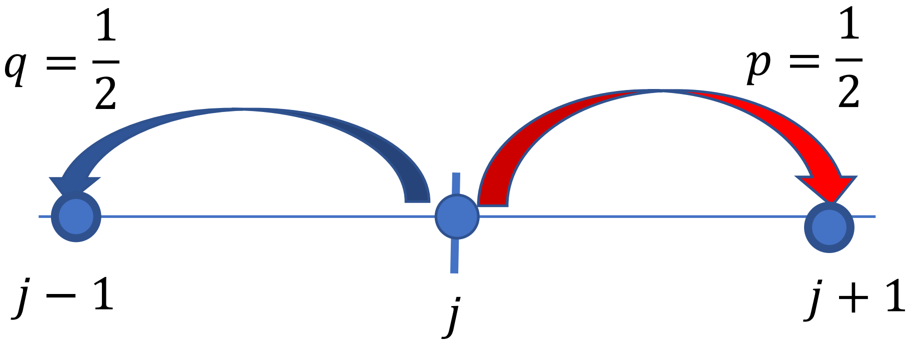


1D Random Walk





1D Random walk



After N steps, we have R steps to the right and L steps to the right

$R + L = N$, $S = R - L$ (net displacement)

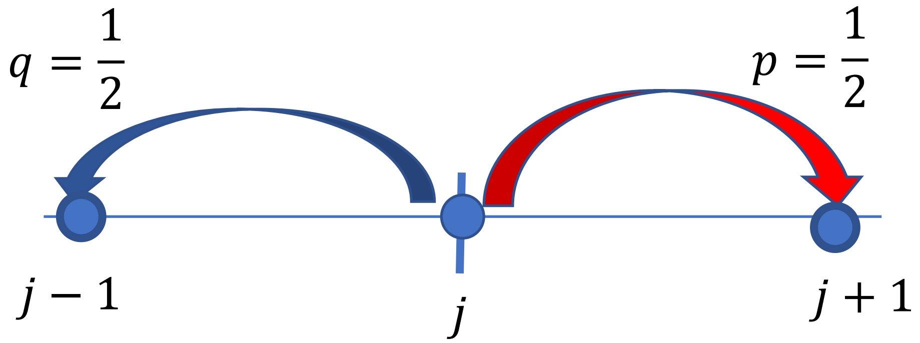
- Number of configurations in which we have R right steps out of N steps

$$\Omega(N, R) = \frac{N!}{R!\,(N-R)!}$$

- Probability for R steps to the right out of N steps

$$P(N, R) = \Omega(N, R)\left(\frac{1}{2}\right)^{R}\left(\frac{1}{2}\right)^{N-R} = 2^{-N}\frac{N!}{R!\,(N-R)!}$$

1D Random walk



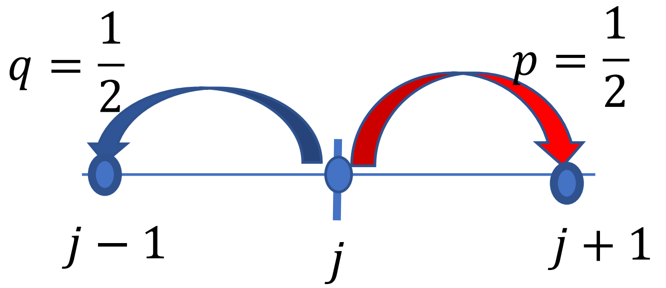
- Probability for R steps to the right out of N steps

$$P(N,R) = 2^{-N}\frac{N!}{R!\,(N-R)!}$$

- Normalization condition: probability for N steps

$$\sum_{R=0}^{N} P(N,R) = 2^{-N}\sum_{R=0}^{N}\frac{N!}{R!\,(N-R)!} = 1$$

Average number of steps to the right



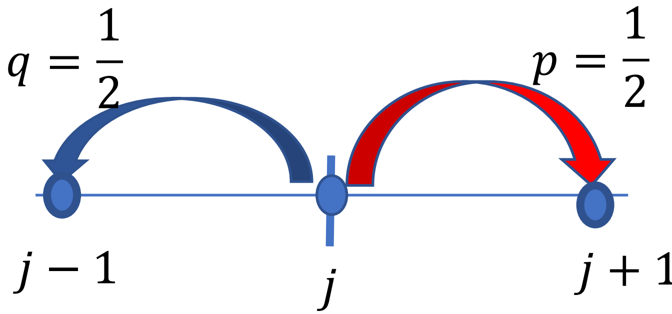
$$\langle R \rangle = \sum_{R=0}^{N} R P(N,R) = \left(\sum_{R=0}^{N} \frac{N!}{R!\,(N-R)!} R p^R q^{N-R} \right)_{p=q=\frac{1}{2}}$$

$$Rp^R \equiv p \frac{d}{dp} p^R$$

$$\langle R \rangle = \left(p \frac{d}{dp} \sum_{R=1}^{N} \frac{N!}{R!\,(N-R)!} p^R q^{N-R} \right)_{p=q=\frac{1}{2}} = \left(p \frac{d}{dp} (p+q)^N \right)_{p=q=\frac{1}{2}}$$

$$\boldsymbol{\langle R \rangle = \frac{N}{2}}$$

Average displacement from the origin

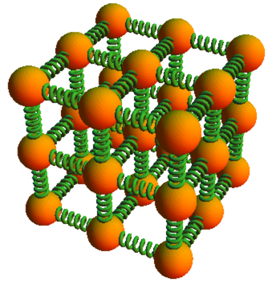


$$\langle R \rangle = \frac{N}{2}$$

$$\langle S \rangle = \langle R \rangle - (N - \langle R \rangle) = 2\langle R \rangle - N$$

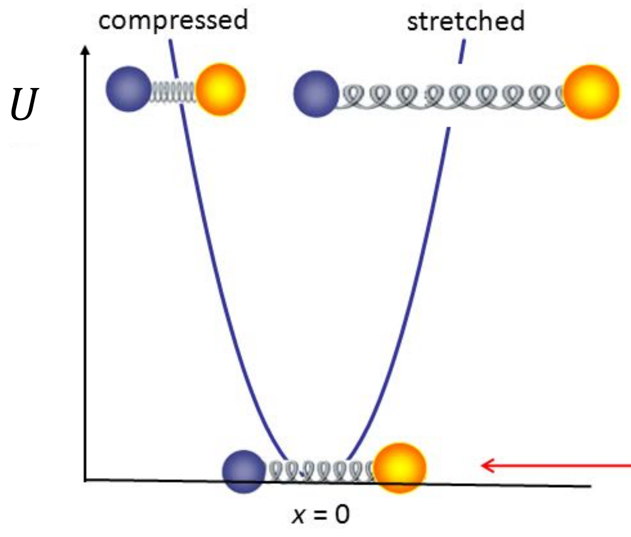
$$\langle S \rangle = 0$$

Thermal vibrations in solids: Einstein crystal



- Collection of identical harmonic oscillators
- *Each atom in 3D has 3 one-dimensional harmonic oscillators*
- Classical harmonic oscillator
- $U_1 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 (x - x_0)^2$
- Frequency $\omega = \sqrt{\frac{\kappa}{m}}$

Classical Harmonic Oscillator



$V = \frac{1}{2}\kappa x^2, T = 0$

$V = 0, T = \frac{p^2}{2m}$

$$U = \frac{p^2}{2m} + \frac{1}{2}\kappa x^2$$

Einstein crystal

One quantum harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}\kappa\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

Quantized energy levels $\epsilon = \left(n + \frac{1}{2}\right)\hbar\omega$

Energy level relative to the ground state

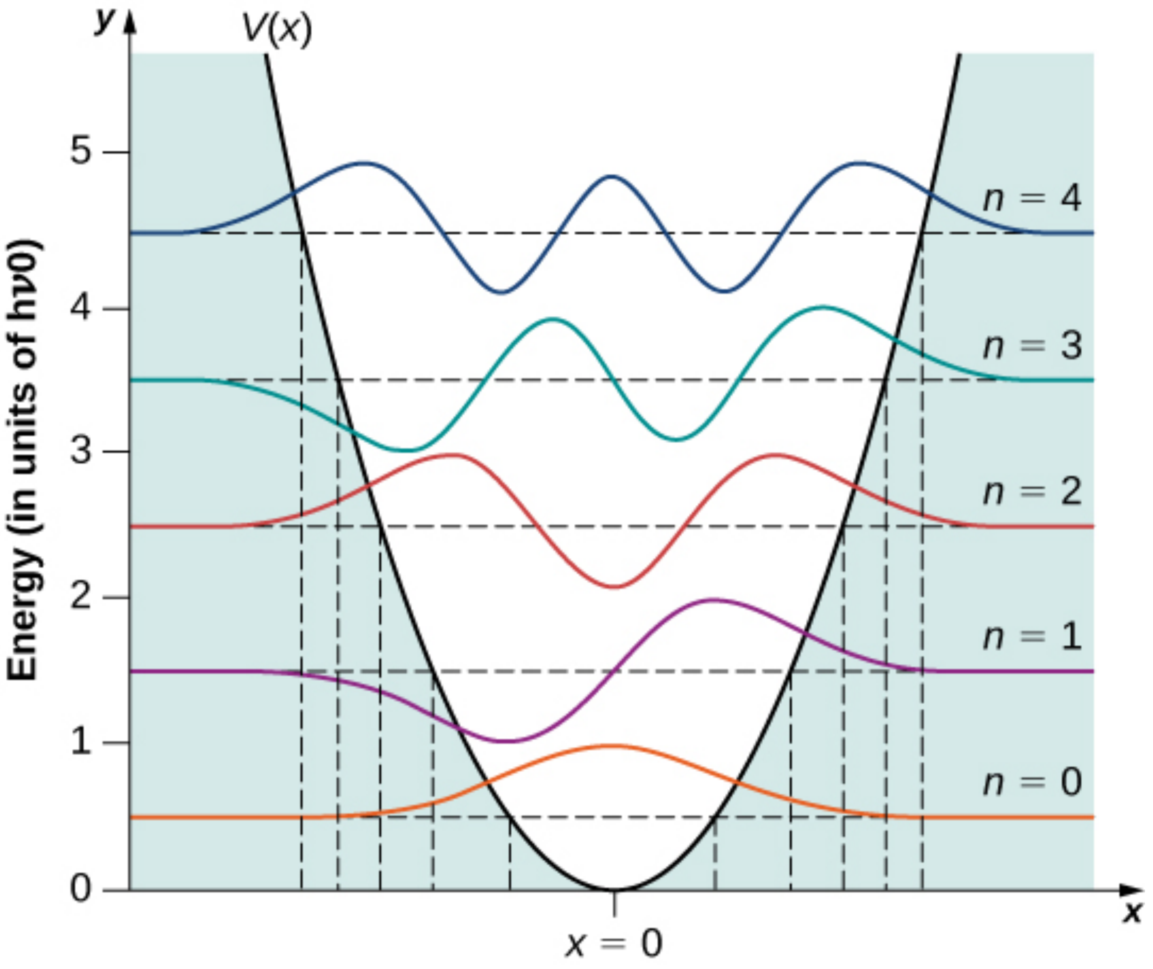
$$\Delta\epsilon = n\hbar\omega$$

Total energy of N harmonic oscillators

$$U_N = \sum_{i=1}^{N} \epsilon_i = \sum_{i=1}^{N} n_i\,\hbar\omega + \frac{N}{2}\hbar\omega$$

Energy units for N quantum harmonic oscillators at frequency $\boldsymbol{\omega}$

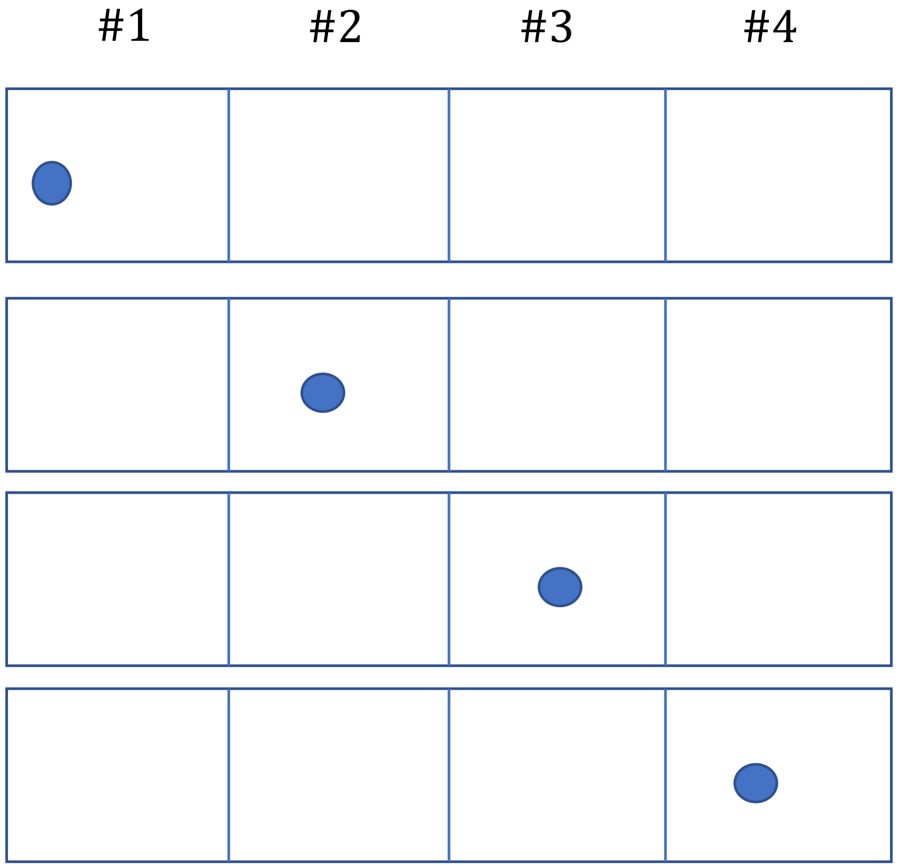
$$\mathbf{q} = \frac{\boldsymbol{U_N - \frac{N}{2}\hbar\omega}}{\boldsymbol{\hbar\omega}}$$



Find multiplicity $\Omega(q, N)$ of a macrostate with N oscillators and q units of energy distributed between them

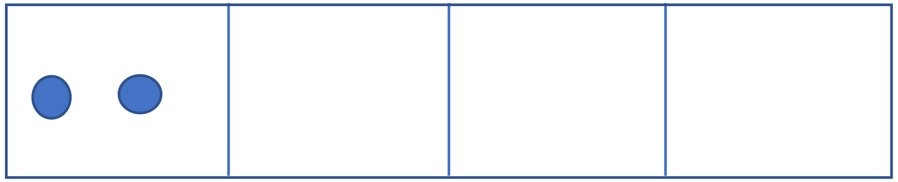
$$q = 1, \qquad N = 4$$

$$\Omega(1{,}4) = 4$$



Find multiplicity $\Omega(q, N)$ of a macrostate with N oscillators and q units of energy distributed between them

1 oscillators has 2 energy quanta, and 3 oscillators are in the ground state

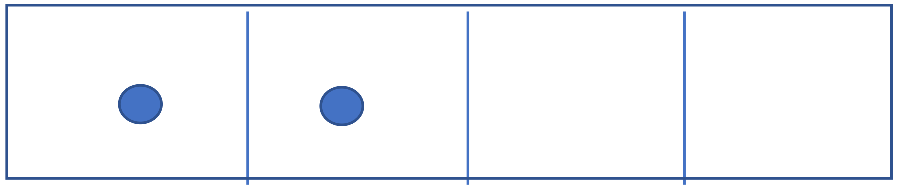


$$q = 2, \qquad N = 4$$

$$\Omega(2,4) = ?$$

$$\Omega(2,4) = 10$$

2 oscillators have 1 energy quanta each, and 2 oscillators are in the ground state

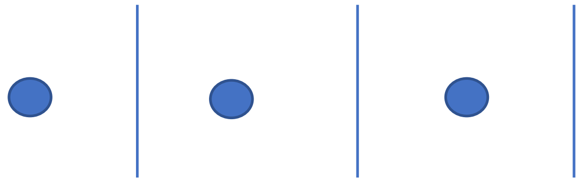


Find multiplicity $\Omega(q, N)$ of a macrostate with N oscillators and q units of energy distributed between them

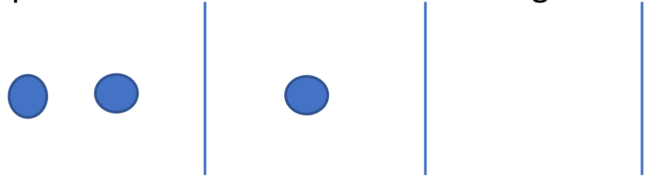
$$\Omega(3,4) =?$$

$$\Omega(3,4) = 20$$

3 oscillators are in an excited state, and the 4th is in the ground state

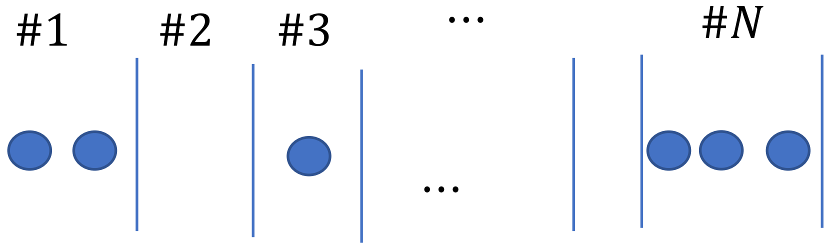


1 oscillators has 2 energy quanta, 1 oscillator has 1 energy quanta and 2 oscillators are in the ground state



1 oscillators has 3 energy quanta, and 3 oscillators are in the ground state

Find multiplicity $\Omega(q, N)$ of a macrostate with N oscillators and q units of energy distributed between them



q energy units $\sim q$ identical balls

N oscillators $\sim$ N identical boxes

Number of ways of distributing q balls between N boxed is the same as the number of combinations with q balls and (N-1)-walls between the lined up boxes

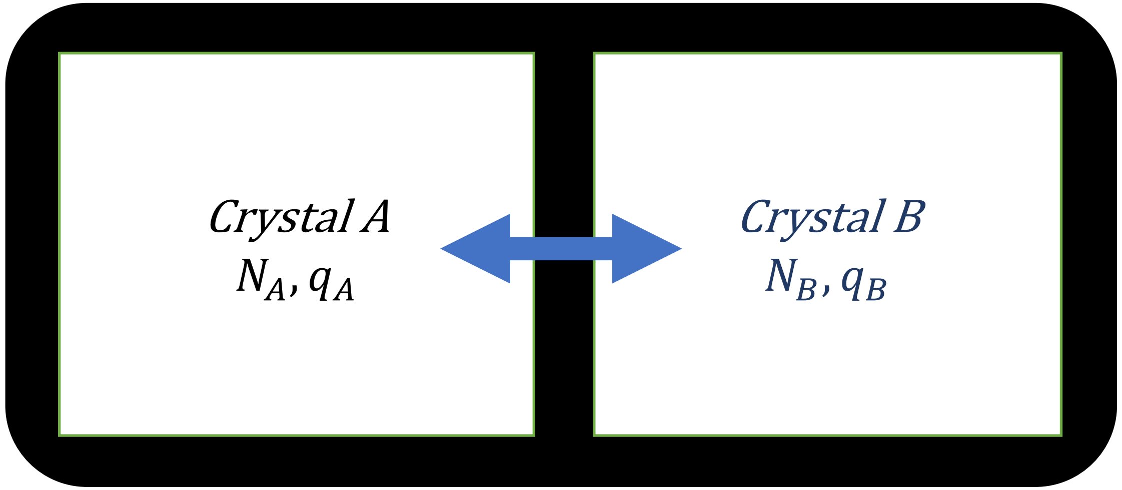
Number of ways of combining *(N-1)-walls* and q balls

$$\Omega(q, N) = \frac{(N-1+q)!}{q!\,(N-1)!}$$

Weakly-coupled Einstein crystals

$$\Omega_{\mathrm{A}}(q_A, N_A) = \frac{(N_A - 1 + q_A)!}{q_A!\,(N_A - 1)!}$$

$$\Omega(q_B, N_B) = \frac{(N_B - 1 + q_B)!}{q_B!\,(N_B - 1)!}$$



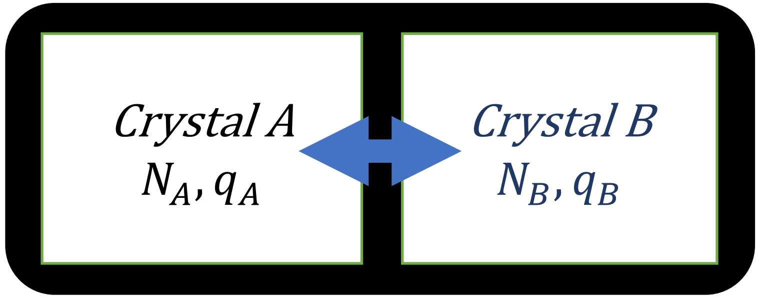
Composite system:

$$q = q_A + q_B, \qquad N = N_A + N_B$$

Multiplicity of a macrostate of the composite systems

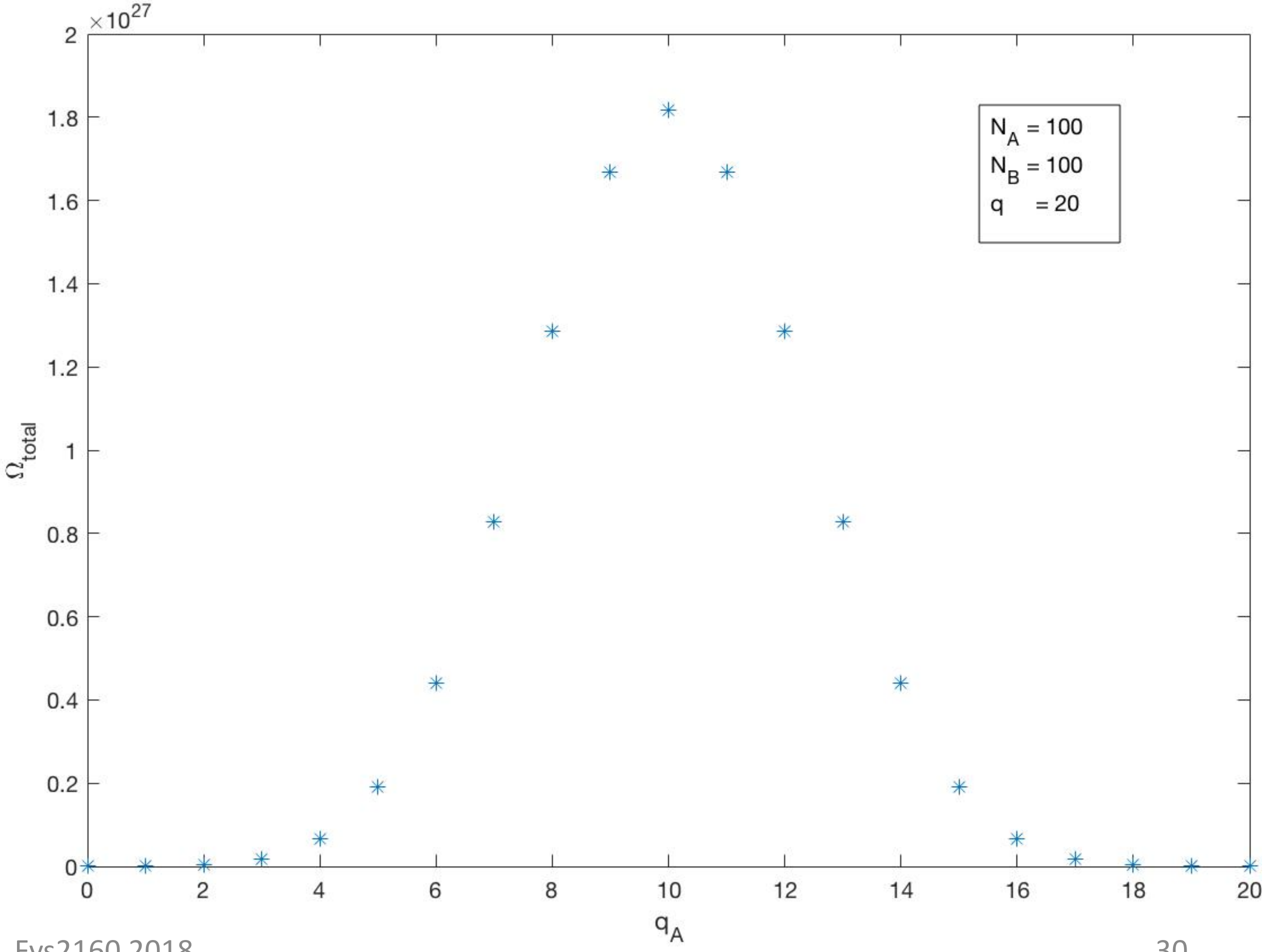
$$\boldsymbol{\Omega_{\mathrm{t}} = \Omega_A(q_A, N_A) \cdot \Omega_B(q_B, N_B)}$$

Weakly-coupled Einstein crystals



Multiplicity of a macrostate with q_A and $q_B = q - q_A$ for two coupled Einstein solids

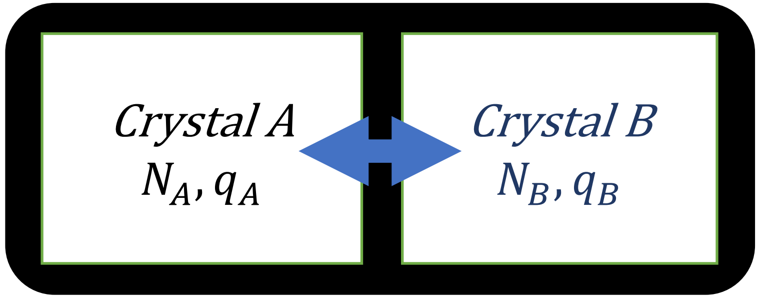
$$\boldsymbol{\Omega_t(q_A, q, N)}$$
$$= \boldsymbol{\Omega_A(q_A, N_A) \cdot \Omega_B(q_B, N_B)}$$



What the macrostate with the maximum multiplicity ?

Matlab tests..

Weakly-coupled Einstein crystals

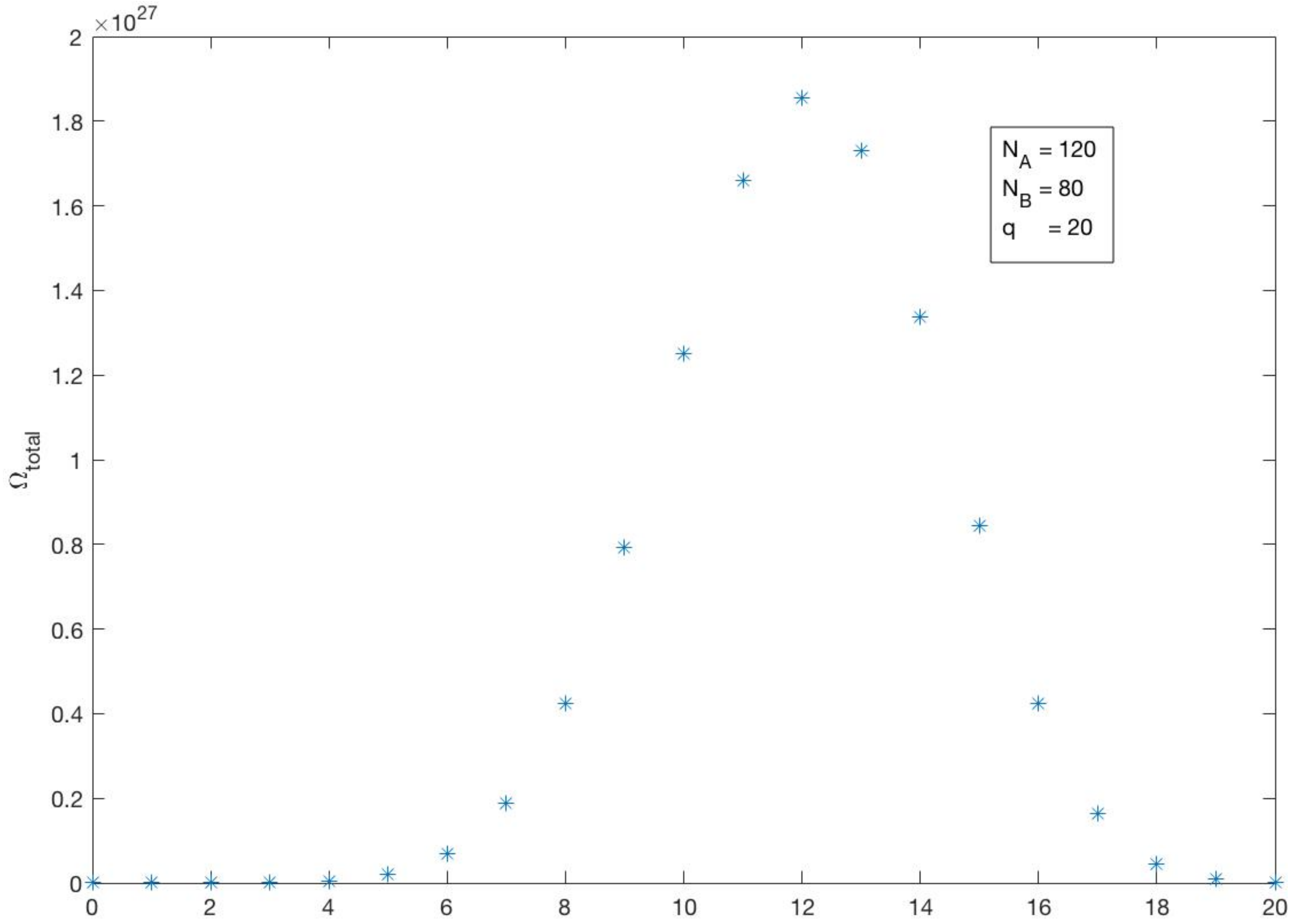


Multiplicity of a macrostate with q_A and $q_B = q - q_A$ for two coupled Einstein solids

$$\boldsymbol{\Omega_t(q_A, q, N) = \Omega_A(q_A, N_A) \cdot \Omega_B(q_B, N_B)}$$

What the macrostate with the maximum multiplicity ?

Matlab tests..



Take home---

- Multiplicity in two-state systems (paramagnets, random walk)

$$\Omega(n, N) = \frac{N!}{n!\,(N-n)!}$$

has a **maximum** peaked around the **average value** $\langle n \rangle$

- Multiplicity in Einstein crystal by analogy with q «identical balls» (energy units) and N «identical bins» (oscillators)

$$\Omega(q, N) = \frac{(N-1+q)!}{(N-1)!\,q!}$$

- Multiplicity of two-coupled Einstein crystal

$$\Omega_{\mathrm{t}} = \Omega_A \cdot \Omega_B$$

has also a maximum around the average value

- Macrostates with maximum multiplicity are the most likely and they correspond to the average values