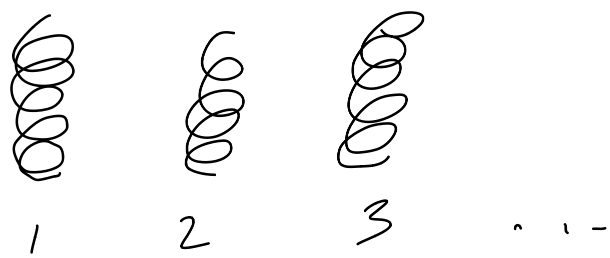
Einstein Solids

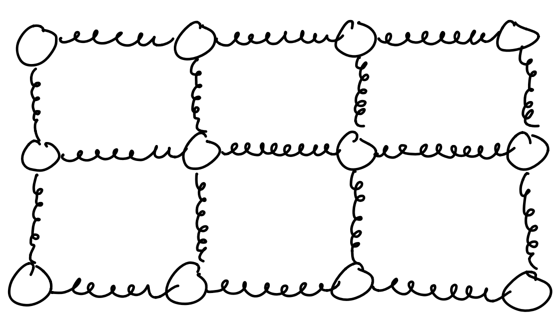
- instead of a bunch of coins, consider a bunch of springs



$$U = \frac{1}{2}k_1x_1^2 + \frac{1}{2}k_2x_2^2 + \frac{1}{2}k_3x_3^2 + \dots$$

Why are we interested in springs?

We can model inter-atomic bonds in a solid this way



Each atom is a quantum harmonic oscillator

Really, each atom is $\underline{\underline{3}}$ quantum HOs

$\uparrow$

x, y, z

This model was proposed by Einstein

$$N_{oscillators} = 3 N_{atoms}$$

Energy of an oscillator

$$E = \frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots$$

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \ldots$$

micro/macro states of a single atom

$N = 3$ oscillators

Minimum Energy: $\frac{1}{2}\hbar\omega$ in each oscillator

$$U_{ground} = \frac{3}{2}\hbar\omega$$

Each oscillator can only increase in units of $\hbar\omega$

Let's look at total energy above the ground state

1	2	3	$U-U_g$
1	4	2	7
$\frac{1}{2}\hbar\omega+\hbar\omega$	$\frac{1}{2}\hbar\omega+4\hbar\omega$	$\frac{1}{2}\hbar\omega+2\hbar\omega$	$\frac{3}{2}\hbar\omega+7\hbar\omega$

No limit on energy, so we can have ∞ # of macrostates

– still finite # Ω per macro

Possible macro states?

0, 1, 2, 3, ...

$$\Omega(0) = 1$$

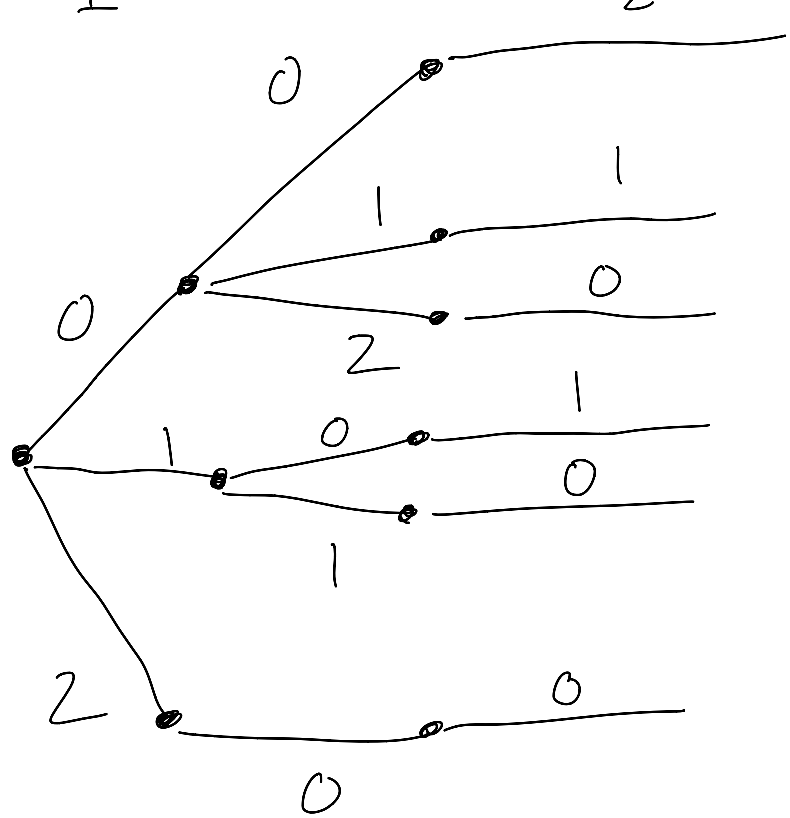
osc #	1	2	3
	0	0	0

$$\Omega(1) = 3$$

1	2	3
1	0	0
0	1	0
0	0	1

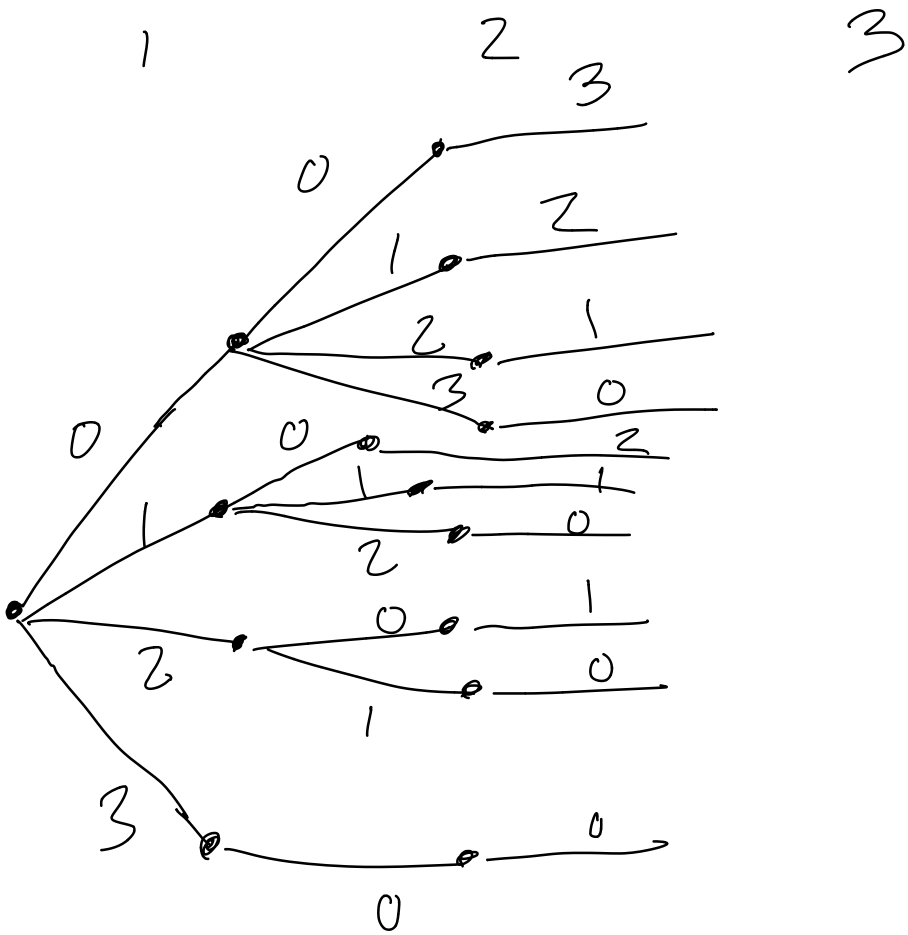
$\Omega(2)$

osc: 1 2 3



0	0	2
0	1	1
0	2	0
1	0	1
1	1	0
2	0	0

$\Omega(2) = 6$



0 0 3
0 1 2
0 2 1
0 3 0
1 0 2
1 1 1
1 2 0
2 0 1
2 1 0
3 0 0

$$\Omega(3) = 10$$

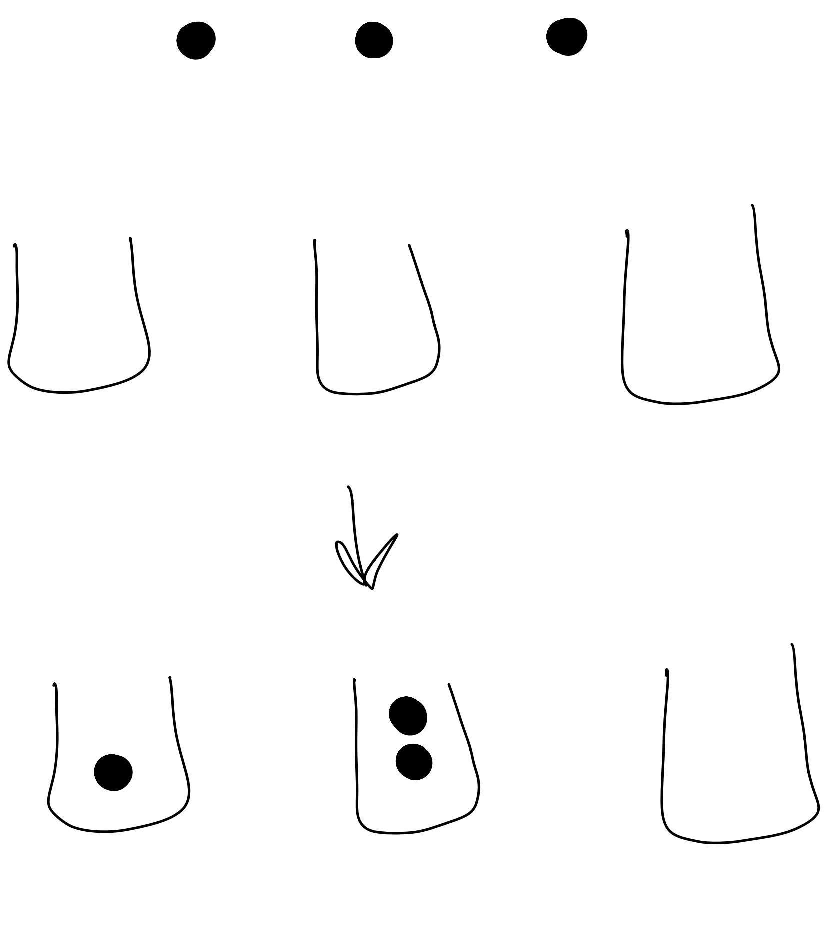
Let's try & generalize this

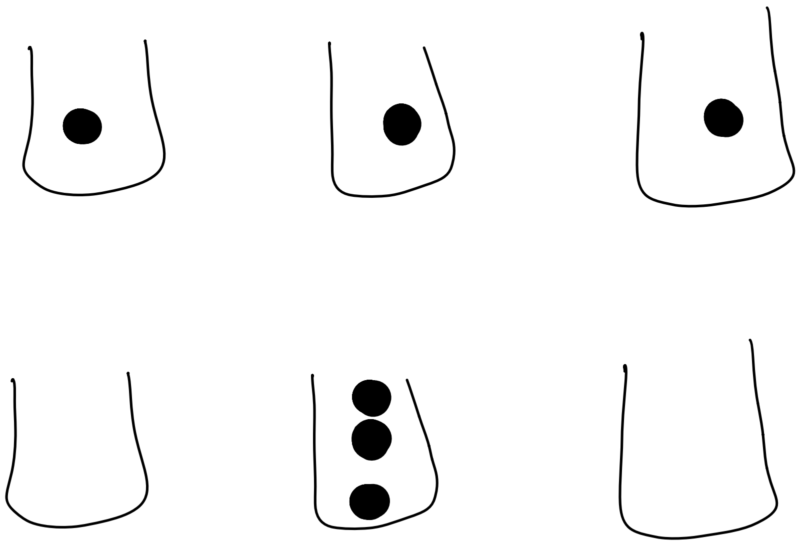
I have some total energy in units of $\hbar\omega$

I have "q" many balls to place,

& "N" many buckets to place them in.

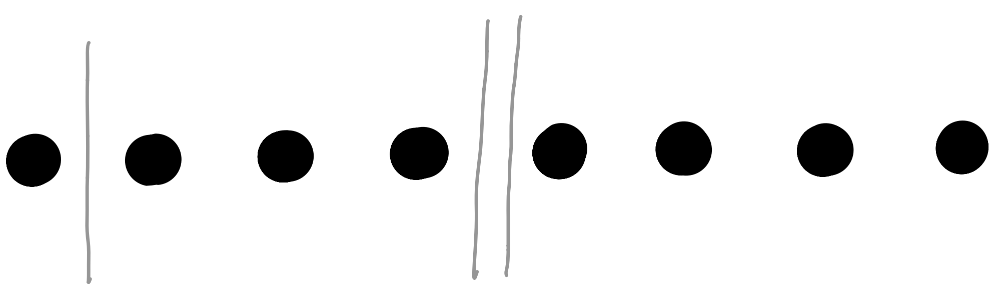
$q = 3$, $N = 3$





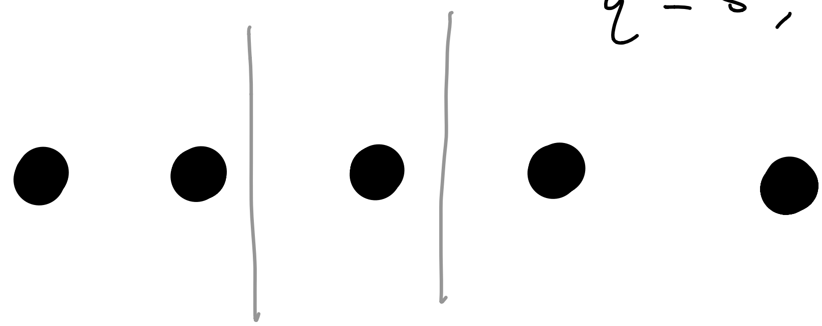
etc . . .

$q = 8, \ N = 4$



1, 3, 0, 4

$q = 5, N = 3$



2 1 2

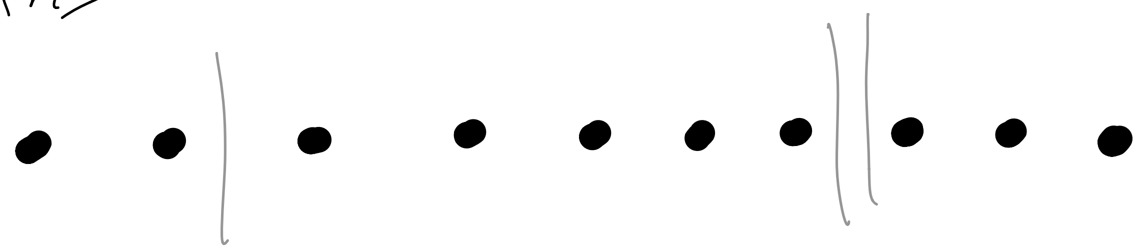
Question

$q = 10, N = 4$

Draw

2, 5, 0, 3

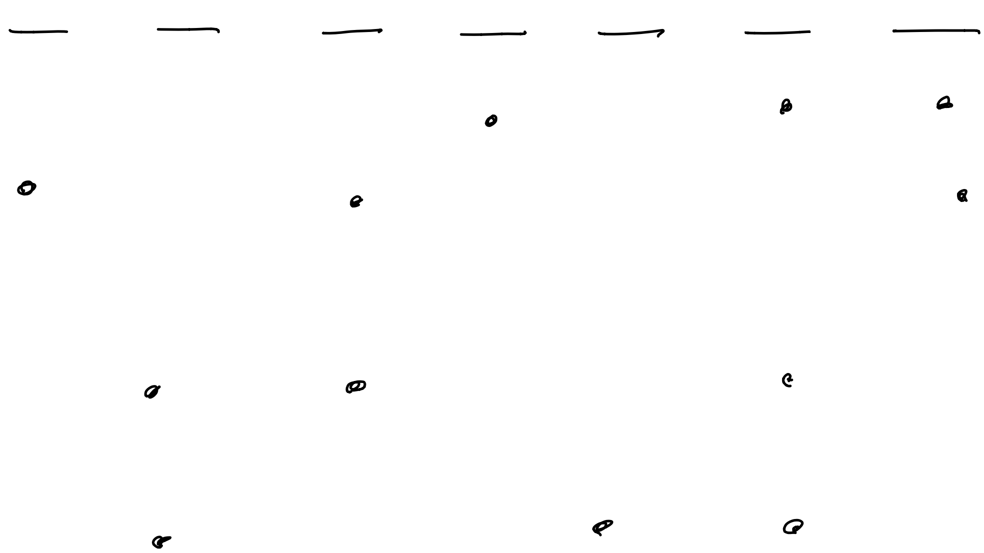
Ans



# of symbols I draw is always $q+N-1$

Out of $q+N-1$ symbols, how many ways to pick q of them to be dots?

$q=3,\ n=4$



1^{st} dot anywhere

$$(q+N-1)$$

2nd dot anywhere but first

$$(q+N-2)$$

3rd dot

$$(q+N-3)$$

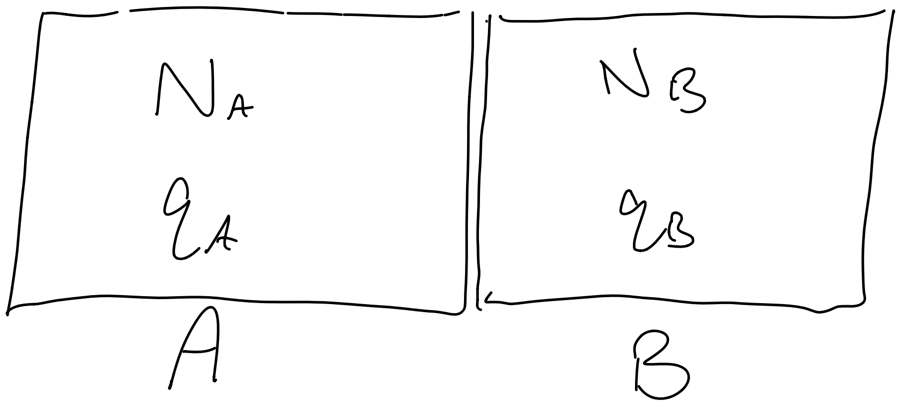
$$\Omega(N,q) = \frac{(q+N-1)!}{(N-1)!}$$

$q!$ many duplicates

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

Show Plot

Now consider 2 of these solids in contact



$$\left.\begin{aligned} U_A &= N_A q_A \hbar\omega \\ U_B &= N_B q_B \hbar\omega \end{aligned}\right\} \text{above } U_{grnd}$$

$$U_{total} = U_A + U_B$$

System is now A + B

$U_A + U_B$ is constant

U_A, U_B can change

Energy can flow

How is energy distributed among them?

Ex

Let's say $N_A = N_B = 3$

3 oscillators in each solid

$U_{total} = q_A + q_B = 6$

Macro states

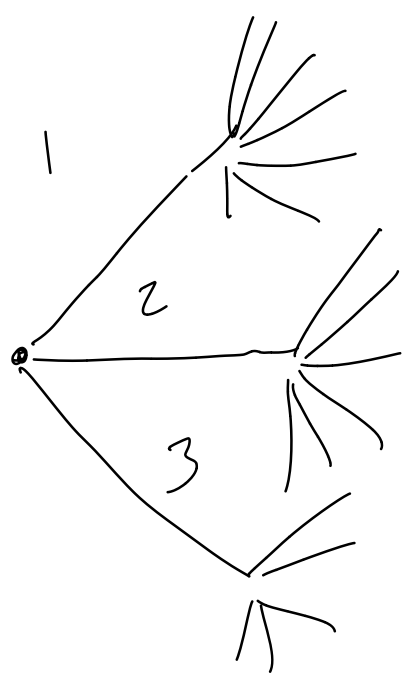
q_A	q_B
6	0
5	1
4	2
3	3
2	4
1	5
0	6

q_A	q_B	Ω_A	Ω_B
0	6	1	28
1	5	3	21
2	4	6	15
3	3	10	10
4	2	15	6
5	1	21	3
6	0	28	1

If there are Ω_A configs in block A, & Ω_B configs in B,

How many are there total?

if $\Omega_A = 3$, $\Omega_B = 21$



$$\Omega_{tot} = \Omega_A \Omega_B$$

q_A	q_B	Ω_A	Ω_B	Ω
0	6	1	28	28
1	5	3	21	63
2	4	6	15	90
3	3	10	10	100
4	2	15	6	90
5	1	21	3	63
6	0	28	1	28
				462

A_1	A_2	A_3	B_1	B_2	B_3
0	2	4	0	0	0
0	1	1	2	2	0

Question: which macrostates are most probable?

Same as with coin flips

$$\text{prob}(q_A) = \frac{\Omega(q_A)}{\Omega(\text{all})}$$

- We just made a big assumption

- this assumes that each individual microstate is equally likely

    - If all microstates have same energy

- Fundamental Assumption of Stat. Mech

$$\text{Prob}(q_A=6, q_B=0) = \frac{28}{462} = 6\%$$

$$\text{Prob}(q_a=5) = \frac{63}{462} = 14\%$$

$$P(q_a=4) = \frac{90}{462} = 19\%$$

$$P(q_a=3) = \frac{100}{462} = 22\%$$

All <u>micro</u>states are equally likely,

but not all <u>macro</u>states!

Most likely state is ~3-4 times more likely than least likely

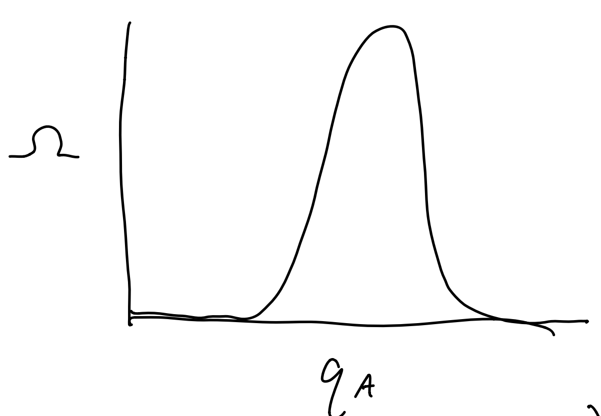
-Now let's bump the numbers up
(Jupyter program)

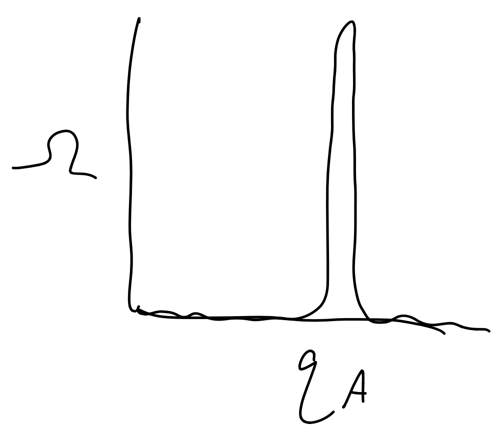
MANY more configurations

-Even the least likely macrostate state has 10^81 microstates
-What matters is not the absolute number, but the *relative* number
-Most likely state has 10^114 microstates
-So most likely state is 10^(114-81) times more likely (10^33)
-Relatively narrow range of probable outcomes

Range narrows as N & q increase

$N, q \approx 100$ $\qquad\qquad$ $N, q \approx 1{,}000$

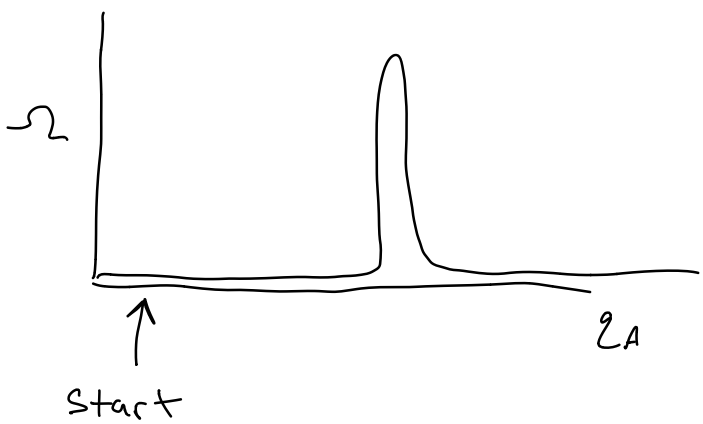




most likely, $q_A = 60$ $\left(\frac{q_A}{q_{tot}} = \frac{3}{5}\right)$ $\frac{N_A}{N_{tot}} = \frac{3}{5}$

We will see that, for "normal" sized systems (N,q >~ 10^20)
- -This function is *very* sharply peaked
- -Outside of the peak, states are *effectively* impossible
  - -You'd have to wait much longer than the Universe!

Consider we arrange the system so that the initial state is with $q_A \sim 0$ (separate the blocks, cool one, heat the other)



Now wait a little while & check again

- Almost certain to find $q_A \approx 60$

- Could wait billions of years, & would never find it back in the $q_A \sim 0$ state

- Flow of energy from B to A is
  - spontaneous
  - irreversible

- We have (sort of) derived heat!
  - Heat is a probabalistic phenomenon
    - most microscopic configurations correspond to ~equally shared energy

- 2ND Law of Thermo

  Spontaneous flow of energy continues until the most likely macrostate