Large Systems and Stirling's Approximation

Prof. Cyr-Racine

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1 Larger Einstein Solids

Consider two larger Einstein solids with

- $N_A = 300$, $N_B = 200$, and $q_{\text{tot}} = 100$.
- There are now 101 macrostates.
- We calculate the multiplicity for each macrostate (defined by q_A) using the general equation

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

q_A	$\Omega_A(300, q_A)$	q_B $(100 - q_A)$	$\Omega_B(200, q_B)$	$\Omega_{\text{tot}} = \Omega_A \Omega_B$
0	1	100	2.8×10^{81}	2.8×10^{81}
1	300	99	9.3×10^{80}	2.8×10^{83}
2	45150	98	3.1×10^{80}	1.4×10^{85}
⋮	⋮	⋮	⋮	⋮
59	2.2×10^{68}	41	3.1×10^{46}	6.7×10^{114}
60	$\mathbf{1.3 \times 10^{69}}$	**40**	$\mathbf{5.3 \times 10^{45}}$	$\mathbf{6.9 \times 10^{114}}$
61	7.7×10^{69}	39	8.8×10^{44}	6.8×10^{114}
⋮	⋮	⋮	⋮	⋮
100	1.7×10^{96}	0	1	1.7×10^{96}

Conclusion:

- The total number of microstates is 9.3×10^{115}.
- The total number of microstates for $q_A = 59, 60,$ and 61 is 2.0×10^{115}, a large fraction of this total.
- The macrostate with $q_A = 60$ and $q_B = 40$ (equipartition of energy, on a per oscillator basis) has the largest multiplicity ($\Omega_{\text{tot}} = 6.9 \times 10^{114}$) and thus the highest entropy. It is the most likely state for the combined system to be in at equilibrium.
- Even for this relatively modest combined solid, the number of microstates involved is already humongous. We will need better computational tools to handle $N \sim 10^{23}$.

2 Large Numbers and Stirling's formula

2.1 Types of numbers

In this course, we will encounter 3 types of numbers

- **Small numbers**: These are the ordinary numbers we encounter all the time: 2, 5, 10,100.
- **Large numbers**: These are typically exponential of small numbers like 10^{23}. One thing to keep in mind is that adding a small number to a large number leaves it unchanged, that is,

$$10^{23} + 20 = 10^{23}. \tag{2}$$

- **Very large numbers**: These are typically exponential of large numbers, e.g. $10^{10^{23}}$. These numbers are so large that it is very difficult to give meanings to them. For example, you can take a very large number and multiply it by a large number and leave it unchanged

$$10^{10^{23}} \times 10^{23} = 10^{10^{23}+23} = 10^{10^{23}}. \tag{3}$$

The above should convince you that these numbers cannot really have physical meaning (they only appear in combinatorics): I can express the same quantity in microns (10^{-6} m) or lightyears (9.46×10^{15} m) and I get the exact same number!

2.2 Stirling's Approximation

As we have seen with the two-state system and the Einstein solid, the multiplicity of microstates typically involves $N!$, where N is a large number like $\sim 10^{23}$. We will need a trick to handle such very large numbers. Stirling's approximation allows us to turn factorials of large numbers into exponentials

$$N! \approx N^N e^{-N} \sqrt{2\pi N}, \qquad (N \gg 1). \tag{4}$$

You will derive the above in the homework. We will often take the logarithm of very large numbers (to compute the entropy, say), in which case, Stirling's approximation takes the form

$$\ln N! \approx N \ln N - N, \tag{5}$$

where we have neglected the $(1/2)\ln(2\pi N)$ term since $\ln N \ll N$ for large N.

Example: Multiplicity of a large Einstein solid Consider an Einstein solid with $N \gg 1$ and $q \gg 1$. The multiplicity of any of its macrostates is

$$\Omega(N,q) = \frac{(q+N-1)!}{q!(N-1)!} \approx \frac{(q+N)!}{q!N!}. \tag{6}$$

Taking the logarithm, we obtain

$$\begin{aligned}
\ln \Omega(N,q) &= \ln\left(\frac{(q+N)!}{q!N!}\right) \\
&= \ln(q+N)! - \ln q! - \ln N! \\
&\approx (q+N)\ln(q+N) - (q+N) - q\ln q + q - N\ln N + N \\
&= (q+N)\ln(q+N) - q\ln q - N\ln N.
\end{aligned} \tag{7}$$

This is a far as we can go without further assumptions. As an example, let's consider the high-energy limit (or high-temperature) limit $q \gg N$.

$$\begin{aligned}
\ln(q+N) &= \ln\left[q\left(1+\frac{N}{q}\right)\right] \\
&= \ln q + \ln\left(1+\frac{N}{q}\right) \\
&\approx \ln q + \frac{N}{q},
\end{aligned} \tag{8}$$

since $\ln(1+x) \approx x$ for $x \ll 1$. Plugging this back into the above, we obtain

$$\begin{aligned}
\ln \Omega(N,q) &\approx (q+N)\left(\ln q + \frac{N}{q}\right) - q\ln q - N\ln N \\
&= N\ln q + N + \frac{N^2}{q} - N\ln N \\
&= N\ln\frac{q}{N} + N + \frac{N^2}{q}.
\end{aligned} \tag{9}$$

The third term is negligible compared to the second one for $q \gg N$. Exponentiating on both sides we get,

$$\Omega(N,q) \approx e^{N\ln(q/N)}e^N = \left(\frac{eq}{N}\right)^N, \qquad (q \gg N). \tag{10}$$