Useful Mathematical Tricks for this Course

In this document, we will always use the convention that

$$\log x = \ln x \tag{1}$$

is the natural logarithm, and not $\log_{10} x$ or $\log_2 x$ as is more common in other courses.

Exercise 1   Understanding the Stirling-Approximation

The goal of this exercise is to better understand where the Stirling-approximation comes from, and why it is justified to use it.

(a) Using properties of the logarithm and the definition $N! = 1 \cdot 2 \cdot \dots \cdot N$, show that

$$\log N! = \log 2 + \dots + \log N \tag{2}$$

(b) Explain how the above sum for $\log N!$ simply corresponds to the total area of the first $N-1$ rectangles shown in grey in Figure 1 from $x = 1$ up to $x = N$. *Hint*: Argue that the area of the "first rectangle" (from $x = 1$ to $x = 2$) is equal to $\log 2$, the area of the "second rectangle" is equal to $\log 3$ etc.
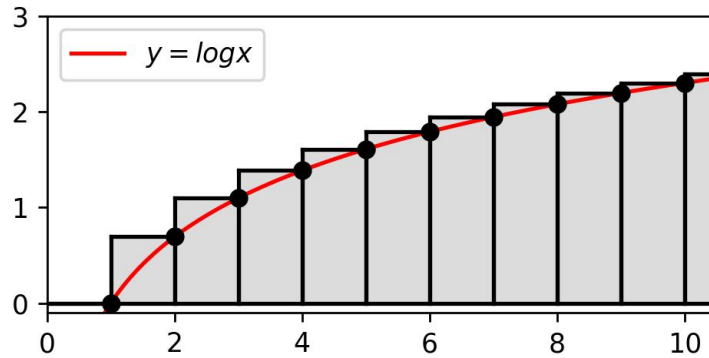

Figure 1: Visual Representation of Stirling-Approximation

(c) When we define integrals for the first time in our lives, we probably visualized the integral $\int_a^b f(x)\,dx$ of a function as the area under the curve of f, for which we can obtain better and better approximations by using rectangles under the curve. In other words, we usually use the area of rectangles as an approximation to the continuous integral. Here, we do the opposite: Use the approximation

$$\log 1 + \dots + \log N \approx \int_1^N \log x \, dx \tag{3}$$

to derive the Stirling-approximation

$$\log N! \approx N \log N - N, \tag{4}$$

where you may need to neglect some terms (see next exercise for a detailed discussion).

(d) The full version of the Stirling formula is

$$\log N! = N \log N - N + \frac{1}{2} \log N + \frac{1}{2} \log 2\pi + \frac{1}{12N} - \frac{1}{360N^3} + O\left(\frac{1}{N^5}\right) \tag{5}$$

If $N = 10^{20}$, explain how big roughly the terms in this expansion are (just the order of magnitude is enough). How can we justify the fact that we usually only keep the first two terms? How precise would our experimental devices need to be to measure the first correction term? *Hint*: $\log 10 \approx 2.3$.

Exercise 2   Stirling-Approximation applied to Combinatorics

We now show a nice trick using the Stirling-approximation that is used a lot in the lecture, which will allow you to do complicated calculations from combinatorics in just a few seconds!

(a) In combinatorics, we will often use the expression

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \tag{6}$$

which is pronounced as "n choose k". Depending on the country, this expression can also be written as $C_{n,k}$ or $_n C_k$. The combinatorial interpretation of this expression is the following: this is the number of ways we have for choosing k objects out of n. Please make sure that you understand this, since this will be used in the lecture multiple times, and also in the next exercise. If you need a refresher, here is a video that explains it. Also, do not hesitate to ask the TAs to explain it to you (not just for this question, but in general)!

(b) Let us now apply the Stirling-Approximation to the logarithm of the combination formula

$$\log\binom{n}{k} = \log\left(\frac{n!}{k!(n-k)!}\right) = \log n! - \log k! - \log(n-k)! \tag{7}$$

Naively, we need to apply the Stirling formula three times, and each of those leads to two terms since $\log n! = n \log n - n$ etc. What a mess! But thankfully, half of the terms will cancel, and we obtain the much simpler formula

$$\log\binom{n}{k} = n \log n - k \log k - (n-k) \log(n-k) \tag{8}$$

which can be obtained by simply using $\log n! \approx n \log n$. Starting from the better expression $\log n! \approx n \log n - n$, show that the second term with $-n$ does indeed cancel out between the three terms.

Remark: the Stirling-approximation used on such combinatorial expressions appears multiple times in the lecture, e.g. in slides 3 pages 10, 11 and 14, slides 4 pages 5 and 8, slides 5 page 19 etc.

How to Calculate Material Properties from the Entropy

Exercise 3   2-Level System in Microcanonical Ensemble

We now study the thermodynamic properties of a simple model system using the microcanonical ensemble: a 2-level system.

The system consists of N atoms, and we assume that each of the N atoms can either have an energy of 0 or an energy of $\epsilon > 0$ if the atom is in the excited state. We will later see that this can (effectively) be used as a simple model of magnetic properties of materials.

Working in the microcanonical ensemble means that we know the total number of atoms N and the total energy E of the system.

(a) Let us assume that $E = M\epsilon$ for some natural number $M = E/\epsilon$. This means that out of all N atoms, M are in the excited state, and $N - M$ are in the ground state. How many ways $\Omega(N, E)$ are there to select the excited atoms?

(b) Show that the entropy $S(E, N)$ of the system can be compactly written as

$$\frac{S(E, N)}{k_B} = N \log N - M \log M - (N - M) \log(N - M). \tag{9}$$

Hint: we used two tricks here: firstly, we use $M = E/\epsilon$ instead of E to save some space. Also, the Boltzmann constant k_B would usually be on the right side, since $S = k_B \log \Omega$, but we write $\frac{S}{k_B} = \log \Omega$ instead. Bringing k_B to the left side is often useful because we will now do some calculations with the right side of the equation, and k_B is just a constant multiplication factor, so there is no need to keep doing all calculations with this extra factor. If we don't use these tricks, we need to write

$$S(E, N) = k_B \left[N \log N - \frac{E}{\epsilon} \log M - (N - \frac{E}{\epsilon}) \log(N - \frac{E}{\epsilon}) \right] \tag{10}$$

which is harder to read and makes the equation look scarier than necessary.

(c) Differentiate the previous equation with respect to E to show that

$$\frac{\epsilon}{k_B T} = \log \frac{N - M}{M} \tag{11}$$

Hint: Instead of working with E, it is easier to work with M. A derivative with respect to E can be turned into a derivative with respect to M by using the chain rule

$$\frac{\partial f}{\partial E} = \frac{\partial f}{\partial M} \frac{\partial M}{\partial E} = \frac{1}{\epsilon} \frac{\partial f}{\partial M} \tag{12}$$

Here, ϵ is just a constant number, so you can multiply the entire equation to bring it to the right side (just like k_B) to simplify your calculations.

(d) The combination $1/k_B T$ appear so often in statistical mechanics that we give it a special symbol: we define $\beta = 1/k_B T$. Using this shortcut, show that

$$E(T, N) = \frac{N\epsilon}{1 + e^{\beta \epsilon}} \tag{13}$$

Hint: Keep using M and first show that $M = \frac{N}{1 + e^{\beta \epsilon}}$

(e) Show that the energy per particle is equal to

$$\frac{E}{N} = \frac{\epsilon}{1 + e^{\beta \epsilon}} = \epsilon \cdot n_{excited} \tag{14}$$

and explain how we can interpret $n_{excited} = \frac{1}{1 + e^{\beta \epsilon}}$ as the fraction of particles that are in the excited state as a function of temperature, or as the probability that a particle is in the excited state.

(f) Show that

$$\lim_{T \to 0} n_{excited} = 0 \qquad \lim_{T \to \infty} n_{excited} = \frac{1}{2} \tag{15}$$

Can you come up with an interpretation of these results?

(g) We now want to connect this with experimentally measurable quantities. Describe which mathematical steps would be necessary (you don't need to do the actual calculation) to calculate material properties like the heat capacity $C(T, N)$ or the entropy $S(T, N)$ (but now as a function of temperature instead of energy!).

The End.