Thu 2 Mar 980032

Total $M = \sum_{e_1} M^{(1)}_{e_1} M^{(2)}_{E-e_1}$

Sharp bounds on M

Let "max" be the largest of $N_{terms} \geq 1$ in sum

$$\max \leq M \leq N_{terms} \cdot \max$$

$$\log(\max) \leq S \leq \log(N_{terms} \cdot \max)$$

Reasonable illustration:

Suppose $N_{terms} \sim N$, $\max \sim e^N$

(spin system $M = 2^N = e^{N \log 2}$)

$$N \lesssim S \lesssim N + \log(N)$$

$N \sim 10^{23}$: $10^{23} \lesssim S \lesssim 10^{23} + 50$

$\rightarrow S \approx 10^{23}$ for all practical purposes

$N_1 = N_2 = 10$ $E = -10$

$E = -(2n_+ - N) = -10, -8, -6, \ldots, 10$

E_1	E_2	n_1^+	n_2^+	$M_1 M_2$
-10	0	10	5	$1 \cdot \binom{10}{5} = 1 \cdot \frac{10\cdot 9\cdot 8\cdot 7\cdot 6}{5\cdot 4\cdot 3\cdot 2} = 4 \cdot 63 = 252$
-8	-2	9	6	
-6	-4	8	7	$\binom{10}{8}\binom{10}{7} = \frac{10\cdot 9}{2}\,\frac{10\cdot 9\cdot 8}{3\cdot 2} = 45 \cdot 120 = 5400$
-4	-6	7	8	
-2	-8	6	9	
0	-10	5	10	252

$\log(5400) \approx 0.89\,S$

$\frac{5400}{252} \sim 20\times$ $\rightarrow$ expect to see even distrib. of spins

"arrow of time"

MATH327: Statistical Physics, Spring 2023

Tutorial activity — Entropy bounds

We met the second law of thermodynamics by considering what happens when two subsystems are brought into thermal contact — allowed to exchange energy but not particles. Conservation of energy means that if subsystem Ω_1 has energy e_1, the other subsystem Ω_2 must have energy $E - e_1$, where E is the total energy of the overall micro-canonical system Ω. We found (in Eq. 21 on page 33 of the lecture notes) that the total number of micro-states of the overall system is

$$M = \sum_{e_1} M^{(1)}_{e_1} M^{(2)}_{E-e_1}$$

where $M^{(S)}_e$ is the number of micro-states of subsystem $S \in \{1, 2\}$ with energy e.

Because M is a sum of strictly positive terms, we can easily set bounds on it. Say the sum over e_1 has $N_{\textsf{terms}} \geq 1$ terms $M^{(1)}_{e_1} M^{(2)}_{E-e_1}$, and define $\max$ be the largest of those terms. Then $\max \leq M$, with equality only when $N_{\textsf{terms}} = 1$. Similarly, $M \leq N_{\textsf{terms}} \cdot \max$, with equality when every term in the sum is the same. All together, we have

$$\max \leq M \leq N_{\textsf{terms}} \cdot \max .$$

This can be more powerful than it may initially appear, thanks to the large numbers involved in statistical physics. For illustration, suppose $\max \sim e^N$ and $N_{\textsf{terms}} \sim N$ for a system with N degrees of freedom. (We have already seen $M = 2^N = e^{N \log 2}$ for a system of N spins with $H = 0$, while $H > 0$ introduces factors of $N!$ that Stirling's formula can recast in terms of $N^N = e^{N \log N}$.) Then

$$e^N \lesssim M \lesssim N e^N .$$

If we take the logarithm and recall $\log M = S$ is the entropy, this gives us

$$N \lesssim S \lesssim N + \log N.$$

With our characteristic $N \sim 10^{23}$, we have $\log N \sim 50$ and $10^{23} \lesssim S \lesssim 10^{23} + 50$, a very tight range in relative terms, with the upper bound only $\sim 10^{-20}\%$ larger than the lower bound.

To see how this works in practice, let each of Ω_1 and Ω_2 be a spin system with $N_1 = N_2 = 10$ spins and $H = 1$. Fix $E = -10$ for the combined system and numerically compute the bounds on its entropy,

$$\log(\max) \leq S \leq \log(N_{\textsf{terms}} \cdot \max) .$$

What fraction of the true entropy S is accounted for by $\log(\max)$? How do these answers change for $N_1 = N_2 = 20, 30, 40, \cdots$, still with fixed $E = -10$?

By considering the sort of spin configurations that produce $\max$, you can see the emergence of an 'arrow of time'!

Stirling's Formula

$$\log(N!) \approx N\log N - N \quad \rightarrow \quad N! = \exp(N\log N - N) = N^N e^{-N} = \left(\frac{N}{e}\right)^N$$

$N \gg 1$

More precise

$$N! = \sqrt{2\pi N}\left(\frac{N}{e}\right)^N \left(1 + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3} + \dots\right)$$

(asymptotic)

1) Simple bounds

$$N\log N - N < \log(N!) < N\log N$$

2) $N! \approx \sqrt{2\pi N}\left(\frac{N}{e}\right)^N$

by showing $N! = \int_0^\infty x^N e^{-x}\, dx$

↳ approximate by gaussian

3) Compute A, B, ...

by comparing $N!$ vs. $(N+1)! = (N+1)N!$

MATH327: Statistical Physics, Spring 2023

Tutorial activity — Stirling's formula

We have already made use of Stirling's formula in the following form:

$$\log(N!) = N \log N - N + \mathcal{O}(\log N) \approx N \log N - N \qquad \text{for } N \gg 1,$$

which implies

$$N! \approx \exp\left[N \log N - N\right] = \left(\frac{N}{e}\right)^N.$$

This can be made more precise:

$$N! = \sqrt{2\pi N}\left(\frac{N}{e}\right)^N \left(1 + \frac{A}{N} + \frac{B}{N^2} + \frac{C}{N^3} + \cdots\right) \tag{1}$$

with calculable coefficients A, B, C, etc.[1] By performing a sequence of analyses of increasing complexity, we can build up these results.

First analysis: Derive the bounds

$$N \log N - N < \log(N!) < N \log N \tag{2}$$

for $N \gg 1$. The second bound is the easier one. There are multiple ways to obtain the first bound. One pleasant approach is to consider the series expansion for e^x. Together, these bounds establish

$$1 - \frac{1}{\log N} < \frac{\log(N!)}{N \log N} < 1 \qquad \Longrightarrow \qquad \log(N!) \sim N \log N$$

Second analysis: Compute the first term in Eq. 1, $N! \approx \sqrt{2\pi N}\left(\frac{N}{e}\right)^N$. This requires several steps, the first of which is to consider the **gamma function**

$$\Gamma(N+1) \equiv \int_0^\infty x^N e^{-x}\, dx.$$

Show that $\Gamma(N+1) = N!$ for integer $N \geq 0$. In other words, derive the Euler integral (of the second kind)

$$N! = \int_0^\infty x^N e^{-x}\, dx. \tag{3}$$

Again, this can be done in multiple ways, including induction with integration by parts or by taking derivatives of

$$\int_0^\infty e^{-ax}\, dx = a^{-1}$$

and then setting $a = 1$.

[1] James Stirling computed the $\sqrt{2\pi}$ while Abraham de Moivre derived the expansion in powers of $1/N$. An interesting aspect of this expansion is that it is **asymptotic** — it has a vanishing radius of convergence but can provide precise approximations if truncated at an appropriate power.

The next step in this second analysis is to approximate the gamma function as a gaussian integral. Show that the integrand $x^N e^{-x} = \exp\left[N \log x - x\right]$ of Eq. 3 is maximized at $x = N$.

For $N \gg 1$, the integrand is sharply peaked around this maximum at $x = N$. You can check this for yourself or take it as given. We can therefore focus on a small region around this peak by changing variables to $y \equiv x - N$ and considering $\left|\frac{y}{N}\right| \ll 1$. Expand the $\log x$ in the integrand, up to and including terms quadratic in $\frac{y}{N}$. You should be left with the desired result, except for the following factor, which can be approximated by a gaussian integral (note the lower bound of integration):

$$\int_{-N}^{\infty} e^{-y^2/(2N)}\, dy \approx \int_{-\infty}^{\infty} e^{-y^2/(2N)} = \sqrt{2\pi N}.$$

The error introduced by extending the integration from $(-N, \infty)$ to $(-\infty, \infty)$ is exponentially small and could be captured by computing the series of corrections suppressed by powers of $\frac{1}{N}$ in Eq. 1.

This leads us to the **third analysis**: Compute some of the leading power-suppressed corrections in Eq. 1. That is, determine the coefficients A, B, etc. Again, there are many ways to achieve this, including higher-order expansions of the $\log x$ considered above. One pleasant approach is to compare $N!$ and $(N+1)!$, now that we have derived the series prefactor $\sqrt{2\pi N}\left(\frac{N}{e}\right)^N$.