

Entropy of a spin system

From the problem “Accessible configurations of a spin system” ...

$$\Omega(E, \Delta E, H, N) = \frac{N!}{\left[\frac{1}{2}(N + E/mH)\right]! \left[\frac{1}{2}(N - E/mH)\right]!} \frac{\Delta E}{2mH}.$$

a.

$$\begin{aligned} \ln \Omega &= \ln N! - \ln \left[\frac{1}{2}(N + E/mH)\right]! - \ln \left[\frac{1}{2}(N - E/mH)\right]! + \ln(\Delta E/2mH) \\ &\approx N \ln N - N - \left[\frac{1}{2}(N + E/mH)\right] \ln \left[\frac{1}{2}(N + E/mH)\right] + \left[\frac{1}{2}(N + E/mH)\right] \\ &\quad - \left[\frac{1}{2}(N - E/mH)\right] \ln \left[\frac{1}{2}(N - E/mH)\right] + \left[\frac{1}{2}(N - E/mH)\right] + \ln(\Delta E/2mH) \\ &= N \ln N - \left[\frac{1}{2}(N + E/mH)\right] \ln \left[\frac{1}{2}(N + E/mH)\right] \\ &\quad - \left[\frac{1}{2}(N - E/mH)\right] \ln \left[\frac{1}{2}(N - E/mH)\right] + \ln(\Delta E/2mH). \end{aligned}$$

b. To prepare for the thermodynamic limit, define $e \equiv E/N$ and $\delta \equiv \Delta E/N$. Then

$$\begin{aligned} S(E, \Delta E, H, N)/k_B &= N \ln N - \left[\frac{1}{2}(1 + e/mH)N\right] \ln \left[\frac{1}{2}(1 + e/mH)N\right] \\ &\quad - \left[\frac{1}{2}(1 - e/mH)N\right] \ln \left[\frac{1}{2}(1 - e/mH)N\right] + \ln(N\delta/2mH). \end{aligned}$$

To separate out “upper case” quantities (dependent on sample size) from “lower case” quantities (independent of sample size), we write

$$\ln \left[\frac{1}{2}(1 \pm e/mH)N\right] = \ln \left[\frac{1}{2}(1 \pm e/mH)\right] + \ln N$$

so that

$$\begin{aligned} S(E, \Delta E, H, N)/k_B &= N \ln N - \left[\frac{1}{2}(1 + e/mH)N\right] \ln N - \left[\frac{1}{2}(1 - e/mH)N\right] \ln N \\ &\quad - \left[\frac{1}{2}(1 + e/mH)N\right] \ln \left[\frac{1}{2}(1 + e/mH)\right] \\ &\quad - \left[\frac{1}{2}(1 - e/mH)N\right] \ln \left[\frac{1}{2}(1 - e/mH)\right] + \ln(N\delta/2mH). \end{aligned}$$

Here comes the miracle of canceling N-dependent terms... the first line above sums to zero!

$$\frac{S(E, \Delta E, H, N)}{Nk_B} = - \left[\frac{1}{2}(1 + e/mH)\right] \ln \left[\frac{1}{2}(1 + e/mH)\right] - \left[\frac{1}{2}(1 - e/mH)\right] \ln \left[\frac{1}{2}(1 - e/mH)\right] + \frac{\ln(N\delta/2mH)}{N}.$$

The rightmost term above vanishes as $N \rightarrow \infty$, so you never need to take the limit $\delta \rightarrow 0$. The result is that, in the thermodynamic limit,

$$s(e, H) = -k_B \left\{ \left[\frac{1}{2}(1 + e/mH)\right] \ln \left[\frac{1}{2}(1 + e/mH)\right] + \left[\frac{1}{2}(1 - e/mH)\right] \ln \left[\frac{1}{2}(1 - e/mH)\right] \right\}. \quad (1)$$

[[One could “simplify” this expression to

$$s(e, H) = -\frac{k_B}{2} \left\{ -2 \ln 2 + \ln [1 - (e/mH)^2] + (e/mH) \ln \left[\frac{1 + e/mH}{1 - e/mH} \right] \right\}, \quad (2)$$

but it’s actually harder to compute with and to understand form (2), so I recommend against it. For example, the function $s(e/mH)$ is even. This is obvious from expression (1) but obscure from expression (2).]]

c. Define $u \equiv e/mH$ and graph

$$s(u) = -k_B \left\{ \left[\frac{1}{2}(1+u) \right] \ln \left[\frac{1}{2}(1+u) \right] + \left[\frac{1}{2}(1-u) \right] \ln \left[\frac{1}{2}(1-u) \right] \right\}.$$

The energy E ranges from $-NmH$ to $+NmH$, so u ranges from -1 to $+1$.

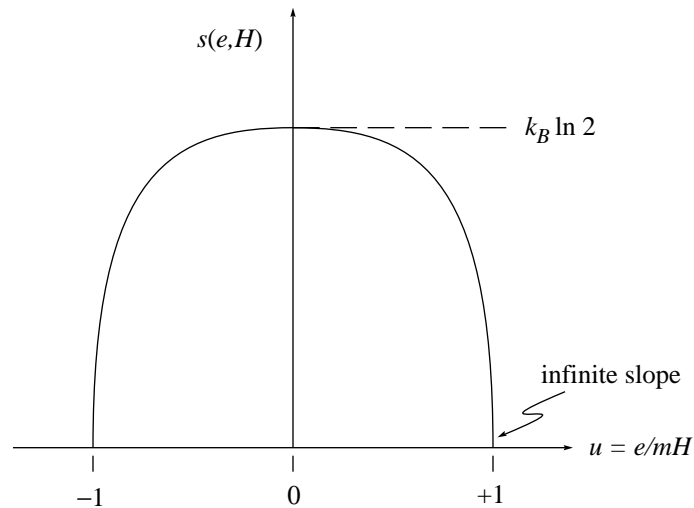
The function $s(u)$ is clearly symmetric about $u = 0$.

The slope

$$\frac{ds}{du} = \frac{k_B}{2} \ln \frac{1-u}{1+u}$$

is positive for $-1 < u < 0$, so $s(u)$ increases monotonically there. (So, despite the minus sign in the formula for $s(u)$, the entropy itself is always positive... good thing, too!)

In sum, the graph of $s(e, H)$ is



This satisfies our expectations at the edge points:

If $e = \pm mH$, we have $\Omega = 1$, so we need $S = k_B \ln \Omega = 0$.