Recap: Friday 14/2/2020

time evolution

output space $\{\omega_1 \ldots \omega_m\}$

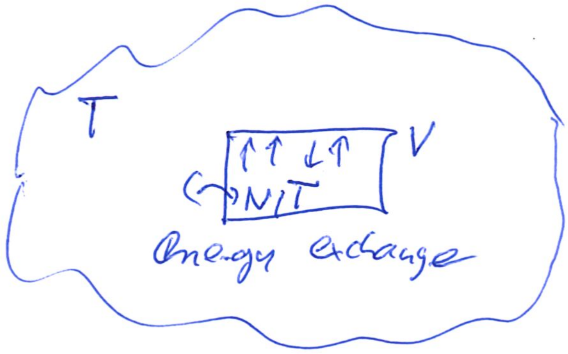
degrees freedom

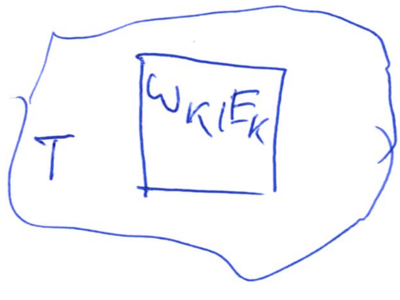
thermodynamical ensemble

probabilities

microcanonical ensemble

Canonical ensemble





probability p_K to find ω_K in the box

$$p_K = \frac{1}{Z} e^{-\beta E_K}$$

$$Z = \sum_{k=1}^{m} e^{-\beta E_k} \quad \text{(partition function)}$$

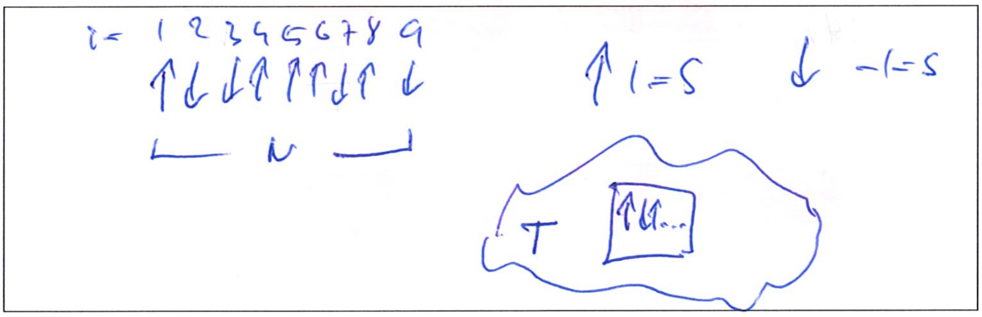
$$\beta = 1/T$$

4.3 Spins in a magnetic fields revisited

Here, we work through a particular example in great detail. However, we will also make a very important observation: whether degrees of freedom are *distinguishable* or *identical* can make a huge difference for the thermal behaviour of the system. This feature is brought to you by quantum physics.

4.3.1 Spins in a solid:

Let us consider N spins in a magnetic field H in a row. The spins are *distinguishable* by their position in the solid[4]. An ensemble (or *event* in probability theory) is a set of N elements each of which is either $+1$ or -1:



We have labelled the spins in a physical way, namely by their postion in the solid. The spins do not interact with each other. The energy of a particular ensemble is given by:

$$E(\{s_i\}) = H \sum_{i=1}^{N} s_i \, .$$

Each state is one-to-one named by the spin values.

Distinguishable: Thus, the sum over all states is given by the sum over all spin configurations.

[4]Properties of individual spins could be measured by a targeted experiment.

notation

The partition function (24) is thus given by:

$$
\begin{aligned}
Z_{\text{dist.}} &= \sum_{s_1=\pm1} \dots \sum_{s_N=\pm1} \exp\Big\{ -\beta\, E(\{s_i\}) \Big\} = \sum_{\{s_i\}} \exp\Big\{ -\beta\, E(\{s_i\}) \Big\} \\
&= \sum_{\{s_i\}} \exp\left\{ -\beta\, H \sum_{i=1}^{N} s_i \right\} \\
&= \sum_{\{s_i\}} \exp\{-\beta\, H\, s_1\} \dots \exp\{-\beta\, H\, s_N\}. \qquad (31)
\end{aligned}
$$

We are now using

$$
(*) \qquad \sum_{i=1}^{N}\sum_{k=1}^{N} a_i b_k = \underbrace{\left(\sum_{i=1}^{N} a_i\right)}_{S} \underbrace{\left(\sum_{k=1}^{N} b_k\right)}_{T} \quad ✓
$$

which also implies

$$
\sum_{i,k,l} a_i b_k c_l = \left(\sum_{i=1}^{N} a_i\right) \left(\sum_{k=1}^{N} b_k\right) \left(\sum_{l=1}^{N} c_l\right) , \qquad \text{etc.}
$$

Let us spent some time to enjoy a bit of mankind's 5000 year legacy - the distributive rule:

$$(a_1 + a_2) b_1 \overset{D}{=} a_1 b_1 + a_2 b_2$$

$$(a_1 + a_2)(b_1 + b_2) \overset{D}{=} a_1 (b_1 + b_2) + a_2 (b_1 + b_2)$$

$$\overset{A}{=} (b_1 + b_2) a_1 + (b_1 + b_2) a_2 \overset{D}{=} a_1 b_1 + a_1 b_2 + b_1 a_2 + b_2 a_2 \quad ✓$$

(*) true for $N=2$: assume: true for N

what? $\left(\sum_{i=1}^{N+1} a_i\right)\left(\sum_{k=1}^{N+1} b_k\right) = \Big(\underbrace{\sum^{N} a_i}_{S} + a_{N+1}\Big)\Big(\underbrace{\sum^{N} b_k}_{T} + b_{N+1}\Big)$

$$= ST + S b_{N+1} + T a_{N+1} + a_{N+1} b_{N+1}$$

(assump.) $\overset{\cdot}{=} \sum_{i,k}^{N} a_i b_k + S b_{N+1} + T a_{N+1} + a_{N+1} b_{N+1}$

$$= \sum_{i,k}^{N+1} a_i b_k \quad ✓$$

We now can re-write (31):

$$
\begin{aligned}
Z_{\text{dist.}} &= \sum_{\{s_i\}} \exp\{-\beta\, H\, s_1\} \ldots \exp\{-\beta\, H\, s_N\} = \\
&= \left(\sum_{s_1} \mathrm{e}^{-\beta H\, s_1} \right) \ldots \left(\sum_{s_N} \mathrm{e}^{-\beta H\, s_N} \right) .
\end{aligned}
$$

If rename the spin variable in each of the sums to, say, s, we find:

$$
Z_{\text{dist.}} = \left(\sum_{s=\pm 1} \mathrm{e}^{-\beta H\, s} \right)^N = \left(\mathrm{e}^{-\beta H} + \mathrm{e}^{\beta H} \right)^N . \tag{32}
$$

$\ln Z = N \cdot \ln(e^{-\beta H} + e^{\beta H})$

The Helmholtz Free Energy F in (27), for our case here

$$
F(T) = -T\, N\, \ln\left(\mathrm{e}^{-\beta H} + \mathrm{e}^{\beta H} \right) , \quad (\beta = 1/T) \tag{33}
$$

is our starting point to calculate the internal energy $\langle E \rangle$ and entropy S:

$$
\langle E \rangle = -T^2 \frac{d}{dT}\left(\frac{F}{T}\right) = T^2 N \frac{d}{dT} \ln\left(e^{-H/T} + e^{H/T}\right)
$$

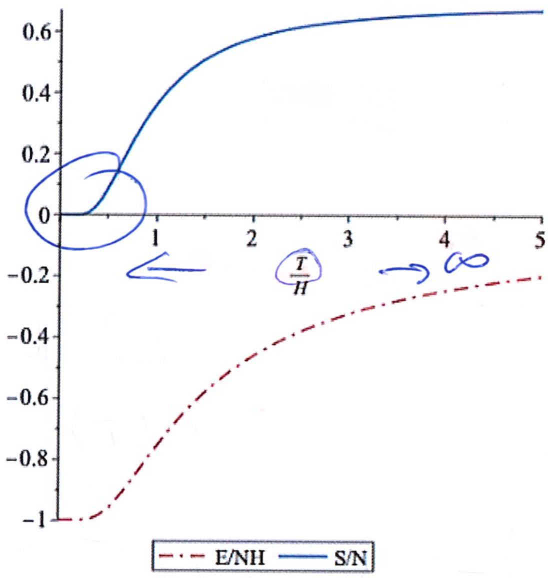
$$
= T^2 N \frac{e^{-H/T} \frac{H}{T^2} + e^{H/T}\left(-\frac{H}{T^2}\right)}{e^{-H/T} + e^{H/T}} = -NH \cdot \tanh(H/T)
$$

$$
\langle S \rangle = -\frac{dF}{dT}
$$

Hence, we have obtained:

$$
\begin{aligned}
\langle E \rangle(T) &= -N\, H \tanh\Big(\beta\, H\Big) , && (34) \\
S(T) &= -N\, H\, \beta \tanh\Big(\beta\, H\Big) + N\, \ln\left(\mathrm{e}^{-\beta H} + \mathrm{e}^{\beta H} \right) . && (35)
\end{aligned}
$$

The figure below shows both in natural units as a function of T/H (dimensionless):



entropy

energy

COMMENTS:

☑ $T \to 0$: $\langle E \rangle = -NH$

$T \to 0$: $\langle E \rangle \to 0$

☑ $T \to 0$: $S \to 0$ ($\ln 1$)

$$\frac{1-\varepsilon}{1+\varepsilon} \doteq (1-\varepsilon)^2 \doteq 1-2\varepsilon$$

Let us study what happens at *low* temperatures as defined by

$$\frac{1}{T} H = \beta H \gg 1 \qquad \Rightarrow \qquad e^{-\beta H} \ll 1\,.$$

Expanding in powers of $\exp\{-\beta H\}$ we find: expansion parameter (Taylor)

$$\langle E \rangle = -NH \frac{e^{+\beta H} - e^{-\beta H}}{e^{\beta H} + e^{-\beta H}} = -NH \frac{1-e^{-2\beta H}}{1+e^{-2\beta H}}$$

$$= -NH \cdot \left[1 - 2e^{-2\beta H}\right] + \ldots$$

With MAPLE, we can get the next order in a convenient way:

$$\frac{E}{NH} = -1 + 2\,e^{-2\beta H} - 2\,e^{-4\beta H} + \mathcal{O}\left(e^{-6\beta H}\right)\,. \tag{36}$$

This has an interesting interpretation: [5]

- In leading order, the energy is $E = -NH$. This energy is as low as it can get. We say all spins are in the so-called *ground state*. In our case, *all* spins are pointing down.
- The next states with slightly higher energy are those where all spins except one are pointing down. The energy difference to the ground state is:

$$\Delta E = -(N-1)H + H - \left[-NH\right] = 2H\,.$$

[5] ATTENTION: physicist chargon.

The probability that this so-called excited state is populated at small temperature is exponentially small, namely: $\exp\{-\Delta E/T\}$. This is generically the case for systems with a gap between ground state and excited states.

For the entropy, we find for low temperatures:

$$\frac{S}{N} = [1 + 2\beta H]\, \mathrm{e}^{-2\beta H} + \mathcal{O}\left(\mathrm{e}^{-4\beta H}\right) . \tag{37}$$

COMMENT:

The entropy vanishes exponentially fast for low temperature (up to power-law corrections). This might be due to the discrete nature of our energy states. It is, however, generic that S vanishes for T approaching zero. Systems are in their ground state. It is generic in quantum mechanics that there is only one ground state. In information theory, the sytem lost its capacity to store information at $T = 0$. The stetting with $T = 0$ is alos called *absolute zero.*

$H/T \ll 1$

Let us also study the *high temperature* limit: $\beta H \ll 1$. In this case, we can expand the exponentials in (34,35) into a Taylor series of powers of βH. We find:

$$\frac{\langle E \rangle}{NH} = -\frac{1}{T/H} + \frac{1}{3(T/H)^3} + \mathcal{O}\left(\frac{1}{T^5}\right) . \tag{38}$$

$$\frac{S}{N} = \ln 2 - \frac{1}{2(T/H)^2} + \mathcal{O}\left(\frac{1}{T^4}\right) . \tag{39}$$