FYS2160 Oblig 9

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I. VARIED QUESTIONS

II. SPIN-SYSTEM IN EXTERNAL MAGNETIC FIELD

In this project we will study the behavior of a spin-system in an external magnetic field. We will address the behavior of N spins that are localized to specific positions in space. Each spin, i, can be in two possible states, $S_i = \pm 1$. The energy of spin i is $\epsilon_i = S_i mB$, where m and B are constants ($mB > 0$).

A. The partition function for a single spin

A single spin has two possible states $S_i = \pm 1$ so the partition function becomes

$$
\begin{aligned}
Z_1 &= \sum_{i=1}^{N} e^{-\epsilon_i \beta} \\
&= \sum_{i=1}^{2} e^{-S_i mB\beta} \\
&= e^{mB\beta} + e^{-mB\beta} \\
&= 2cosh(mB\beta)
\end{aligned}
$$

where $\beta = \frac{1}{kT}$

B. The partition function for N spins

In a system of N spins the energy of a microstate is the sum $\sum_{i=1}^{N} \epsilon_i$. Since we know that $\epsilon_i = \epsilon(S_i) = S_i mB = \pm mB$ the possible values of the total energy depends on the number of positive spins $n_\uparrow$ and the number of negative spins $n_\downarrow$. Since one is given by the other ($n_\uparrow = N - n_\downarrow$) it suffices to say that the energy depends on $n_\downarrow$. For a microstate with a number $n_\downarrow$ of negative spins the energy must be

$$
E_{n_\downarrow} = \sum_{i=1}^{N} \epsilon(S_i) = (N - 2n_\downarrow)mB
$$

where we have the possible microstates $n_\downarrow = 0, 1, ..., N$.
The partition function is given

$$
\begin{aligned}
Z_N &= \sum_{n_\downarrow=0}^{N} e^{-E_{n_\downarrow}\beta} \\
&= \sum_{E} \Omega(E) e^{-E\beta}
\end{aligned}
$$

We see that we can rewrite the sum over microstates as a sum over energies, as long as we multiply the Boltzman factors by the multiplicity, or degeneracy, $\Omega(E)$ of the corresponding energy. How do we find this quantity? E is a function of $n_\downarrow$. Furthermore each of the N spins are distinguishable because they are localized to specific locations in space. Thus the multiplicity of E is the number of ways we can choose $n_\downarrow$ spins to point down out of the total N and we can express it in terms of the binomial coefficient:

$$
\Omega(E) = \Omega(n_\downarrow, N) = \binom{N}{n_\downarrow}
$$

where $\binom{N}{n_\downarrow} = \frac{N!}{n_\downarrow!(N-n_\downarrow)!} = \frac{N!}{n_\downarrow! n_\uparrow!}$.
Thus we get the partition function

$$
\begin{aligned}
Z_n &= \sum_{E} \binom{N}{n_\downarrow} e^{-E\beta} \\
&= \sum_{n_\downarrow=0}^{N} \binom{N}{n_\downarrow} e^{-(N-2n_\downarrow)mB\beta} \\
&= \sum_{n_\downarrow=0}^{N} \binom{N}{n_\downarrow} e^{-mB\beta(N-n_\downarrow-n_\downarrow)} \\
&= \sum_{n_\downarrow=0}^{N} \binom{N}{n_\downarrow} (e^{-mB\beta})^{N-n_\downarrow} (e^{mB\beta})^{n_\downarrow}
\end{aligned}
$$

Here I use the binomial formulae $(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k$ to get

$$
\begin{aligned}
Z_N &= (e^{mB\beta} + e^{-mB\beta})^N \\
&= (2cosh(mB\beta))^N \\
&= Z_1^N
\end{aligned}
$$

C. Helmholtz free energy for the spin system

We have that the Helmholtz free energy of the system is

$$
\begin{aligned}
F &= -kTln(Z_N) \\
&= -kTln((2cosh(mB\beta))^N) \\
&= -kTln[(cosh(mB\beta))^N 2^N] \\
&= -kT[Nln(cosh(mB\beta)) + Nln(2)] \\
&= -NkTln(cosh(\frac{mB}{kT})) - NkTln(2)
\end{aligned}
$$

D. The entropy of the system

The entropy $S(T, V, N)$ of the system is, taking the derivative of the Helmholtz free energy F with respect to temperature T keeping volume V and the number of particles N constant, given by

$$\begin{aligned}
S &= -(\frac{\delta F}{\delta T})_{V,N} \\
&= NkT[\frac{1}{cosh(mB\beta)}\frac{\delta}{\delta T}cosh(mB\beta)] \\
&+ Nkln(cosh(mB\beta)) + Nkln(2) \\
&= Nk[T\frac{sinh(mB\beta)}{cosh(mB\beta)} + ln(2cosh(mB\beta))] \\
&= k[NTtanh(mB\beta) + ln(Z_N)]
\end{aligned}$$

E. $\bar{S_i}$ for spin i

We want to determine the average value $\bar{S_i}$ of S_i for spin i. We use our knowledge of each state's probability to determine an average value by applying the following equation

$$\begin{aligned}
\bar{S_i} &= \sum_{i=1}^{2} S_i P(S_i) \\
&= \frac{1}{Z_1}\sum_{i=1}^{2} S_i e^{-\epsilon_i \beta} \\
&= \frac{1}{Z_1}(e^{-mB\beta} - e^{mB\beta}) \\
&= -\frac{2sinh(mB\beta)}{2cosh(mB\beta)} \\
&= -tanh(mB\beta)
\end{aligned}$$

F. $\bar{S_i}$ when B is large and when T is large

When B is large, we have

$$\lim_{B\to\infty} \bar{S_i} = -\lim_{B\to\infty} tanh(mB\beta) = -1$$

When T is large, we have

$$\lim_{T\to\infty} \bar{S_i} = -\lim_{T\to\infty} tanh(\frac{mB}{kT}) = -tanh(0) = 0$$

The probability of state S_i is $P(S_i) = \frac{e^{-\frac{S_i mB}{kT}}}{Z_1}$ and this explains the behavior above. A large B indicates that the external magnetic field is strong and since $\epsilon_i = \pm mB$ this means the difference between the two energy levels increase. A system is drawn towards the lowest energy level and here this corresponds to the magnetic dipole moments' directions aligning parallel to that of the external field. Since the direction of a particle's spin is the opposite of that of the magnetic moment, this also compels the spins to align in one specific direction (opposite to that of the external field). This is reflected in $P(S_i)$ as a large B makes $P(S_i = 1) \to 0$ and $P(S_i = -1) \to 1$ - corresponding to one direction becoming highly unlikely while the other highly favorable.

A large T, on the other hand, makes the exponential of the Boltzman factor go to zero, causing the probabilities to even out. The distribution of states available to our system is described by the canonical ensemble which means that its potential is the Helmholtz free energy, which in addition to the definition given earlier can be expressed $F = U - TS$. The system is driven to minimize this energy. This then explains how a large T can override the initial drive towards the lowest energy state - it strengthens the drive towards increasing entropy and disorder. As $S_i = \pm 1$ becomes equally probable states the average value $\bar{S_i}$ goes to zero.

G. Are all states $(S_1, S_2, ..., S_N)$ equally probable