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