Collaborators

I worked with **Andrew Binder** to complete this homework assignment.

Problem 1

Show that for N non-interacting spin $\frac{1}{2}$ particles in a magnetic field B the energy U is given by

$$U = -N\mu_B B \tanh\left(\frac{\mu_B B}{k_B T}\right)$$

the heat capacity is given by

$$\frac{C}{Nk_B} = \left(\frac{\mu_B B}{k_B T}\right)^2 \operatorname{sech}^2\left(\frac{\mu_B B}{k_B T}\right)$$

and the entropy is given by

$$\frac{S}{Nk_B} = \ln\left[2\cosh\left(\frac{\mu_B B}{k_B T}\right)\right] - \frac{\mu_B B}{k_B T}\tanh\left(\frac{\mu_B B}{k_B T}\right)$$

We have from the textbook:

$$\begin{aligned}
Z_N &= Z_1^N = 2^N \cosh^N(\beta\mu_B B) \\
\therefore \ln Z_N &= N\ln(2\cosh(\beta\mu_B B)) \\
&= N\ln 2 + N\ln\cosh(\beta\mu_B B)
\end{aligned}$$

Now, let's compute $U = -\frac{\mathrm{d}\ln Z}{\mathrm{d}\beta}$:

$$\begin{aligned}
U &= -\frac{\partial \ln Z_N}{\partial \beta} \\
&= -N\frac{\partial}{\partial\beta}\ln(\cosh(\beta\mu_B B)) \\
&= -N\mu_B B\tanh\left(\frac{\mu_B B}{k_B T}\right) && \text{computed using WolframAlpha}
\end{aligned}$$

Which is exactly the expression that we wanted to derive. Now, since we know that $C = \left(\frac{\partial U}{\partial T}\right)_V$:

$$
\begin{aligned}
C &= \frac{\partial}{\partial T}\left[-N\mu_B B \tanh\left(\frac{\mu_B B}{k_B T}\right)\right] \\
&= -N\mu_B B \,\mathrm{sech}^2\left(\frac{\mu_B B}{k_B T}\right)\cdot\frac{-\mu_B B}{k_B T^2} \\
&= N\left(\frac{\mu_B B}{T}\right)^2\cdot\frac{1}{k_B}\,\mathrm{sech}^2\left(\frac{\mu_B B}{k_B T}\right) \\
\therefore \frac{C}{Nk_B} &= \left(\frac{\mu_B B}{k_B T}\right)^2 \mathrm{sech}^2\left(\frac{\mu_B B}{k_B T}\right)
\end{aligned}
$$

Similarly, we know that since $F = -Nk_B T \ln\left(2\cosh\left(\frac{\mu_B B}{k_B T}\right)\right)$, then:

$$
\begin{aligned}
S = \frac{U-F}{T} &= \frac{1}{T}\left[-N\mu_B B \tanh\left(\frac{\mu_B B}{k_B T}\right) + Nk_B T \ln\left[2\cosh\left(\frac{\mu_B B}{k_B T}\right)\right]\right] \\
&= \frac{Nk_B T}{T}\left[-\frac{\mu_B B}{k_B T}\tanh\left(\frac{\mu_B B}{k_B t}\right) + \ln\left[2\cosh\left(\frac{\mu_B B}{k_B T}\right)\right]\right] \\
\therefore \frac{S}{Nk_B} &= \ln\left[2\cosh\left(\frac{\mu_B B}{k_B T}\right)\right] - \frac{\mu_B B}{k_B T}\tanh\left(\frac{\mu_B B}{k_B T}\right)
\end{aligned}
$$

And so we're done. ■

Problem 2

A certain magnetic system contains n independent molecules for unit volume, each of which has four energy levels given by 0, $\Delta - g\mu_B B$, Δ, $\Delta + g\mu_B B$ (g is a constant). Write down the partition function, compute teh Helmholtz function and hence compute the magnetization M. Hence show that the magnetic susceptibility χ is given by

$$\chi = \lim_{B\to 0} \frac{\mu_0 M}{B} = \frac{2n\mu_0 g^2 \mu_B^2}{k_B T(3 + e^{\Delta/k_B T})}$$

The partition function is defined as $Z = \sum e^{-\beta E_i}$, so if we substitute in the energies we get:

$$Z = 1 + e^{-\beta\Delta + \beta g\mu_B B} + e^{-\beta\Delta} + e^{-\beta\Delta - \beta g\mu_B B}$$

So therefore, since $F = -nk_B T \ln Z$, then

$$F = -nk_B T \ln\big(1 + e^{-\beta\Delta + \beta g\mu_B B} + e^{-\beta\Delta} + e^{-\beta\Delta - \beta g\mu_B B}\big)$$

From here, it's useful to rewrite the partition function as:

$$Z = 1 + e^{\beta\Delta}\left(1 + 2\cosh\left(\frac{g\mu_B B}{k_B T}\right)\right)$$

Now, the magnetization M is defined as $M = -\left(\frac{\partial F}{\partial B}\right)_T$, so if we take the derivative of F:

$$\begin{aligned} M &= nk_B T \frac{\partial}{\partial B}\left(\ln\left[1 + e^{-\beta\Delta}\left(1 + 2\cosh\left(\frac{g\mu_B B}{k_B T}\right)\right)\right]\right) \\ &= nk_B T \frac{\frac{1}{k_B T} 2g\mu_B \sinh\left(\frac{g\mu_B B}{k_B T}\right)}{2\cosh\left(\frac{g\mu_B B}{k_B T}\right) + 1 + e^{\beta\Delta}} \end{aligned}$$

The derivative was computed by hand then checked using WolframAlpha. Since we're on the order of molecules, it's appropriate to assume that $\sinh x \approx x$ and $\cosh x \approx 1$:

$$\begin{aligned} M &= \frac{2ng^2\mu_B\left(\frac{g\mu_B B}{k_B T}\right)}{3 + e^{\beta\Delta}} \\ &= \frac{2ng^2\mu_B^2 B}{k_B T(3 + e^{\beta\Delta})} \end{aligned}$$

Now we can compute the limit:

$$\begin{aligned} \chi &= \lim_{B\to 0} \frac{\mu_0 M}{B} = \lim_{B\to 0} \frac{\mu_0}{B} \frac{2ng^2\mu_B^2 B}{k_B T(3 + e^{\beta\Delta})} \\ &= \frac{2n\mu_0 g^2 \mu_B^2}{k_B T(3 + e^{\Delta/k_B T})} \end{aligned}$$

And so we're done. ■

Problem 3

The energy E of a system of three independent harmonic oscillators is given by

$$E = \left(n_x + \frac{1}{2}\right)\hbar\omega + \left(n_y + \frac{1}{2}\right)\hbar\omega + \left(n_z + \frac{1}{2}\right)\hbar\omega$$

Show that the partition function Z is given by

$$Z = Z_{SHO}^3$$

where Z_{SHO} is the partition function of a simple harmonic oscillator given in eqn. 20.3. Hence show that the Helmholtz function is given by:

$$F = \frac{3}{2}\hbar\omega + 3k_BT\ln\left(1 - e^{-\beta\hbar\omega}\right)$$

and that the heat capacity tends to $3k_B$ at high temperature.

Call $E = E_x + E_y + E_z$ for the n_x, n_y and n_z components. Now we write out the partition function:

$$\begin{aligned} Z &= \sum e^{-\beta(E_x+E_y+E_z)} \\ &= \sum e^{-\beta E_x} e^{-\beta E_y} e^{-\beta E_z} \end{aligned}$$

Now notice that since x, y, z are orthogonal, we can actually combine them under a common n. Therefore:

$$Z = \sum e^{-3\beta E_x} = Z_{SHO}^3$$

Now to show the Helmholtz function, we use the fact that $F = -k_BT\ln Z$:

$$\begin{aligned} F &= -k_BT\ln Z_{SHO}^3 \\ &= -3k_BT\ln Z_{SHO} \\ &= 3\left(\frac{\hbar\omega}{2} + k_BT\ln\left(1 - e^{-\beta\hbar\omega}\right)\right) \\ &= \frac{3}{2}\hbar\omega + 3k_BT\ln\left(1 - e^{-\beta\hbar\omega}\right) \end{aligned}$$

Note that $\ln Z_{SHO} = \left(\frac{\hbar\omega}{2} + k_BT\ln\left(1 - e^{-\beta\hbar\omega}\right)\right)$ is given in the textbook, which is what I used to simplify this expression. Now to compute the heat capacity, we first have

$$U = \frac{3\hbar\omega}{2} + \frac{3\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

So therefore, we take the derivative with respect to T:

$$
\begin{aligned}
\frac{\partial U}{\partial T} &= 3\hbar\omega \frac{\frac{\hbar\omega}{k_B T} e^{\hbar\omega/k_B T}}{T^2\left(e^{\hbar\omega/k_B T}-1\right)^2} \\
&= 3k_B(\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}
\end{aligned}
$$

And we know that at high temperatures, $e^{\beta\hbar\omega} - 1 \approx \beta\hbar\omega$ (by a Taylor expansion). therefore,

$$
\begin{aligned}
\frac{\partial U}{\partial T} &= 3k_B(\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(\beta\hbar\omega)^2} \\
&= 3k_B
\end{aligned}
$$

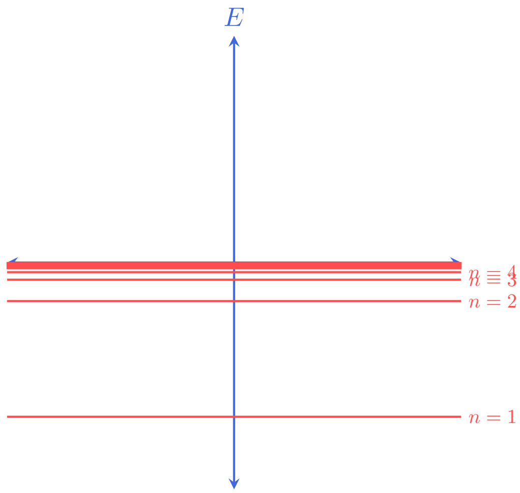
As desired. ■

Problem 4

The internal levels of an isolated hydrogen atom are given by $E = -R/n^2$ where $R = 13.6\text{eV}$. the degeneracy of each level is given by $2n^2$.

(a) Sketch the energy levels

A sketch is shown below:



As we can see, the energy levels approach $E = 0$, which makes sense since as $n \to \infty$, $E \propto 1/n^2$ so $E \to 0$. Thanks to **Andrew Binder** for the Ti*k*Z diagram.

(b) Show that

$$Z = \sum_{n=0}^{\infty} 2n^2 \exp\left(\frac{R}{n^2 k_B T}\right)$$

Summing over the energy levels, we get

$$Z = \sum_n e^{-\beta E_n} = \sum_1^{\infty} 2n^2 e^{\beta R/n^2} = \sum_1^{\infty} 2n^2 e^{\frac{R}{n^2 k_B T}} = \sum_{n=0}^{\infty} 2n^2 \exp\left(\frac{R}{n^2 k_B T}\right)$$

And so we're done. ■