

Statistical thermodynamics

Hw 2

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Problem 1

1. We will treat the system as a system of N independent particles, where the possible energy of each particle is mB or $-mB$.
The partition function is defined as $Z = \sum_{\alpha} e^{-\beta E_{\alpha}}$ and $\beta = \frac{1}{K_B T}$.
Since the particles are independent we can calculate the partition function for each particle \mathfrak{z} . The total partition function would be $Z = \mathfrak{z}^N$.

$$\mathfrak{z} = e^{-\beta mB} + e^{\beta mB} = 2 \cosh(\beta mB)$$

$$Z(T, N, B) = 2^N \cdot \cosh^N(\beta mB)$$

2. Using $A = -K_B T \ln(Z)$ we find

$$A = -K_B T \ln(2^N \cdot \cosh^N(\beta mB)) = -NK_B T \ln(2 \cdot \cosh(\beta mB))$$

$$A = -N \cdot K_B \cdot T \cdot (\beta mB + \ln(1 + e^{(-2\beta mB)})) = - (NmB + NK_B T \ln(1 + e^{(-2\beta mB)}))$$

Using $S = - \left(\frac{\partial A}{\partial T} \right)_{N, V}$ we find

$$S = NK_B \ln(1 + e^{(-2\beta mB)}) + \frac{2NmB}{T(1 + e^{2\beta mB})}$$

Since $A = U - TS$ we get

$$U = A + TS = \frac{2NmB}{(1 + e^{2\beta mB})} - NmB$$

Comparing the results with Hw1 we see that we got the same expressions. For U we got the exact same one.

For S we got

$$S = -K_B N \left(\frac{N_\uparrow}{N} \ln \left(\frac{N_\uparrow}{N} \right) + \left(1 - \frac{N_\uparrow}{N} \right) \ln \left(1 - \frac{N_\uparrow}{N} \right) \right)$$

where

$$\frac{N_\uparrow}{N} = \frac{1}{e^{2mB\beta} + 1} = \frac{e^{-2mB\beta}}{e^{-2mB\beta} + 1}$$

So it can be easily verified that the two expressions are the same.

3. The total energy U is given by the particles with energy mB (written N_\uparrow) and the particles with energy $-mB$ (written N_\downarrow) so

$$U = \frac{2NmB}{(1 + e^{2\beta mB})} - NmB = N_\uparrow mB + N_\downarrow (-mB) = (N_\uparrow - N_\downarrow) mB$$

Therefore

$$N_\uparrow - N_\downarrow = \frac{2N}{(1 + e^{2\beta mB})} - N$$

and

$$M(T, N, B) = m(N_\uparrow - N_\downarrow) = \frac{2Nm}{(1 + e^{2\beta mB})} - Nm$$

Results are identical to those of Hw1.

4. We will now calculate $-\left(\frac{\partial A}{\partial B}\right)_{T,N}$

$$-\left(\frac{\partial A}{\partial B}\right)_{T,N} = -Nm + NK_B T \frac{2\beta m}{1 + e^{2\beta mB}} = \frac{2Nm}{(1 + e^{2\beta mB})} - Nm$$

obviously $M(T, N, B) = -\left(\frac{\partial A}{\partial B}\right)_{T,N}$.

Problem 2

1. Following the same routine from question 1, we shall calculate the partition function of one harmonic oscillator and then raising it to the power of $3N$ we will obtain the total partition function.

The energy spectrum for a one dimensional harmonic oscillator is given by $E_n = (n + 1/2)\hbar\omega$, thus

$$\mathfrak{z} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)} = e^{-\frac{\beta\hbar\omega}{2}} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$$

$$\mathfrak{z} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}}$$

$$\mathfrak{z} = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$Z = \mathfrak{z}^{3N} = \left(2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)^{-3N}$$

2. Following the same path we shall find A and derive S and U .

$$A = -K_B T \ln(Z) = 3NK_B T \ln\left(2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)$$

$$S = -\frac{\partial A}{\partial T} = -3NK_B \ln\left(2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right) + \frac{3N\hbar\omega}{2T} \cot\left(\frac{\beta\hbar\omega}{2}\right)$$

$$S = 3\frac{N\hbar\omega}{T} \frac{1}{e^{\beta\hbar\omega} - 1} - 3NK_B \ln\left(1 - e^{-\beta\hbar\omega}\right)$$

Once again simple mathematics will reveal that the expression for the entropy is the same as the one in Hw1.

$$U = A + TS$$

Using

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

We get

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

and you guessed right it does fit the results of Hw1.

Last thing to do is to calculate the heat capacity given by $C_v = T \left(\frac{\partial S}{\partial T} \right)_{N,V}$.

$$C_v = T \left(\frac{\partial S}{\partial T} \right)_{N,V} = \left(\frac{\partial U}{\partial T} \right)_{N,V} = \frac{3N(\hbar\omega)^2 e^{\beta\hbar\omega}}{K_B T^2 (e^{\beta\hbar\omega} - 1)^2}$$

Well so far theory and practice go hand in hand.