Problem 1

1.1 Obtain the partition function of a distinguishable particle in a one-dimensional simple harmonic oscillator potential.

Solution:
The energy levels of a quantum harmonic oscillator is given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{1}$$

Since energy of this oscillator is allowed to change, we use the partition function of the canonical ensemble which is defined as

$$Z \equiv \sum_s e^{-\beta E_s} \tag{2}$$

where $\beta = 1/(k_B T)$ in which k_B is the Boltzmann constant. Substituting Eq. (1), we obtain

$$Z = \sum_n e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega} = e^{-\frac{1}{2}\beta\hbar\omega}\sum_n \left(e^{-\beta\hbar\omega}\right)^n \tag{3}$$

Note that we have obtained an infinite geometric series. The sum of such a series is

$$1 + x + x^2 + x^3 \ldots = (1-x)^{-1} \tag{4}$$

Applying this relation, the Z becomes

$$Z = \frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} = \frac{1}{e^{\frac{1}{2}\beta\hbar\omega} - e^{-\frac{1}{2}\beta\hbar\omega}} = \frac{1}{2\sinh\frac{\beta\hbar\omega}{2}} \tag{5}$$

with the use of hyperbolic functions.

1.2 From your result in 1.1, obtain the system's internal energy and heat capacity.

Solution:
It is first important to find the natural logarithm of the partition function as follows:

$$\ln Z = \ln\frac{1}{2\sinh\frac{\beta\hbar\omega}{2}} = -\ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right) \tag{6}$$

Then, using this result, we obtain the system's internal energy as

$$U = -\frac{\partial \ln Z}{\partial\beta} = \frac{\partial}{\partial\beta}\left[\ln\left(2\sinh\frac{\beta\hbar\omega}{2}\right)\right] = \frac{2\cosh\frac{\beta\hbar\omega}{2}}{2\sinh\frac{\beta\hbar\omega}{2}}\cdot\frac{\hbar\omega}{2} = \frac{\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2} \tag{7}$$

Thus, we get

$$U = \frac{\hbar\omega}{2}\coth\frac{\hbar\omega}{2k_BT} \tag{8}$$

We use this U to get the heat capacity of the system:

$$C_V = \left(\frac{\mathrm{d}U}{\mathrm{d}T}\right)_{V,N} = \frac{\hbar\omega}{2}\frac{\mathrm{d}}{\mathrm{d}T}\left[\coth\frac{\hbar\omega}{2k_BT}\right] = \frac{\hbar\omega}{2}\left(-\operatorname{csch}^2\frac{\hbar\omega}{2k_BT}\right)\left(-\frac{\hbar\omega}{2k_BT^2}\right) \tag{9}$$

Thus, we have

$$C_V = \frac{1}{k_B}\left(\frac{\hbar\omega}{2T}\operatorname{csch}\frac{\hbar\omega}{2k_BT}\right)^2 \tag{10}$$

1.3 Discuss your result in 1.2, as T approaches infinity.

Solution:
Ignoring the effect the constants in the expressions, we plot the system's internal energy and heat capacity in Fig. 1 and Fig. 2 respectively. We see in Fig. 1 that the internal energy is proportional to temperature. On the other hand, the heat capacity asymptotes to some value as T approaches infinity as shown in Fig. 2.

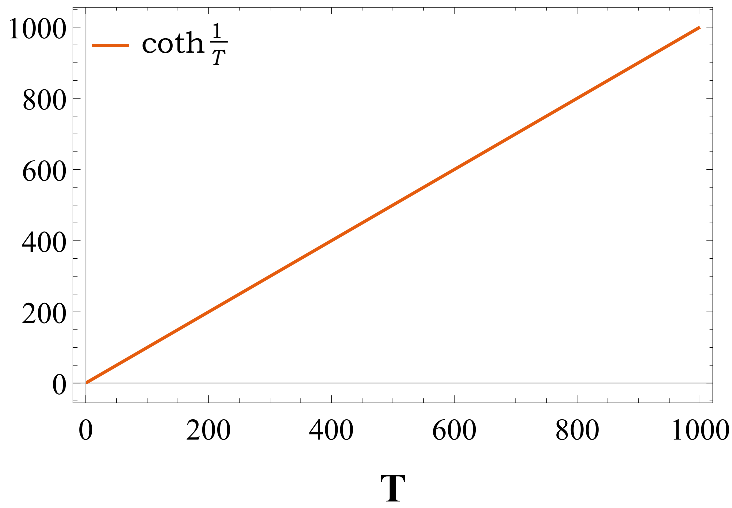

Figure 1: A plot of $\coth T^{-1}$

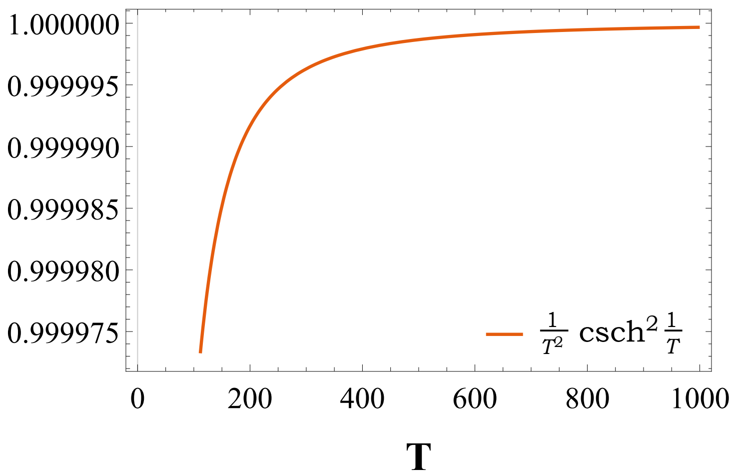

Figure 2: A plot of $T^{-2}\coth^2 T^{-1}$

Problem 2

Consider a one-dimensional array of N spins in a paramagnet with each spin having a magnetic moment μ. In the presence of a magnetic field B, the spins can align parallel (-) or antiparallel (+) to the field with energy $\pm\mu B$.

2.1 Obtain the partition function of this system.

Solution:
It is given that the energy of the system can either be

$$E = \pm\mu B \tag{11}$$

As the energy of a spin can change, we again use the partition function of the canonical ensemble as given in Eq. (2). Let us first obtain the partition function of a single spin:

$$Z_1 = e^{-\beta\mu B} + e^{\beta\mu B} = 2\cosh\beta\mu B \tag{12}$$

For a system with N spins, the partition function is given by

$$Z_N = (Z_1)^N = (2\cosh\beta\mu B)^N \tag{13}$$

2.2 From your result in 2.1, obtain the system's internal energy.

Solution:
In the same manner as in the previous problem, we first calculate for $\ln Z_N$:

$$\ln Z_N = \ln(2\cosh\beta\mu B)^N = N\ln(2\cosh\beta\mu B) \tag{14}$$

Then, the internal energy of the given system is

$$U = -\frac{\partial \ln Z_N}{\partial \beta} = -N\frac{\partial}{\partial \beta}\left[\ln(2\cosh\beta\mu B)\right] = -N\frac{2\sinh\beta\mu B}{2\cosh\beta\mu B}\cdot\mu B = -N\mu B\tanh\beta\mu B \tag{15}$$