Experiment 7
Partition Function-02
Canonical Ensemble - Maxwell Boltzmann (Ideal Gas)

1. METHOD
   (a) Connection between State function and Partition function ?
   (b) Difference between Micro-Canonical, Canonical and Grand-Canonical ensemble ?

2. CODING
   Generate a matrix that stores for different V and T the values of $Z(V,T)$ according to

$$Z(V,T) = \frac{\pi}{2}\int_0^\infty n_j^2\, exp\Big(-\frac{h^2}{8mV^{2/3}\,k_BT}\,n_j^2\Big)dn_j$$

   What is ∞ here in the integration ?

   (a) **(Pressure, Internal Energy and Entropy)**
   The intensive function pressure P can be found as

$$P = NkT\left(\frac{\partial \ln Z}{\partial V}\right)_T$$

   The extensive function internal energy U can be found as the average energy is

$$< E >= \frac{U}{N} = kT^2\left(\frac{\partial \ln Z}{\partial T}\right)_V$$

   The entropy S can be found as

$$S = \frac{U}{T} + Nk(\ln Z - \ln N + 1)$$

   (b) **(Internal Energy)**
   The specific heat capacity is

$$C_v = \frac{\partial < E >}{\partial T}$$

   and the variance in energy or the "Energy fluctuations" are

$$\Big\langle (\Delta E)^2 \Big\rangle = \frac{\partial^2 ln Z}{\partial \beta^2} = kT^2 C_v$$

3. PLOTS
   (a) **(Figure 1)**
   Use the integral expression for the partition function to Plot $\ln Z$
   (a) versus temperature T and $ln\ T$ for different values of V and $ln\ V$ and label the curves
   (b) versus volume V for different values of T and label the curves.
   Take ranges as $T = 150 - 450\ K$, $V = 20 - 50 \times 10^{-3} m^3$ and $P = 30 - 90\ kPa$.
   Hint: the upper limit of the integral can be anywhere between 10^{11} to 10^{15}
   Also check if this matches with the analytical expression $Z(V,T) = V\left(\frac{2\pi mk}{h^2}\right)^{3/2} T^{3/2}$

(b) **(Figure 2)**
Plot the pressure P
(a) versus temperature T *for different values of* V *and label the curves*
(b) versus volume V *for different values of* T *and label the curves*

(c) **(Figure 3)**
Plot the internal energy U **versus temperature** T.
Evaluate the specific heat capacity from the slope of graph using inbuilt function . Take $V = 20 \times 10^{-3} m^3$

(d) **(Figure 4)**
Plot the entropy S
(a) versus temperature T *for different values of* V *and label the curves*
(b) versus volume V *for different values of* T *and label the curves.*

4. APPLICATIONS

(a) Thermodynamics of magnetic systems : negative temperatures