PROBLEMS ON STATISTICAL MECHANICS

(Based on Class taken on Classical Stat. Mech: Canonical and Grand Canonical Ensembles)

1. Show that, $\langle E^2 \rangle = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}$, (Z is partition function for Canonical ensemble)

2. Show that, the standard deviation in the value of energy is given by, (consider Canonical ensemble)

$$\sigma = \sqrt{\langle E^2 \rangle - \langle E \rangle^2} = \sqrt{\frac{\partial^2 (lnZ)}{\partial \beta^2}}$$

3. Consider, a one level system having energy $\varepsilon = -NK_BT \ ln\left(\frac{V}{V_0}\right)$; where, V_0 is a constant.

(i) Write down the partition function for the system.

(ii) Calculate the average pressure for this system as a function of volume and temperature.

4. Show that, the expression of enthalpy H is given by (Z= partition function of canonical ensemble),

$$H = \frac{1}{\beta}\left[\left(\frac{\partial \ln Z}{\partial \ln T}\right)_{V,N} + \left(\frac{\partial \ln Z}{\partial \ln V}\right)_{T,V}\right]$$

5. Show that , the Gibb's free energy G is given by (Z= partition function of canonical ensemble),

$$G = -\frac{1}{\beta}\left[\ln Z - \left(\frac{\partial \ln Z}{\partial \ln V}\right)_{T,\ N}\right]$$

6. The oxygen atom has three low lying energy levels 3_{P_2} with energy $\varepsilon = 0\ cm^{-1}$, 3_{P_1} with energy $\varepsilon = 157.4\ cm^{-1}$ and 3_{P_0} with energy $\varepsilon = 226.1\ cm^{-1}$. The degeneracy of the levels is $g_J = 2J + 1$ .Calculate the partition function of this system at room temperature.

7. A two state system has energies $-\frac{\Delta}{2}$ and $+\frac{\Delta}{2}$. Compute the partition function Z for the system. What is the internal energy U of the system? (Assume that the energy states are non-degenerate).

8. Starting from the canonical partition function of ideal gas, $Z = \left[\left(\frac{2\pi m K_B T}{h^2}\right)^{\frac{3}{2}} V\right]^N$, establish the equation of state.

9. Evaluate the sum $Z = \sum_{n=0}^{\infty} e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega}$ and then calculate U= $-\frac{\partial \ln Z}{\partial \beta}$, where $\beta = \frac{1}{K_BT}$. Finally, evaluate the specific heat starting from the expression of U.

10. Starting from the expression of canonical partition function for a system having discrete energy levels, show that $\langle E^2 \rangle - \langle E \rangle^2 = K_B T^2 C_v$; where, 'C_v' is the specific heat at constant volume of the system.

11. A system of N particles contains one dimensional linear harmonic oscillators whose Hamiltonian is given by $H = \sum_{i=1}^{N}\left(\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 q_i^2\right)$,

(i) Write down the partition function in canonical ensemble.

(ii) Using the connection of partition function to the Helmholtz Free Energy (F= $-K_BT\ln Z$) in thermodynamics, calculate the entropy of the systems.

(iii) Hence show that C_p and C_v are the same for this system.

(iv) What is the thermodynamic pressure 'P' of the system.

12. Consider a system of N non-interacting particles each having two energy levels $+\varepsilon$ or $-\varepsilon$ respectively, at a temperature T.

(i) Write down the single particle partition function.

(ii) Extend it for 'N' non-interacting system of particles.

(iii) Calculate the average energy for the system.

(iv) Calculate the Free Energy and the Entropy.

13. A system has two energy levels at energies 0 and ε having degeneracy g_0 and g_1 respectively.

(i) Write down the partition function.
(ii) Calculate the average energy.
(iii) Calculate the entropy of the system.
(iv) What is the specific heat of the system?
(v) Figure out the high temperature and low temperature behaviour of the specific heat.

14. Show that, for ideal gas system, the partition function is given by the relation $Z = N\left(\frac{r_0}{\lambda}\right)^3 \pi^{3/2}$; where, λ is the De- Broglie wavelength, r_0 is the average separation and *N* is the number of particles.

15. For a system of N one-dimensional harmonic oscillators, obtain the canonical partition function. Calculate average energy and obtain the quantum limit.

16. Calculate the canonical partition function for an ensemble of localised magnetic dipoles in a magnetic field. Hence, find out the average dipole moment along the magnetic field. Sketch the function as function of temperature.

17. Give the classical statistical definition of partition function. Consider an ideal Boltzmann gas of *N* indistinguishable particles confined to a volume *V* at temperature *T*, in which the energy of each particle (ε) is related to its momentum by ε=C P .

(i) Determine the partition function of the system.
(ii) Find the pressure and specific heat at constant volume.
(iii) Calculate the chemical potential of the gas.

18. The partition function of a system is given by ln *Z* = a T^4 V; where 'a' is a constant, T is the absolute temperature and V is the volume. Calculate

(i) the internal energy
(ii) the pressure
(iii) the entropy.

19. A system in thermal equilibrium at a temperature T has energies 0 and E. Calculate the partition function of system. Calculate

(i) Helmholtz free energy (F)
(ii) Entropy (S)
(iii) Internal energy (U)
(iv) Specific heat at constant volume.

Discuss the trend of specific heat at

(i) low temperature
(ii) high temperature

20. The total energy of the system of *N* one dimensional classical oscillator is given by

$$E(q,p)=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+\frac{1}{2}m\omega^2 q_i^2\right]$$

Where , q_i and p_i are position and momentum of the i^{th} oscillator, respectively.

(i) Write down the partition function.

(ii) Helmholtz free energy
(iii) Internal energy
(iv) Specific heat at constant volume

21. In quantum mechanics, energy of an oscillator is quantized. Then the energy of a system consisting of *N* such oscillators is given by,

$E_{n_i} = \sum_{i=1}^{N} \left(n_i + \frac{1}{2}\right) \hbar\omega$; where, n_i is an integer ; n_i = 0,1,2,3,4,.....

Now find

(i) the partition function of the system.
(ii) entropy
(iii) Helmholtz free energy
(iv) internal energy
(v) specific heat at constant volume.

Also discuss the case of low temperature and high temperature behaviour of specific heat.

22. An ideal gas of *N* spinless atoms occupies a volume *V* at temperature *T*. Each atom has only two energy levels separated by an energy Δ. Find the chemical potential, free energy and average energy of the system.

23. If *Z* is partition function of a one dimensional harmonic oscillator having energy $\left(n + \frac{1}{2}\right)\hbar\omega$.

(i) What's the probability that the system has energy $\frac{\hbar\omega}{2}$?
(ii) What's the probability that the system has energy lower than $4\hbar\omega$?
(iii) What's the probability that system has energy greater than $4\hbar\omega$?

24. A paramagnetic system consists of N magnetic dipoles. Each dipole carries magnetic moment, μ , which can be treated classically. If the system is at a finite temperature *T* in a uniform magnetic field *H* ,then

(i) Find partition function.
(ii) Find internal energy.
(iii) Find average magnetic moment.

25. The Hamiltonian of a classical ideal gas is given by

$$E_N(q,p) = \sum_{i=1}^{3N} \frac{p_i^2}{2m}$$

(i) Write down expression of grand canonical partition function.
(ii) Find mean value of grand potential.
(iii) Find average number of particles.
(iv) Find pressure of system.
(v) Find an expression for entropy of the system.

26. A system consists of three energy levels which are E_1 = 0 , E_2 = 1.38 × 10^{-23} *J* , E_3 = 2.76 × 10^{-23} *J*. Determine the partition function and calculate the probability that the system is in each level.
Given that the system is at a temperature of 1 *K*.

27. A system has three energy levels of energy 0, 100 K_B and 200 K_B with degeneracies 1,3 and 5 respectively. Calculate the partition function, the relative population of each level and the average energy at a temperature of 100 *K* .

28. The partition function of a system is given by the equation $Z = e^{\alpha T^3 V}$; where , α is a constant. Calculate the pressure, entropy and internal energy of the system.

29. The lowest energy of O_2 is three fold degenerate. The next level is doubly degenerate and lies 0.97 *eV* above the lowest. Take the lowest level to have energy of 0.
Calculate the partition function at 1000K & 3000*K* .

30. Calculate the free enegy of a system with spin one on each site.
Given that, the levels associated with the three spin states have energies ε , 0 , - ε.

31. Consider, two identical particles which are to be placed in four single particle states. Two of these states have energy 0, one has ε and the last one has 2ε. Calculate the partition function ,given that the particles are (i) fermions
(ii) bosons

32. A system consists of three independent particles localised in space. Each particle has two states of energy 0 and E. When the system is in thermal equilibrium with a heat bath at temperature *T*. Calculate its partition function.

33. Consider, a system of *N* identical non-interacting, magnetic ions of spin $^1/_2$, magnetic moment μ , in a crystal at temperature *T* in a uniform magnetic induction field *B* .
Calculate the partition function, Z_n for this system and from this obtain a formula for the entropy *S*.

34. A gas of *N*-particles is enclosed in a volume *V* and at a temperature *T* . The partition function is given by $ln\ Z = N\ ln\left[(V - bN)(K_B T)^{3/2}\right]$; where, b is a constant with appropriate dimension. If *P* is the pressure , find the equation of state of the system.

35. Consider, a solid surface to be a 2-D lattice with N_s sites. Assume that N_a atoms ($N_a \ll N_s$) are adsorbed on the surface, so that each site has either 0 or 1 adsorbed atom. An adsorbed atom possesses energy E = - ε ; where, E > 0.
(Assume that atoms on the surface do not interact with each other.)

(i) If the surface is at temperature *T*, compute considered potential of the adsorbed atoms as a function of *T* and E = - ε (use the canonical ensemble) .
(ii) If the surface is in equilibrium with an ideal gas of similar atoms at temperatre *T* , compute the ratio $\frac{N_a}{N_s}$ as a function of pressure, *P* , of the gas. Assume , the gas has number density *n* .

36. Show that , the partition function of two independent (non-interacting) systems *i* and *j* is given by $Z_{ij} = Z_i \times Z_j$.