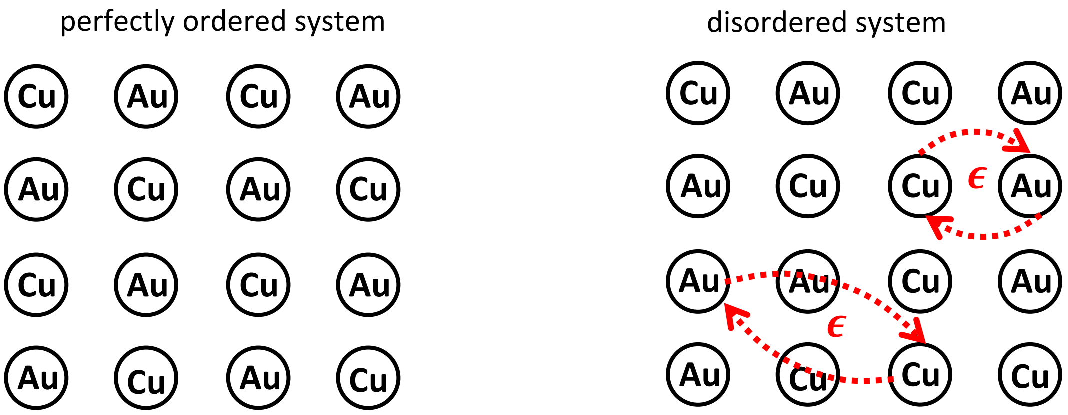
Question 1.

CuAu (Copper-Gold) binary alloy crystal consists of N Cu atoms and N Au atoms. The structure can be modelled as follows. At $T = 0K$ perfectly ordered system has N Cu-sites occupied by N Cu atoms, and N Au-sites occupied by N Au atoms. At a finite temperature T, n Cu atoms are displaced to Au-sites, and n Au atoms are displaced to Cu-sites. For one site exchange ε is given to the crystal.



In microcanonical ensemble, find the number of exchanged atoms $n(T)$ as a function of temperature using the minimization of free energy.

Question 2.

Consider a solid formed by N hydrogen molecules which are localized on lattice sites. The energy of a hydrogen molecule is determined by the quantum numbers l_1 and l_2 where $l_1 = -1, 0, +1$ and $l_2 = 0, +1$. A hydrogen molecule can exist in two forms: ortho hydrogen where the energy of the molecule is $+\varepsilon$; and para hydrogen where the energy of the molecule is 0. The state $l_1 = l_2$ is not allowed. If $l_1 > l_2$ a hydrogen molecule has the energy value of $\varepsilon_i = 0$. If $l_1 < l_2$ a hydrogen molecule has the energy value of $\varepsilon_i = +\varepsilon$. Let n be the number of molecules in ortho state.

a) Fill the following table of possible quantum states of a hydrogen molecule with the possible pairs of quantum numbers and corresponding the energy values according to the information given in the text.

l_1	l_2	ε_i

b) Find the number of molecules in ortho state $n(T)$ in microcanonical ensemble.

c) Find the energy of the hydrogen solid in canonical ensemble $E(T)$

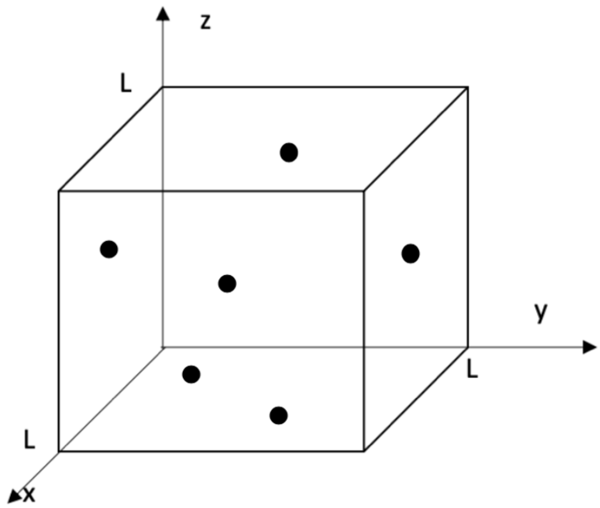
Question 3.

Consider an ultra-relativistic classical ideal gas of N particles in a volume V=LxLxL. Each particle have the energy of $\varepsilon(p) = cp$ where c is the speed of light and p is the momentum.

a) Find the N particle partition function for the gas.

Use the formula for single particle partition function $Z_1 = \frac{1}{h^3}\iint e^{-E(\vec{p},\vec{r})/k_BT} d^3\vec{p}d^3\vec{r}$

b) Find the equation of states $f(P, V, T)$.



Question 4.

Consider N non-interacting particles contained in a three dimensional cavity of unit volume ($V = 1$). Excitation energy of a particle is given by $\varepsilon(k) = \hbar ck$

a) Find the single particle density of states in energy.

b) Find the single particle partition function

c) Find the grand partition function for the system. (Leave you result in summation form, don't do further calculation)

Question 5.

Consider a system of three particles with three energy eigenstates of $0, 3\varepsilon$ and 5ε. Write the partition function for three particle system.

a) If the particles are non-identical

b) If the particles are obeying Bose-Einstein statistics.

c) If the particles are obeying Fermi-Dirac statistics.