

## Module S1

### Statistical Mechanics

This module requires you to read material from a textbook such as Kittel & Kroemer relevant to the following topics:

Topics:

Definition of entropy, temperature, and chemical potential

Boltzmann factor

Partition function

Grand partition function

Black body radiation

Statistical treatment of the ideal gas

Fermi-Dirac distribution

Bose-Einstein distribution

References: Kittel and Kroemer *Thermal Physics* 2<sup>nd</sup> edition chapters 1 through 7.

Daniel V. Schroeder *An Introduction to Thermal Physics* chapters 2, 6 and 7.

**Assignment:**

1. Suppose the internal energy of a closed system is represented by the variable,  $U$ . It is known that the number of microscopic states for a given value of  $U$  is equal to  $CU^{kN}$ , where  $N$  is the number of particles in the system and  $C$  and  $k$  are constants that depend on the details of the system. Using the fundamental definition of temperature,  $\frac{1}{T} = \left( \frac{\partial S}{\partial U} \right)_{N,V}$ , find  $U$  as a function of temperature for this system when it is brought into thermal equilibrium.
  
2. A system consists of a single particle that can be in one of three states, the energy of which is  $0$ ,  $E_0$  or  $2E_0$ , where  $E_0 > 0$ .
  - a. Write out the partition function for this system.
  - b. Calculate the Helmholtz free energy.
  - c. Calculate the entropy and plot  $S/k_B$  as a function of  $k_B T/E_0$ .
  - d. Calculate the thermal energy and plot  $U/E_0$  as a function of  $k_B T/E_0$ .
  - e. Discuss the zero temperature limits of the functions you calculated in parts (c) and (d) and then discuss why those limits make sense physically.
  - f. Repeat part (e) for the infinite temperature limits.
  
3. A simple model of two interacting, spin 1 dipoles is that their energy is given by  $-JS_1S_2$ , where  $J$  is a positive constant and  $S_1$  and  $S_2$  can each independently take on the value of  $-1$ ,  $0$ ,  $+1$ .
  - a. How many states of this system are there?
  - b. Write out the partition function for this system.
  - c. Determine the thermal energy, the Helmholtz free energy and entropy of this system.
  - d. For each of the functions in (c), evaluate mathematically the limit as temperature approaches zero and then as temperature approaches infinity. Next, discuss why physically each result makes sense.

4. Consider a black body at three different temperatures, room temperature, 100°C, and 500°C. In each case,
- calculate the frequency at which the radiant energy peaks.
  - name the portion of the electromagnetic spectrum for the peak frequencies.
  - calculate the fraction of the radiant energy in the visible portion of the spectrum, 400nm-700nm, for each of these temperatures (you will need to make a suitable approximation to evaluate the integral).
5. Consider a site which can be occupied by 0 particles ( $E=0$ ), 1 particle ( $E=-\alpha$ ) or two particles ( $E=-3\alpha$ ). That is, this site shows a strong preference for being doubly occupied.
- Write out the grand partition function for this system.
  - Calculate  $\langle N \rangle$  as a function of chemical potential and temperature.
  - Plot  $\langle N \rangle$  as a function of  $k_B T / \alpha$  for  $\mu=0$ ,  $-\alpha$ , and  $-2\alpha$ .
6. (Modified from Kittel and Kroemer's text): Hemoglobin molecules (Hb) in the blood provide attachment points for  $O_2$ . Let us consider a simple model in which each Hb molecule has just one point of attachment.
- Suppose it is known that when the absolute activity of  $O_2$  (i.e.,  $e^{\mu/k_B T} \equiv \lambda_A$ ) is  $1 \times 10^{-5}$ , 90% of Hb molecules have an  $O_2$  attached to them. Take the body temperature to be 37°C. Determine the energy  $E_A$  associated with the state in which an  $O_2$  is attached to Hb. Express your answer in eV, and take the zero on your energy scale to correspond to the state in which no molecule is attached to Hb.
  - Now suppose both  $O_2$  and CO molecules are present. Write out an expression for the probability that a CO molecule is attached. Your answer should be in terms of  $E_A$ ,  $E_B$  (the energy associated with CO being attached),  $\lambda_A$  (the absolute activity of  $O_2$ ),  $\lambda_B$  (the absolute activity of CO), and the temperature  $T$ .
  - Repeat part (b) for the probability that the Hb has an  $O_2$  molecule attached.
  - Evaluate the above expressions numerically if  $E_B = -0.548 \text{ eV}$  and  $\lambda_B = 10^{-7}$ , and  $E_A$ ,  $\lambda_A$ , and  $T$  are as above.

7. Using your own words and format, derive the Fermi-Dirac and Bose-Einstein distribution functions and describe their qualitative similarities and differences.

8. Silver has  $5.76 \times 10^{22}$  conduction electrons per cubic centimeter.

a. Calculate the Fermi energy in eV and the Fermi temperature in Kelvin.

b. What does the Fermi temperature tell us about the behavior of the conduction electrons at room temperature?

c. Calculate the electronic contribution of the electrons to the specific heat of silver at room temperature. Look up a value for the total specific heat of silver at room temperature and comment on the difference.

9. (Modified from Schroeder's text) Fried et al (*Phys Rev Lett* **81** 3811 (1998)) formed a Bose-Einstein condensate by cooling *atomic* hydrogen. The density of hydrogen was  $1.8 \times 10^{14}$  atoms/cm<sup>3</sup>. Calculate the condensation temperature, treating these atoms as non-interacting bosons. Compare this to the experimentally observed value of  $50 \mu\text{K}$ .

10. Fluctuations

a. Defining  $U = \langle E \rangle$  and  $C_v$  as the heat capacity of a system at constant volume  $\left(\frac{\partial U}{\partial T}\right)_v$ , show that  $k_B T^2 C_v = \langle (E - \langle E \rangle)^2 \rangle$ . Hint: express  $\langle E \rangle$  in terms of the partition function.

b. Defining  $\langle N \rangle$  as the average number of particles in a system in thermal equilibrium at temperature  $T$  and diffusive equilibrium at chemical potential  $\mu$ , show that  $\langle (N - \langle N \rangle)^2 \rangle = k_B T \frac{\partial \langle N \rangle}{\partial \mu}$ . This calculation is somewhat similar to that of (a), but you must consider the grand partition function.

MODULE S1

Name:

Term:

Problem	Max	1 <sup>st</sup>	2 <sup>nd</sup>	Final
1	5			
2	15			
3	10			
4	5			
5	5			
6	5			
7	5			
8	5			
9	5			
10	5			
TOTAL	65			