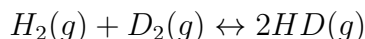


Problem Set 4

1. Compute  $K_p$ , the pressure-based equilibrium constant for the dissociation reaction of  $O_2$  at  $T = 3000K$ . The electronic ground-state degeneracy for oxygen atoms,  $g_0(O) = 9$ , while for oxygen molecules,  $g_0(O_2) = 3$ .
2. Do problem 9-1 in McQuarrie's Statistical Mechanics book.
3. Using the translational partition function and the partition functions for harmonic oscillators and rigid rotators, do problem 9-9 in McQuarrie's Statistical Mechanics book.
4. Consider the reaction given by:



Using molecular parameters (see table 6-1 in McQuarrie), show that the equilibrium constant for this reaction has a temperature dependence of roughly:

$$K(T) = 4.24e^{-77.7K/T}$$

5. Heat capacities of liquids
  - a)  $C_V$  for liquid argon (at  $T = 100K$ ) is  $18.7 \text{ J K}^{-1} \text{ mol}^{-1}$ . How much of this heat capacity can you rationalize on the basis of your knowledge of gases?
  - b)  $C_V$  for liquid water at  $T = 10^\circ\text{C}$  is about  $75 \text{ J K}^{-1} \text{ mol}^{-1}$ . Assuming water has three vibrations, how much of this heat capacity can you rationalize on the basis of gases? What is responsible for the rest?
6. For the nearest-neighbor Ising model,

$$\mathcal{H} = -H \sum_n \sigma_n - \frac{J}{2} \sum_{n,n'}^{N.N.} \sigma_n \sigma_{n'}$$

with external magnetic field ( $H \neq 0$ ), determine the zero-temperature states as a function of  $J$  and  $H$ . Present the results on a H-J zero-temperature diagram marking clearly which states are favored in the various regions of the diagram.

7. For the one-dimensional Ising model, plot the average energy (actually  $E/NJ$ ), the magnetic susceptibility, and the specific heat all against  $kT/J$  between values of 0 and 5. Discuss the specific heat maximum at around  $kT/J = 1$ .

8. Extra credit: Maximum Entropy in Las Vegas

You play a slot machine in Las Vegas. For every \$1 coin you insert there are three outcomes:

- a) you lose \$1.
- b) you win \$1, so your profit is \$0.
- c) you win \$5, so your profit is \$4.

Suppose you find that your average expected profit over many trials is \$0 (i.e. you play slots at a casino owned by someone exceedingly generous or stupid). Find the maximum entropy distribution for the probabilities  $p_1$ ,  $p_2$  and  $p_3$  of observing each of these three outcomes.