Physical Chemistry of Materials 2

Due date: September 26, 2012

Homework #1

1. The Korea Lottery consists of drawing five balls numbered 1 to 43, and a single ball numbered 1 to 23 from a separate machine.
   (a) What is the probability of hitting the jackpot in which the values for all six balls are correctly predicted?
   (b) What is the probability of predicting just the five balls correctly?
   (c) What is the probability of predicting just the first five balls in the exact order they are picked?

2. Consider the 25 players on a professional baseball team. At any point, 9 players are on the field.
   (a) How many 9–player batting orders are possible given that the order of batting is important?
   (b) How many 9–player batting order are possible given that the all-star designated hitter must be in the order batting in the fourth spot?
   (c) How many 9–player fielding teams are possible, under the assumption that the location of the players on the field is not important?

3. Consider a random walk in one dimension. In such process, the probability to moving an individual step with the step distance of λ in the $+x$ or $-x$ direction is equal. Image starting at x=0 and performing a random walk in which 20 steps are taken.
   (a) What is the farthest distance the particle can possibly move in the $+x$ direction? What is the probability of this occurring?
   (b) What is the probability the particle will not move at all?
   (c) What is the probability of the particle moving half the maximum distance in the x–direction?
   (d) Plot the probability of the particle moving a given distance versus distance. What does the probability distribution look like? Is the probability normalized?

4. Consider the probability distribution for molecular velocities in one dimension (v_x) given by $P(v_x)dv_x = Ce^{-\frac{mv_x^2}{2kT}}dv_x$.
   (a) Determine the normalization constant C.
   (b) Determine $\langle v_x \rangle$.
   (c) Determine $\langle v_x^2 \rangle$.
   (d) Determine the variance.

5. Simplify the following expressions:
   (a) $\frac{n!}{(n-2)!}$ (b) $\frac{n!}{\left(\frac{n}{2}!\right)^2}$

6. (a) Realizing the most probable outcome from a series of N coins is $N/2$ heads and $N/2$ tails, what is the expression for W_{max} corresponding to this outcome?

   (b) Given your answer for part (a), derive the following relationship between the weight for an outcome other than the most probable and W_{max}.

$$\log\left(\frac{W}{W_{\max}}\right) = -\log\left(\frac{H}{N/2}\right) - T\log\left(\frac{T}{N/2}\right)$$

   (c) We can define the deviation of a given outcome from the most probable outcome using a 'deviation index", $\alpha = (H - T)/N$. Show that the number of heads or tails can be expressed as $H = (N/2)(1+\alpha)$ and $T = (N/2)(1-\alpha)$.

   (d) Finally, demonstrate that $W/W_{\max} = e^{-N\alpha^2}$.

7. A set of 13 particles occupies states with energies of 0, 100, and 200 cm^{-1}. Calculate the total energy and number of microstates for the following energy configurations:

   (a) a_0=8, a_1=5, and a_2=0

   (b) a_0=9, a_1=3, and a_2=1

   (c) a_0=10, a_1=1, and a_2=2

   Do any of these configurations correspond to the Boltzmann distribution?

8. The vibrational frequency of I_2 is 208 cm^{-1}. At what temperature will the population in the first excited state be half that of the ground state?

9. Atkin's 9th edition: 15.1(b), 15.3(a), 15.4(a), and 15.4(b).