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**Equalizing energies.** For the two 10-particle two-state systems of Example suppose the total energy to be shared between the two objects is  $U = U_A + U_B = 4$ . What is the distribution of energies that gives the highest multiplicity?

However, we can assume the systems are of the same format (the first energy level is  $e=0$  and the second is  $e=1$ ) and that there are again 10 particles in each system. And, let's denote the number of particles in state  $i$  by  $n_i$ . So, the multiplicity of each system individually is:

$W = \binom{10!}{n_1!(10-n_1)!}$  so the total multiplicity is:

$$W_{tot} = \binom{10!}{n_{1,A}!(10-n_{1,A})!} \binom{10!}{n_{1,B}!(10-n_{1,B})!} = \frac{(10!)^2}{n_{1,A}!(10-n_{1,A})!(4-n_{1,A})!(6+n_{1,A})!}$$

We can evaluate this for all possible values of  $n_{1,A}$ :

$n_{1,A}$	W
0	210
1	1200
2	2025
3	1200
4	210

**Calculating the entropy of dipoles in a field.** You have a solutions of dipolar molecules with a positive charge at the head and a negative charge at the tail. When there is no electric field applied to the solution, the dipoles point north (n), east (e), west (w), or south (s) with equal probabilities. The probability distribution is shown in Figure 6.7(a). However when you apply a field to the solution, you now observe a different distribution: the dipole points north with probability 7/16, east or west with probability 1/4 and south with probability 1/16.

- (a) What is the polarity of the applied field? (In which direction does the field have its most positive pole?)

The positive heads of the dipole should point away from the positive pole of the field. Therefore the field must have its positive pole to the south.

- (b) Calculate the entropy of the system in the absence of the field.

Use the formula:  $S = -k \sum_i p_i \log p_i$

Since all directions are equally likely,  $S = -k * 4 * (\frac{1}{4} \log \frac{1}{4}) = k \log 4$ .

- (c) Calculate the entropy of the system in the applied field.

$$S = -k \left( \frac{7}{16} \log \frac{7}{16} + 2 * \left( \frac{1}{4} \log \frac{1}{4} \right) + \frac{1}{16} \log \frac{1}{16} \right) = k \left( 3 \log 2 - \frac{7}{16} \log 7 \right) \approx 1.228k$$

- (d) Does the system become more ordered or disordered when the field is applied?

The entropy decreases when the field is turned on so the system becomes more ordered.

**Calculating the entropy of mixing.** Consider a lattice with  $N$  sites and  $n$  green particles. Consider another lattice, adjacent to the first, with  $M$  sites and  $m$  red particles. Assume that the green and red particles cannot switch lattices. This is state A.

(a) What is the total number of configurations  $W_A$  of the system in state A?

$$W_A = W_N * W_M = \frac{N!}{n!(N-n)!} \frac{M!}{m!(M-m)!}$$

(b) Now assume that all  $N+M$  sites are available to all the green and red particles. The particles remain distinguishable by their color. This is state B. Now what is the total number of configurations  $W_B$  of the system?

$$W_B = \frac{(N+M)!}{n!m!(N+M-n-m)!}$$

Now take  $N=M$  and  $n=m$  for the following two problems:

(c) Using Stirling's approximation on page 56, what is the ratio  $W_A/W_B$ ?

$$\frac{W_A}{W_B} = \left[ \frac{N!}{n!(N-n)!} \right]^2 \frac{(n!)^2 (2N-2n)!}{(2N)!} \approx \frac{\left(\frac{N}{e}\right)^{2N} \left(\frac{2N-2n}{e}\right)^{2N-2n}}{\left(\frac{2N}{e}\right)^{2N} \left(\frac{N-n}{e}\right)^{2N-2n}} \approx \frac{2^{2N-2n}}{2^N} \approx 2^{-2n}$$

(d) Which state, A or B has the greatest entropy? Calculate the entropy difference given by:  $\Delta S = S_A - S_B = k \ln(W_A/W_B)$ .

$$\Delta S = S_A - S_B = k \log \left( \frac{W_A}{W_B} \right) \approx k \log 2^{-2n} \approx -2nk \log 2 < 0$$

so  $S_A < S_B$ .

**Maximum entropy for a three-sided die.** You have a three-sided die, with numbers 1,2 and 3 on the sides. (So the values we can observe are  $\epsilon_1=1$ ,  $\epsilon_2=2$ ,  $\epsilon_3=3$ . For a series of  $N$  dice rolls, you observe an average score  $\langle \epsilon \rangle$  per roll using the maximum entropy principle.

(a) Write expressions that show how to compute the relative probabilities of occurrence of the three sides,  $n_1^*/N$ ,  $n_2^*/N$  and  $n_3^*/N$ , if  $\alpha$  is given.

Like the example in the book, we can use the Boltzmann probabilities to maximize the

entropy. So the general form for each probability is:  $p_i = \frac{e^{-\beta \epsilon_i}}{\sum_{i=1}^3 e^{-\beta \epsilon_i}}$

To simplify, take  $x = e^{-\beta}$  so  $p_1 = \frac{x}{x+x^2+x^3}$ ,  $p_2 = \frac{x^2}{x+x^2+x^3}$ ,  $p_3 = \frac{x^3}{x+x^2+x^3}$ .

We know that:  $\langle \epsilon \rangle = \sum_{i=1}^3 \epsilon_i p_i$  so  $\alpha = \frac{x+2x^2+3x^3}{x+x^2+x^3}$

We can solve this for  $x$  in terms of  $\alpha$  by using the quadratic equation:

$$x = \frac{\alpha - 2 + \sqrt{(2 - \alpha)^2 - 4(3 - \alpha)(1 - \alpha)}}{2(3 - \alpha)} = \frac{\alpha - 2 + \sqrt{-3\alpha^2 + 12\alpha - 8}}{2(3 - \alpha)}$$

To get the probability of turning up a 1, 2, or 3, we would first calculate x and then plug back in to the equations for p<sub>1</sub>, p<sub>2</sub>, and p<sub>3</sub>.

(b) Compute n<sub>1</sub>\*/N, n<sub>2</sub>\*/N and n<sub>3</sub>\*/N if α=2.

x=1 so p<sub>1</sub>=p<sub>2</sub>=p<sub>3</sub> = 1/3.

(c) Compute n<sub>1</sub>\*/N, n<sub>2</sub>\*/N and n<sub>3</sub>\*/N if α=1.5.

$$x = \frac{\sqrt{13} - 1}{2} \approx 0.4343 \text{ so } p_1 = 0.6162 \text{ } p_2 = 0.2627 \text{ and } p_3 = 0.1162$$

(d) Compute n<sub>1</sub>\*/N, n<sub>2</sub>\*/N and n<sub>3</sub>\*/N if α=2.5.

$$x = \frac{\sqrt{13} - 1}{6} \approx 2.3028 \text{ so } p_1 = 0.1162 \text{ } p_2 = 0.2627 \text{ and } p_3 = 0.6162.$$