MATH 280: HOMEWORK #3

DUE IN LECTURE ON FEB. 14, 2019.

1. The multinomial theorem, dice rolls and thermodynamics.

Chapter 2 of E. Schrodinger's book "Statistical Thermodynamics" sketches how the multinomial theorem can be used to explain the relative likelihood of the possible energy levels of a system given only the average energy of the system.

This problem is about another way to understand these arguments using the toy model of repeated rolls of a fair six-sided die. This model provides another way to understand the Gibbs approach to statistical thermodynamics which Schrodinger describes in chapter 1 of his book.

A fair die has the numbers $1, 2, 3, 4, 5, 6$ on its six sides. Suppose you make a sequence of N-independent rolls of the die. Each such sequence can be described by a ordered sequence

$$B = (b_1, \ldots, b_N) \tag{1.1}$$

of integers $b_i \in \{1, 2, 3, 4, 5, 6\}$. There are N^6 sequences which arise in this way, and since we are assuming the die is fair and that the rolls are independent, each sequence has probability $\frac{1}{N^6}$ of occurring.

The average outcome of the sequence of rolls described by (1.1) is

$$E(B) = \frac{1}{N} \sum_{i=1}^{N} b_i \tag{1.2}$$

For $j = 1, \ldots, 6$, we can also consider the number a_j of rolls in the sequence (1.1) equal to j. In other words

$$a_j(B) = \#\{i : 1 \le i \le N \quad \text{and} \quad b_i = j\} \quad \text{for} \quad j = 1, \ldots, 6 \tag{1.3}$$

We can rewrite (1.2) as

$$E = \frac{1}{N} \sum_{j=1}^{6} j \cdot a_j(B) = a_1(B) + 2 \cdot a_2(B) + 3 \cdot a_3(B) + 4 \cdot a_4(B) + 5 \cdot a_5(B) + 6 \cdot a_6(B) \tag{1.4}$$

since there are a_j values of i for which $b_i = j$ contribute $a_j \cdot j$ to $\sum_{i=1}^{N} b_i$.

We can now state a toy model of the fundamental question of statistical mechanics (!):

Question 1.1. *Suppose that both N and E are given. Let $S(E)$ be the set of all ordered sequences B as in (1.1) for which $E(B)$ is equal to E. Suppose that each element of $S(B)$ has the same likelihood of occurring.*

1. *What are all the 6-tuples $a = (a_1, \ldots, a_6)$ of integers which could arise as $a(B) = (a_1(B), \ldots, a_6(B))$ for some element B of S? Here $a_j(B)$ is defined as in (1.3). Let $A(E)$ be the set of all such $a = (a_1, \ldots, a_6)$.*
2. *For each 6 tuple $a = (a_1, \ldots, a_6) \in A$, what is the likelihood $P(a)$ of a arising as $a = a(B)$ for some B in $S(E)$? Since every sequence of rolls is assumed to have the same likelihood of occurring,*

$$P(a) = \frac{\#\{B \in S(E) : a(B) = (a_1, \ldots, a_6)\}}{\#S(E)} \tag{1.5}$$

3. *What is the average value of $a_j(B)/N$ as B ranges over $S(E)$? This is the expect proportion of times that j will arise in a sequence of N rolls that leads to average value E.*

4. *Which 6 tuple $(a_1, \ldots, a_6)$ arises most often as $a(B)$ for some $B \in S(E)$? For this choice of $(a_1, \ldots, a_6)$, what is a_j/N? How close is a_j/N to the expected value of $a_j(B)/N$ from part (3)?*

This question relates to thermodynamics in the following way.

Suppose that a system consists of many, many parts, each of which can have one of 6 energy levels. We know the average energy E of all the particles. We would like to guess the most likely proportion of the particles which will have one of the 6 allowed energy knowing only the average energy E of all the particles.

One approach is to let N be the total number of particles, and to consider how each particle could have been labelled with one of the 6 energy levels. Schrodinger, however, prefers a different approach due to Gibbs for analyzing the question.

Imagine that we observe the system some large number N of times. Each time we do this, we pull out a sample from the system. This sample of the 6 possible energy levels. Say that b_i is the energy level of the sample obtained on the i^{th} observation. Assuming that we are pulling out samples in an unbiased way, the average

$$E = \frac{1}{N} \sum_{i=1}^{N} b_i$$

will tend toward the average energy of all the particles as N gets very large. Since we suppose that this average energy is known, we will consider the sequences

$$B = (b_1, \ldots, b_N)$$

that lie in the set $S(E)$ above. The answer to part 3 of Question 1.1 then gives the expected fraction of the particles that will have a given energy level, i.e. the expected distribution of energies among the particles. What Schrodinger actually analyzes is part 4 of Question 1.1, and we will see later how this leads to the usual formalism of thermodynamics.

The object of this homework is to work through some explicit small examples of the toy problem to have some feeling for the general case.

Problem 1. Concerning part 1 of question 1.1, show that $a = (a_1, \ldots, a_6)$ can arise as $a(B) = (a_1(B), \ldots, a_6(B))$ for some $B \in S(E)$ if and only if

$$\sum_{j=1}^{6} a_j = N \quad \text{and} \quad \sum_{j=1}^{6} j \cdot a_j = E.$$

Show that if these conditions hold for a given $a = (a_1, \ldots, a_6)$ then the number of $B \in S(E)$ for which $a(B) = a$ is the multinomial coefficient

$$\frac{N!}{a_1! \cdots a_6!}.$$

Problem 2. Recall from part 1 of question 1.1 that $A(E)$ is the set of all $a = (a_1, \ldots, a_6)$ arising as $a(B)$ for some $B \in S(E)$. Show that

$$\#S(E) = \sum_{a \in A(E)} \frac{N!}{a_1! \cdots a_6!}.$$

Deduce from Problem 1 that

$$P(a) = \frac{1}{S(E)} \cdot \frac{N!}{a_1! \cdots a_6!}.$$

if $a \in A(E)$.

Problem 3. Part 3 of Question 1.1 is to find the average value of $a_j(B)/N$ as B ranges over $S(E)$. Show that this average is the same as

$$\sum_{a=(a_1,\ldots,a_6)\in A} p(a)\cdot \frac{a_j}{N}.$$

Here $p(a)$ is the probability of a occurring, so this is the expected value of the random variable a_j/N on the sample space A.

Problem 4. Suppose now that $N = 10$ and that $E = 1.3$. Find $A(E)$, $\#S(E)$ and $P(a)$ for each $a \in A(E)$. Find the expected value of $a_j(B)/N = a_j(B)/10$ as B ranges over $S(E)$ as in part 3 of Question 1.1 and $j = 1,\ldots,6$. How do these compare to a_j/N when $a = (a_1,\ldots,a_6)$ is the element of $A(E)$ for which $P(a)$ is largest, as in part 4 of Question 1.1?