

## Solution 4: Free Energy and Partition Functions

**Preface:** In this assignment, we apply our understanding of free energy to compute how the average spin of a spin system is affected by an external magnetic field. We then compute partition functions for various systems. In the penultimate problem, we derive the formula for the number of derangements of a list, and thus establish the mathematical groundwork for the final problem: the statistical physics of permutations.

### 1. Spins in a Magnetic Field: Macrostates

- (a) (4 points) We have  $N$  spins in an external magnetic field  $H$  and we seek to find the free energy  $F_N(m, T)$  for this system. Mathematically, the only difference between this system and that considered in Section 6 of Lecture Notes 05 is the energy term. In the lecture notes, the energy was quadratic in the average magnetization  $m$ . In this problem, the energy is given by

$$E_N(m) = -\mu H \sum_{i=1}^N s_i = -\mu H N \frac{1}{N} \sum_{i=1}^N s_i = -\mu H N m, \quad (1)$$

which is linear in  $m$ . The entropy for the two systems is the same, so we can simply take Eq.(31) from the notes, and state that the entropy for our system is

$$S_N(m) = k_B \ln \Omega_N(m) = k_B \left[ N \ln 2 - \frac{N}{2} \ln(1 - m^2) - \frac{N}{2} m \ln \frac{1 + m}{1 - m} \right], \quad (2)$$

where we neglected sub-leading terms. Using Eq.(1) and Eq.(2), the free energy for the system is therefore

$$\begin{aligned} F_N(m, T) &= E_N(m) - T S_N(m) \\ &= \boxed{-\mu H N m - k_B T \left[ N \ln 2 - \frac{N}{2} \ln(1 - m^2) - \frac{N}{2} m \ln \frac{1 + m}{1 - m} \right]}. \end{aligned} \quad (3)$$

- (b) (4 points) We now want to compute the value of  $m$  at which Eq.(3) is at a local minimum. We determine the local minimum of  $F_N(m, T)$  by finding the  $\bar{m}$  that satisfies

$$\frac{\partial}{\partial m} F_N(m = \bar{m}, T) = 0, \quad \frac{\partial^2}{\partial m^2} F_N(m = \bar{m}, T) > 0. \quad (4)$$

Computing the first condition in Eq.(4), we have

$$\begin{aligned} 0 &= \frac{\partial}{\partial m} F_N(m = \bar{m}, T) \\ &= -\mu H N - \frac{N k_B T}{2} \left( \frac{2m}{1 - m^2} - \ln \frac{1 + m}{1 - m} + m \frac{1}{1 + m} + m \frac{1}{1 - m} \right) \Big|_{m=\bar{m}} \\ &= -\mu H N + \frac{N k_B T}{2} \ln \frac{1 + \bar{m}}{1 - \bar{m}}, \end{aligned} \quad (5)$$

which yields the condition

$$\frac{2\mu H}{k_B T} = \ln \frac{1 + \bar{m}}{1 - \bar{m}}. \quad (6)$$

We can write Eq.(6) in a more useful form by using the definition of the hyperbolic tangent function. First, we take the exponential of both sides of Eq.(6) in order to obtain

$$e^{2\mu H/k_B T} = \frac{1 + \bar{m}}{1 - \bar{m}}. \quad (7)$$

Then we solve Eq.(7) for  $\bar{m}$  to find

$$\bar{m} = \frac{e^{2\mu H/k_B T} - 1}{e^{2\mu H/k_B T} + 1} = \frac{e^{\mu H/k_B T} - e^{-\mu H/k_B T}}{e^{\mu H/k_B T} + e^{-\mu H/k_B T}}, \quad (8)$$

or, with the the definition,

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}, \quad (9)$$

we obtain

$$\boxed{\bar{m} = \tanh\left(\frac{\mu H}{k_B T}\right)}. \quad (10)$$

Checking the second condition in Eq.(4), we have

$$\begin{aligned} \frac{\partial^2}{\partial m^2} F_N(m = \bar{m}, T) &= \frac{\partial}{\partial m} \frac{N}{2} \left[ -2\mu H + k_B T \ln(1 + m) - k_B T \ln(1 - m) \right] \Big|_{m=\bar{m}} \\ &= N \frac{k_B T}{1 - \bar{m}^2}, \end{aligned} \quad (11)$$

which is always greater than zero for valid values of  $\bar{m}$  (because  $m = \sum_i s_i/N$  it can only be within the range  $[-1, +1]$ ). Therefore, with both conditions in Eq.(4) satisfied, Eq.(10) defines the local minimum of the free energy. ■

- (c) (4 points) Since Eq.(10) gives  $\bar{m}$  as a function of  $H$ , we can easily plot it. For three different temperature values, we have

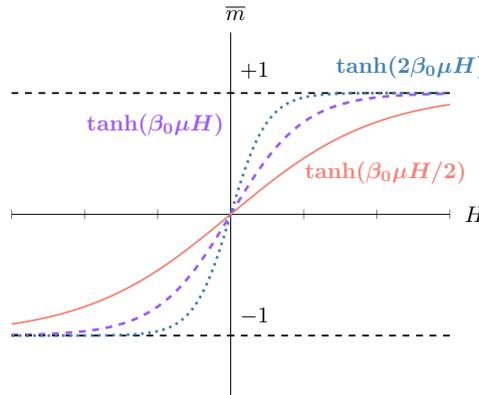


Figure 1: Plot of  $\bar{m}$  as a function of  $H$  for various temperatures. As we decrease temperature (or increase  $\beta$ ), the response of  $\bar{m}$  to  $H$  increases (i.e.,  $\partial m/\partial H$  increases). ■

- (d) (4 points) As  $T \rightarrow 0$ ,  $\mu H/k_B T$  goes to  $\infty$  and Eq.(10) and Eq.(9) tell us that the  $\bar{m}$  goes to  $+1$ .

$$\boxed{\text{As } T \rightarrow 0, \bar{m} \rightarrow 1}. \quad (12)$$

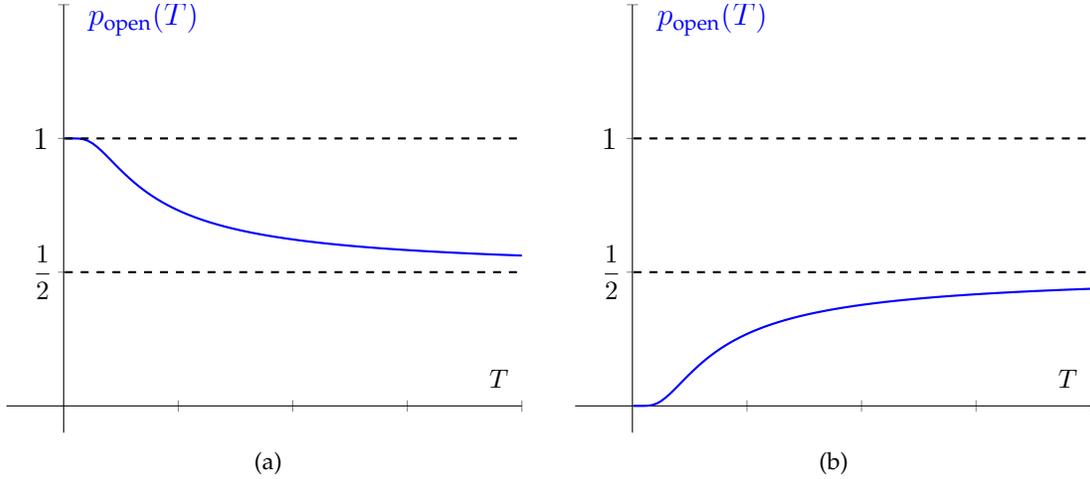


Figure 2: Plot of  $p_{\text{open}}$  as a function of  $T$ . Plot (a) is based on the assumption that  $\varepsilon_{\text{open}} < \varepsilon_{\text{closed}}$  and plot(b) is based on the assumption that  $\varepsilon_{\text{open}} > \varepsilon_{\text{closed}}$ . We note that at  $T = 0$  we either have  $p_{\text{open}} = 1$  (if  $\varepsilon_{\text{open}} < \varepsilon_{\text{closed}}$ ) or  $p_{\text{open}} = 0$  (if  $\varepsilon_{\text{open}} > \varepsilon_{\text{closed}}$ ) both of which reflect the fact that at  $T = 0$ , the system only wants to be in its lowest energy microstate. As  $T \rightarrow \infty$ ,  $p_{\text{open}} \rightarrow 1/2$  meaning that at high temperatures, the open and closed microstates are equally likely.

When  $\bar{m} = 1$ , this means that  $\sum_{i=1}^N s_i = N$  and thus all the spins are pointed upwards. There is only a single microstate for which all the spins are pointed upwards, so  $\Omega_N(\bar{m}) = 1$  at this temperature. We thus find that the entropy is

$$\boxed{\lim_{T \rightarrow 0} S_N(\bar{m}) = \lim_{T \rightarrow 0} k_B \ln \Omega_N(\bar{m}) = \ln 1 = 0,} \quad (13)$$

which is consistent with the third law of thermodynamics (i.e., that the entropy of systems with a single lowest energy state goes to zero as temperature goes to zero). ■

## 2. Open and Closed Ion Channel

- (a) (2 points) We want to compute the partition function of the ion channel system. The ion channel has two microstates. One microstate has energy  $\varepsilon_{\text{open}}$  corresponding to the open microstate and the other has energy  $\varepsilon_{\text{closed}}$  corresponding to the closed microstate. The partition function for a general system is

$$Z = \sum_{\{i\}} e^{-\beta E_i}, \quad (14)$$

where  $i$  is a particular microstate,  $\sum_{\{i\}}$  defines the summation over microstates, and  $E_i$  is the energy of microstate  $i$ . For this system, we therefore have

$$\boxed{Z = e^{-\beta \varepsilon_{\text{closed}}} + e^{-\beta \varepsilon_{\text{open}}},} \quad (15)$$

where  $\beta = 1/k_B T$ . ■

(b) (4 points) In general, the probability to be in a microstate  $i$  of a thermodynamic system is

$$p_i = \frac{e^{-\beta E_i}}{Z}, \quad (16)$$

where  $E_i$  is the energy of the microstate, and  $Z$  is the partition function of the system. For our system, given the result Eq.(15) and that the energy of the open microstate is  $\varepsilon_{\text{open}}$ , the probability to be in the open state is

$$p_{\text{open}} = \frac{e^{-\beta \varepsilon_{\text{open}}}}{e^{-\beta \varepsilon_{\text{closed}}} + e^{-\beta \varepsilon_{\text{open}}}} = \frac{1}{e^{-\beta(\varepsilon_{\text{closed}} - \varepsilon_{\text{open}})} + 1}, \quad (17)$$

where we divided the numerator and the denominator by  $e^{-\beta \varepsilon_{\text{closed}}}$  in the final line. With the definition  $\Delta\varepsilon = \varepsilon_{\text{closed}} - \varepsilon_{\text{open}}$  and writing this result in terms of  $T$ , we have

$$p_{\text{open}} = \frac{1}{e^{-\Delta\varepsilon/k_B T} + 1}. \quad (18)$$

Plots of this function (contingent on whether  $\Delta\varepsilon > 0$  or  $\Delta\varepsilon < 0$ .) are shown in Fig. 2. ■

(c) (4 points) By the Gibbs definition, the entropy of a two-state system where there is a probability  $p_{\text{open}}$  to be in one state and a probability  $p_{\text{closed}}$  to be in the other state is

$$S = -k_B p_{\text{open}} \ln p_{\text{open}} - k_B p_{\text{closed}} \ln p_{\text{closed}}, \quad (19)$$

We computed  $p_{\text{open}}$  in Eq.(18). By probability normalization, we must have  $p_{\text{open}} + p_{\text{closed}} = 1$ . And so, we have

$$p_{\text{closed}} = 1 - \frac{1}{e^{-\Delta\varepsilon/k_B T} + 1} = \frac{e^{-\Delta\varepsilon/k_B T}}{e^{-\Delta\varepsilon/k_B T} + 1} = \frac{1}{1 + e^{\Delta\varepsilon/k_B T}}, \quad (20)$$

where we multiplied the numerator and the denominator by  $e^{\Delta\varepsilon/k_B T}$  in the final equality. Returning to Eq.(19), and using Eq.(18) and Eq.(20), we find that the entropy is

$$S = k_B \frac{\ln(e^{-\Delta\varepsilon/k_B T} + 1)}{e^{-\Delta\varepsilon/k_B T} + 1} + k_B \frac{\ln(e^{\Delta\varepsilon/k_B T} + 1)}{e^{\Delta\varepsilon/k_B T} + 1}. \quad (21)$$

Now we will consider the  $T \rightarrow 0$  limit. Let us assume  $\Delta\varepsilon > 0$ . If we take  $T \rightarrow 0$ , then the  $e^{-\Delta\varepsilon/k_B T} + 1$  goes to 1 since the exponential goes to zero. Since  $\ln 1 = 0$ , the first term of Eq.(21) is zero when  $T \rightarrow 0$  (and  $\Delta\varepsilon > 0$ ). For the second term, taking  $T \rightarrow 0$ , results in a limit like

$$\lim_{x \rightarrow \infty} \frac{\ln x}{x}. \quad (22)$$

Because  $x$  faster than  $\ln x$  increases as we increase  $x$ , this limit is also zero. Therefore, as  $T \rightarrow 0$ , **the entropy Eq.(21) also goes to zero. This result is consistent the third law of thermodynamics.** ■

### 3. Lattice Model of a Single Dimer

(a) (4 points) We want to determine the partition function of the system consisting of  $L$  distinct lattice sites and two identical particles where the particles have energy  $-E_0$  when they are next to one

another. There are “ $L$  choose 2” ways to select lattice sites for the two particles, and thus there are “ $L$  choose 2” microstates. Of the total number of ways to select lattice sites for the two particles, there are  $L - 1$  ways to select these lattice sites such that the particles are next to one another. This is because having the particles be next to one another is like having a larger particle that occupies *two* lattice sites, and for  $L$  total lattice sites, such a large particle can be in one of  $L - 1$  positions. The counting of our microstates and their associated energies is therefore as follows

State of System	Number of Microstates	Energy of Microstate
Dimer microstates	$L - 1$	$-E_0$
Non-dimer microstates	$\binom{L}{2} - (L - 1)$	0

Therefore, by the definition of the partition function for a thermal system, we obtain

$$\begin{aligned}
 Z &= \sum_{\{i\}} e^{-\beta E_i} \\
 &= \sum_{\text{dimers}} e^{-\beta E_{\text{dimer}}} + \sum_{\text{non-dimers}} e^{-\beta E_{\text{non-dimers}}} \\
 &= (L - 1)e^{\beta E_0} + \binom{L}{2} - L + 1 \\
 &= \boxed{(L - 1)e^{\beta E_0} + \binom{L}{2} - L + 1}. \tag{23}
 \end{aligned}$$

- (b) (4 points) We want to compute the probability to be in the dimerized state. Given the above table, the probability to be in the dimerized state is

$$\begin{aligned}
 p_{\text{dimer}} &= \frac{(L - 1)e^{\beta E_0}}{(L - 1)e^{\beta E_0} + \binom{L}{2} - L + 1} \\
 &= \frac{(L - 1)e^{\beta E_0}}{(L - 1)e^{\beta E_0} + L(L - 1)/2 - (L - 1)} \\
 &= \boxed{\frac{1}{1 + (L/2 - 1)e^{-\beta E_0}}}, \tag{24}
 \end{aligned}$$

where in the second line we used  $\binom{L}{2} = L!/(2!(L - 2)!) = L(L - 1)/2$  and in the final line we divided the numerator and the denominator by  $(L - 1)e^{\beta E_0}$ . We note that as  $T \rightarrow \infty$ , (i.e.,  $\beta \rightarrow 0$ ) the probability to be in the dimerized state becomes  $2/L$  which is simply the number of dimer microstates divided by the total number of microstates. Alternatively as  $T \rightarrow 0$ ,  $\beta \rightarrow \infty$  and the probability to be in the dimerized state goes to 1. This makes sense, because the dimerized state is the lowest energy state and the system falls to the lowest energy state as  $T \rightarrow 0$ .

- (c) (4 points) Our task is to find the temperature ranges for which there is a higher likelihood to be in the dimer state than there is to be in the non-dimer state. Since there are only two states, there is a higher likelihood to be in the dimer state if  $p_{\text{dimer}} > 1/2$ . Thus, our task (reformulated) is to find the temperature ranges for which  $p_{\text{dimer}}$  in Eq.(24) is greater than  $1/2$ .

Setting up the associated inequality and solving, we find

$$1/2 < p_{\text{dimer}}$$

$$\begin{aligned}
&= \frac{1}{1 + (L/2 - 1)e^{-\beta E_0}} \\
2 &> 1 + (L/2 - 1)e^{-\beta E_0} \quad [\text{Flip inequality when inverting both sides}] \\
1 &> (L/2 - 1)e^{-\beta E_0} \\
\ln 1 &> \ln [(L/2 - 1)e^{-\beta E_0}] \\
0 &< \ln(L/2 - 1) - \frac{E_0}{k_B T}. \tag{25}
\end{aligned}$$

Isolating  $T$  in the final inequality, we have

$$\boxed{T < \frac{E_0}{\ln(L/2 - 1)}}. \tag{26}$$

■

#### 4. Spins in a Magnetic Field: Microstates

- (a) (4 points) Our objective is to derive an alternative expression for the partition function of a collection of spins  $\{s_i\}$  each of which has a magnetic dipole moment  $\mu$  and all of which exist in an external magnetic field  $H$ . We begin with the expression for the partition function as it was derived in Lecture 06:

$$Z_N(\beta\mu H) = \sum_{\{s_j=\pm 1\}} \exp\left(\beta\mu H \sum_{i=1}^N s_i\right) = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\left(\beta\mu H \sum_{i=1}^N s_i\right) \tag{27}$$

In Eq.(27), we are computing the sum of  $\exp\left(\beta\mu H \sum_{i=1}^N s_i\right)$  over the possible values of  $s_1, s_2, \dots, s_N$ . For this summation, the microstates are written out explicitly, but we can also write Eq.(27) in terms of *collections* of microstates. If our system has  $n_\uparrow$  up spins and  $n_\downarrow$  down spins, then we have the equation

$$\sum_{i=1}^N s_i = \sum_{\text{num. up spins}} (+1) + \sum_{\text{num. down spins}} (-1) = n_\uparrow - n_\downarrow. \tag{28}$$

The energy of the system can thus be written as

$$E(n_\uparrow) = -\mu H \sum_{i=1}^N s_i = -\mu H(n_\uparrow - n_\downarrow). \tag{29}$$

For this spin system,  $n_\uparrow$  can go from 0 to  $N$ . Now, there are " $N$  choose  $n_\uparrow$ " microstates for every choice of  $n_\uparrow$ . Therefore, if we were to compute the partition function of this system using the energy Eq.(29), we would need to weigh our Boltzmann factor  $e^{-\beta E(n_\uparrow)}$  by the number of microstates associated with this energy. We therefore find that the partition function is

$$Z_N(\beta\mu H) = \sum_{n_\uparrow=0}^N (\# \text{ of microstates for } n_\uparrow) e^{-\beta E(n_\uparrow)} = \sum_{n_\uparrow=0}^N \binom{N}{n_\uparrow} e^{\beta\mu H(n_\uparrow - n_\downarrow)}. \tag{30}$$

■

- (b) We want to use Eq.(30) to complete the calculation of the partition function for this system. We

first note that  $n_{\downarrow} = N - n_{\uparrow}$  so that

$$\beta\mu H(n_{\uparrow} - n_{\downarrow}) = \beta\mu H(n_{\uparrow} - (1 - n_{\uparrow})) = \beta\mu H(2n_{\uparrow} - 1). \quad (31)$$

Eq.(30) then becomes

$$\begin{aligned} Z_N(\beta\mu H) &= \sum_{n_{\uparrow}=0}^N \binom{N}{n_{\uparrow}} e^{\beta\mu H(2n_{\uparrow}-N)} \\ &= e^{-\beta\mu HN} \sum_{n_{\uparrow}=0}^N \binom{N}{n_{\uparrow}} e^{2\beta\mu H n_{\uparrow}} \\ &= e^{-\beta\mu HN} \sum_{n_{\uparrow}=0}^N \binom{N}{n_{\uparrow}} (e^{2\beta\mu H})^{n_{\uparrow}} \\ &= e^{-\beta\mu HN} (1 + e^{2\beta\mu H})^N \quad \text{[Binomial Theorem]} \\ &= [e^{-\beta\mu H} (1 + e^{2\beta\mu H})]^N \\ &= (e^{-\beta\mu H} + e^{\beta\mu H})^N \end{aligned} \quad (32)$$

With the fact that  $e^x + e^{-x} = 2 \cosh(x)$ , we then find

$$Z_N(\beta\mu H) = 2^N \cosh^N(\beta\mu H), \quad (33)$$

as we previously found. ■

## 5. Number of Derangements

- (a) (2 points) We want to find the number of derangements of the list  $(1, 2, 3)$  where a derangement is defined as a permutation in which no element is in its original ordering. Listing out all the permutations of  $(1, 2, 3)$  we have

$$(1, 2, 3) \quad (1, 3, 2) \quad (2, 3, 1) \quad (2, 1, 3) \quad (3, 1, 2) \quad (3, 2, 1). \quad (34)$$

Inspecting Eq.(34), we see that the first four permutations have either 1, 2, or 3 in the same ordering that the respective number has in the original permutation  $(1, 2, 3)$ . Thus only the last two permutations satisfy the definition of a derangement. Therefore

$$\boxed{\text{Number of derangements of } (1, 2, 3) = 2.} \quad (35)$$

■

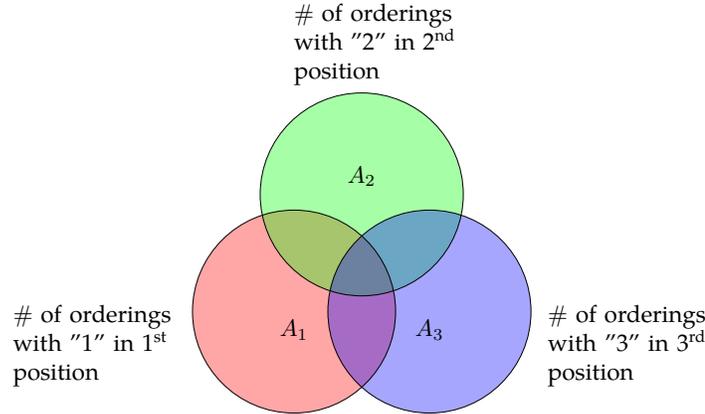


Figure 3: The circle  $A_k$  represents all the orderings such that  $k$  is in the  $k$ th position. To find the number of derangements, we will count the number of unique elements in the above diagram and subtract the result from the total number of permutations of three elements.

- (b) i. (4 points) We want to express the total number of unique orderings in the Venn diagram Fig. 3. In the Venn diagram, each circle represents the orderings with a particular number in its original ordering. For example,  $A_k$  is the collection of orderings in which  $k$  is in the  $k$ th position. The Venn diagrams have overlapping elements because some permutations have multiple numbers remaining in their original positions. If we had two Venn diagrams, we would add all the elements from the single Venn diagrams and then subtract the contributions arising from the overlap. We would then find

$$\text{Total number of elements for two circle Venn diagram} = |A_1| + |A_2| - |A_1 \cap A_2| \quad (36)$$

For the three circle Venn diagram, to count the total number of unique permutations contained in all three Venn diagrams, we **add** all the elements in all **single** Venn diagrams, **subtract** the contributions arising from all overlaps of **two** Venn diagrams, and then **add** the contributions arising from the overlap of the **three** Venn diagrams. The end result is that the number of unique elements in Fig. 3 is

$$|A_1| + |A_2| + |A_3| - |A_1 \cap A_2| - |A_2 \cap A_3| - |A_3 \cap A_1| + |A_1 \cap A_2 \cap A_3| \quad (37)$$

- ii. (4 points) Now we want to express Eq.(37) in terms of factorials. We note that  $A_k$  is the set of permutations where the number  $k$  is in the  $k$ th position, and  $|A_k|$  is the number of elements in that set. Since the number  $k$  has a fixed position in  $A_k$ , we can count the number of elements comprising  $A_k$  (i.e., find  $|A_k|$ ) by counting the number of ways to reorder the numbers which are not fixed.

For a list of three numbers, if we fix one number, then there are  $(3-1)! = 2!$  ways to rearrange the remaining numbers.

Similarly,  $|A_k \cap A_\ell|$  is the number of permutations such that *both*  $k$  and  $\ell$  are in their respective positions. For a list of three numbers, if we fix two numbers, then there is  $(3-2)! = 1$  way to arrange the remaining number.

Continuing with this argument, we therefore find

$$\begin{aligned} |A_1| &= |A_2| = |A_3| = (3-1)! = 2! \\ |A_1 \cap A_2| &= |A_2 \cap A_3| = |A_3 \cap A_1| = (3-2)! = 1! \\ |A_1 \cap A_2 \cap A_3| &= (3-3)! = 0!. \end{aligned} \quad (38)$$

Rewriting Eq.(37) in terms of factorials, we see that the number of unique elements in Fig. 3 (i.e., the number of permutations of (1, 2, 3) where either 1, 2, or 3 is in its original position) is

$$\boxed{3 \cdot 2! - 3 \cdot 1! + 1 \cdot 0!} \quad (39)$$

- iii. (4 points) Eq.(39) is the number of permutations of (1, 2, 3) where either 1, 2, or 3 is in its original position. To find the number of permutations where neither 1, 2, nor 3 is in its original position (i.e., the number of derangements), we need to subtract the total number of permutations from the number calculated in Eq.(39). There are  $3!$  total permutations for a list with three unique numbers. Therefore, computing the number of derangements, we have

$$\boxed{d_3 = 3! - (3 \cdot 2! - 3 \cdot 1! + 1 \cdot 0!) = 3! - 3 \cdot 2! + 3 \cdot 1! - 1 \cdot 0!} \quad (40)$$

- iv. (4 points) Inspecting Eq.(40), we see that the factorial terms descend in integer steps from 3 to 0. We also see that the magnitude of the coefficients of the factorial terms, are 1, 3, 3, 1 in sequence. These coefficients are the same as those in the binomial expansion of  $(x + y)^3$ , namely they are  $\binom{3}{j}$  for  $j$  running from 0 to 3. Finally, we see that the signs in Eq.(40) alternate with the first term being positive, the second term negative, the third term positive again, and the fourth term negative again. We can thus write Eq.(40) in summation notation if we make the following translations

$$3!, 2!, 1!, 0! \rightarrow (3 - j)! \text{ for } j = 0, 1, 2, 3 \quad (41)$$

$$1, 3, 3, 1 \rightarrow \binom{3}{j} \text{ for } j = 0, 1, 2, 3 \quad (42)$$

$$+1, -1, +1, -1 \rightarrow (-1)^j \text{ for } j = 0, 1, 2, 3 \quad (43)$$

In result, Eq.(40) becomes

$$\boxed{d_3 = \sum_{j=0}^3 \binom{3}{j} (-1)^j (3 - j)!} \quad (44)$$

- v. (2 points) We would like to generalize Eq.(44) to the case where we have  $N$  unique elements and we are trying to find the number of derangements. If we were to work through the derivation again, we would find that the  $d_N$  could be gleaned from Eq.(44) if we took every 3 and replaced it with an  $N$ . We thus have

$$\boxed{d_N = \sum_{j=0}^N \binom{N}{j} (-1)^j (N - j)!} \quad (45)$$

- (c) (6 points) In order to use Eq.(45) to fill out the given table, we need to compute  $d_1$ ,  $d_2$ ,  $d_3$ , and  $d_4$ . Doing so, according to the given formula, we have

$$\begin{aligned} d_1 &= \sum_{j=0}^1 \binom{1}{j} (-1)^j (1 - j)! \\ &= \binom{1}{0} 1! - \binom{1}{1} 0! \end{aligned}$$

$$= 1 - 1 = 0 \tag{46}$$

$$\begin{aligned} d_2 &= \sum_{j=0}^2 \binom{2}{j} (-1)^j (2-j)! \\ &= \binom{2}{0} 2! - \binom{2}{1} 1! + \binom{2}{0} 0! \\ &= 2 - 2 + 1 = 1 \end{aligned} \tag{47}$$

$$\begin{aligned} d_3 &= \sum_{j=0}^3 \binom{3}{j} (-1)^j (3-j)! \\ &= \binom{3}{0} 3! - \binom{3}{1} 2! + \binom{3}{2} 1! - \binom{3}{3} 0! \\ &= 3! - 3 \cdot 2! + 3 \cdot 1! - 0! = 6 - 6 + 3 - 1 = 2 \end{aligned} \tag{48}$$

$$\begin{aligned} d_4 &= \sum_{j=0}^4 \binom{4}{j} (-1)^j (4-j)! \\ &= \binom{4}{0} 4! - \binom{4}{1} 3! + \binom{4}{2} 2! - \binom{4}{3} 1! + \binom{4}{4} 0! \\ &= 4! - 4 \cdot 3! + 6 \cdot 2! - 4 \cdot 1! + 0! = 24 - 24 + 12 - 4 + 1 = 9 \end{aligned} \tag{49}$$

Collecting these results and placing them in a table, gives us the summarized result

Number of Elements in List	Number of Derangements
1	0
2	1
3	2
4	9

■

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