Problem : Directed Polymer 1

Problem statement

A directed polymer consists of atoms $i = 0, 1, 2, .., N$ at positions $(x_i, y_i) \in \mathbb{Z}^2$ of a square lattice. The atom at the origin is fixed at the position $x_0 = y_0 = 0$ and the other atoms are chained together such that $x_i - x_{i-1} = 1$ and $|y_i - y_{i-1}| = 1$.
This polymer is hence oriented in the x-direction and does not self intersect.

Before starting with sub-questions, let us draw this polymer to get an intuition.
Using the following properties we will graph points on a $\mathbb{Z}^2$ (The elements of this set are (n, m) such that $n, m \in \mathbb{Z}$). The polymer will be the curve that will be formed by connecting these points

- $\mathcal{O} = (0, 0)$: This means that our first point has to be at the origin (i.e. Polymer/curve starts at the origin)
- $x_i - x_{i-1} = 0$: This means that, no matter what, the next point as to be one unit to the right. (This property tells us how the polymer moves in the x-direction)
- $|y_i - y_{i-1}| = 1$ which can be written as

$$y_i - y_{i-1} = \{\begin{cases} 1 \\ -1 \end{cases}$$

  This property tell us how the subsequent points have to be placed in y direction. It could go one unit up or one unit down.

Combining all the three points, we can draw the following diagram of all the possible

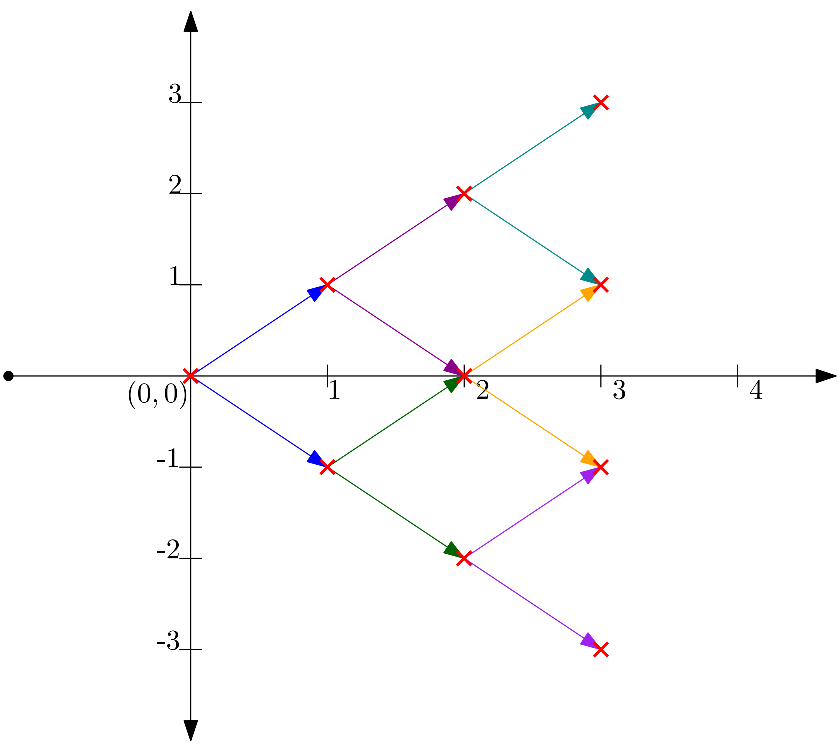

Figure 1: All possible paths till $n = 3$

The "x" marks on the diagrams are the possible points we can have till n=3. At every node you choose one of the colored arrow. Doing this you can trace a curve (the curve essentially represents the polymer, so I'll use both the words interchangeably from now on)
Here are three examples of valid polymers of length 3 (we can define the "length" by the number of units the curve reaches in x-axis)

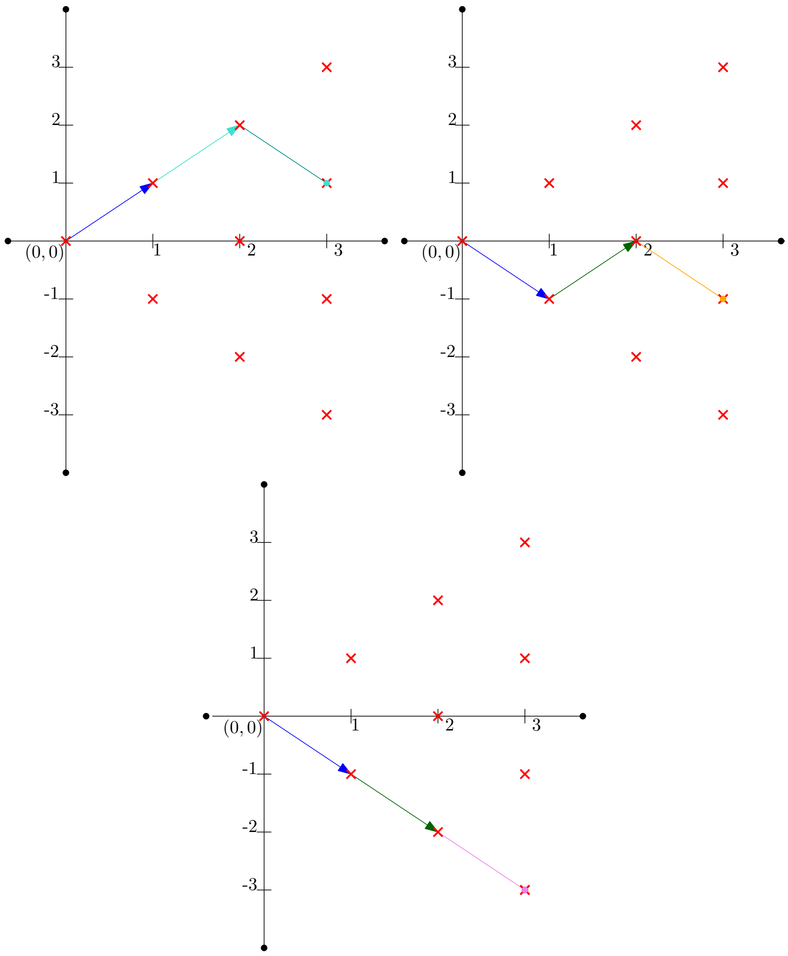

Figure 2: Top left : Polymer a, Top right : Polymer b, Bottom : Polymer c

For a polymer of length 3, we can have

$$(2 \text{ choices after origin}) \times (2 \text{ choices after reaching node 1}) \times (2 \text{ choices after reaching node 2}) \\ = 2^3 \text{ choices} = 8 \text{ choices}$$

We can easily generalize this by saying that a polymer of length N will have 2^N choices.

This should help get a better picture of what is happening in the problem. Let's get down to business and solve the problems at hand.

Problem (a)

Determine the total number of micro-states of the polymer.

Solution

Now that we already have a visual representation, we can think about a particle on every node (every "x" in the diagram would be a particle. For every available x-position, there can be only one particle). The first particle will be fixed at the origin. All the other particles have a choice of being either one unit up or down compared to the previous particle.

We can summarize it the following way

Particle number	1	2	3	...	N	N+1
Choices	1	2	2	2	2	2
Node number (x_coordinate)	0	1	2	...	N-1	N

Table 1: Counting microstates

From this table we can see that for N positions on the x-axis, including the 0th position, we need $N+1$ particles.

The microstates $\mathcal{W}$ are the total number of polymers we can have for given N nodes. Therefore,

$$\mathcal{W} = \underbrace{1}_{\text{Fixed particle 1}} \times \underbrace{2 \times 2 \times \ldots \times 2}_{N} = 2^N$$

Problem (b)

Determine the total number of micro-states $\mathcal{W}(y)$ having the property $y_N = y$.
Hint : Write y_N in terms of $\sigma_i = y_i - y_{i-1} \in \pm 1$, where $i = 1, \ldots, N$, and then in terms of the number ν of $+1$'s in σ_i

Solution

The hint here is absolutely crucial. But, if you don't understand it, it can confuse you even more

Let us call σ_i as the "sign" of a particular polymer. We know that polymer must start at $(0,0)$, then it has to go one unit right. After that, it has a choice of going one unit up or down.

Let us define n_+ as the number of times a particular polymer takes the unit up step and n_- as the number of times it takes a step down.

Then the total sign of the polymer can be defined by

$$y_N = \sum_i \sigma_i = n_+ - n_- = y$$

i.e. for every $\nearrow$ we count it in n_+ and for every $\searrow$ we count it in n_-

We also know

$$n_+ + n_- = N \quad \implies \quad n_- = N - n_+$$

In the following table we count the n_+, n_- and y_N for the $N = 3$ unit polymers that we illustrated on page 2 of this problem.

Figure	a	b	c
Structure	$\nearrow + \nearrow + \searrow$	$\searrow + \nearrow + \searrow$	$\searrow + \searrow + \searrow$
n_+	2	1	0
n_-	1	2	3
y_N	1+1-1=1	-1+1-1=-1	-1-1-1=-3

All the preparations are done, now we can get back to the problem at hand. In the previous problem we counted all microstates. Now, we want to find the microstates with a certain property. The certain property for this problem being, $y(N) = y$.
What does this mean? It means that we are trying to find for a given ensemble of states, what is the probability of having $y(N)$ to be equal to y. The probability can be calculated by $\frac{\text{Number of states having this property}}{\text{Total number of states}}$

From the math above the table we can write the following equation,

$$y_N = n_+ - n_- = n_+ - (N - n_+) = 2n_+ - N \overset{!}{=} y$$

The equation till the exclamation mark should be clear. Due to poor choice of variables, it can get misleading. The "y" at the end of the equation is a pure number.

Now is the crucial step. For a given N, how many states will have the property $y(N) = y$ It will be

$$\binom{N}{y} = \binom{N}{n_+}$$

The equation comes from the fact that for a given N and y, we can find the corresponding n_+, and n_+ is just the number of $\nearrow$ steps, which is easy to measure.

Therefore,

$$\text{Number of microstates with } n_+ \text{ states} = \binom{N}{n_+} = \binom{N}{\frac{y_N+N}{2}} = \mathcal{W}(y)$$

$$\text{Probability of finding such a mircostate} = \frac{\mathcal{W}(y)}{\mathcal{W}}$$

Problem (c)

Calculate the typical deflection of the chain end,

$$\langle y_N^2 \rangle = \frac{\sum_y y^2 \mathcal{W}(y)}{\sum_y \mathcal{W}(y)}$$

Hint : Consider the partition function of the canonical ensemble $Z(\beta) = \sum_y e^{\beta y}\mathcal{W}(y)$. Write $\langle y_N^2 \rangle$ in terms of the β-derivative of $Z(\beta)$.

Solution

There are multiple ways to go around this calculation, the best one is to remember this trick, Define (we will see why, it is just for simplicity purposes)

$$Z(\beta) = \sum_y e^{\beta y}\mathcal{W}(y)$$

Here we can see that

$$Z(0) = \sum_y \mathcal{W}(y) = \text{Denominator}$$

which is the denominator of the expression we are trying to calculate. Maybe $Z''(0)$ is the numerator (Prime is differentiation with respect to β)?

Checking,

$$\left(Z''(\beta)\right)|_{\beta=0} = \left.\frac{\partial^2 Z(\beta)}{\partial\beta^2}\right|_{\beta=0} = \left.\left(\sum_y e^{\beta y} y^2 \mathcal{W}(y)\right)\right|_{\beta=0} = \sum_y (1) y^2 \mathcal{W}(y) = \text{Numerator}$$

So, we can write down our equation as

$$\langle y_N^2 \rangle = \frac{Z''(0)}{Z(0)}$$

Let's calculate the numerator and denominator explicitly from scratch, i.e. for arbitrary β, we can then just plug $\beta = 0$ and get the expressions we want (remember we have already established this relation : $y = 2n_+ - N$

$$\begin{aligned}
Z(\beta) &= \sum_y e^{\beta y} \mathcal{W}(y) \\
&= \sum_{n_+} e^{\beta(2n_+ - N)} \binom{N}{n_+} \\
&= \sum_{n_+} e^{\beta(n_+ + n_+ - N)} \binom{N}{n_+} \\
&= \sum_{n_+} \left(e^{\beta}\right)^{n_+} \left(e^{-\beta}\right)^{N-n_+} \binom{N}{n_+}
\end{aligned}$$

Now we use the binomial identity : $(a+b)^n = \sum_{k=0}^{n} \binom{n}{k} a^{n-k} b^k$ (You can easily check for $n = 2$ you get $(a+b)^2 = a^2 + 2ab + b^2$)

If we take $a = e^{-\beta}$, $b = e^{\beta}$, then we can use the identity in the equation above it.

$$\begin{aligned}
Z(\beta) &= \sum_k b^k a^{N-k} \binom{N}{k} \\
&= (a+b)^N \\
&= (e^{\beta} + e^{-\beta})^N
\end{aligned}$$

Now, recall the definition of hyperbolic cosine

$$\cosh(\beta) = \frac{e^{\beta} + e^{-\beta}}{2} \implies 2\cosh(\beta) = e^{\beta} + e^{-\beta}$$

Using this definition into what we had,

$$Z(\beta) = (2\cosh(\beta))^N = 2^N \cosh^N \beta$$

Recalling the quantity we were calculating for : $\langle y_N^2 \rangle = \frac{Z''(0)}{Z(0)}$. So, we need to calculate $Z(0)$ and $Z''(0)$

$$Z(0) = 2^N \cosh^N(0) = 2^N$$

$$\begin{aligned}
Z'(\beta) &= 2^N \frac{\partial(\cosh(\beta))^N}{\partial\beta} = 2^N \Big[N(\cosh(\beta))^{N-1} \cdot \sinh(\beta) \Big] \\
Z''(\beta) &= 2^N \Big[N(N-1)(\cosh(\beta))^{N-2} \cdot \sinh^2(\beta) + N(\cosh(\beta))^{N-1} \cdot \cosh(\beta) \Big] \\
&= 2^N \cdot (\cosh(\beta))^{N-2} \cdot N \cdot \Big[(N-1) \cdot \sinh^2(\beta) + \cosh^2(\beta) \Big]
\end{aligned}$$

Giving us

$$Z''(0) = 2^N (1)^{N-2} N \cdot [0+1] = 2^N \cdot N$$

Finally,

$$\langle y_N^2 \rangle = \frac{Z''(0)}{Z(0)} = \frac{2^N \cdot N}{2^N} = N$$

Which absolutely makes sense, as the probability of going up or down in the chain is 50/50.