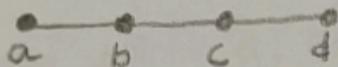


BT2042  
Fundamentals of Biophysical Chemistry

Assignment - 1

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Monte Carlo Simulation:



Monte - Carlo simulation is a model used to predict the probability of different outcomes when the intervention of random variables is present.

Now, in this given simulation a polymer consisting of 4 coarse-grained beads is present. Then, a total of 6 polymers is plotted in a lattice at random positions. Then based on interaction with the beads simulations of polymer is done for  $10^6$  Monte-Carlo moves. Then, similarly 10 such simulations are done and an average position of final plot is drawn.

## Algorithm of Simulation:

- 1] Initial position  $x_i$  is determined.
- 2] Then, randomly a move is done, creating new position  $x_{i+1}$   
$$x_{i+1} = x_i + \Delta x_{\text{rand}}$$
- 3] Energy of both positions is calculated  $[E_i, E_{i+1}]$ .
- 4] If,  $E_{i+1} \leq E_i$ , accept  $x_{i+1}$ .  
Else, choose random variable  $a$ ,  $0 \leq a \leq 1$   
Calculate  $\exp(-(E_{i+1} - E_i)/k_b T)$

given,  $K_b T = 1$ , so,

$$\exp(-(E_{i+1} - E_i)) = \exp(-\Delta E) \quad \text{, where } \Delta E = E_{i+1} - E_i$$

If,  $\exp(-\Delta E) > a$ , accept  $x_{i+1}$

Else, reject  $x_{i+1}$ , keep  $x_i$

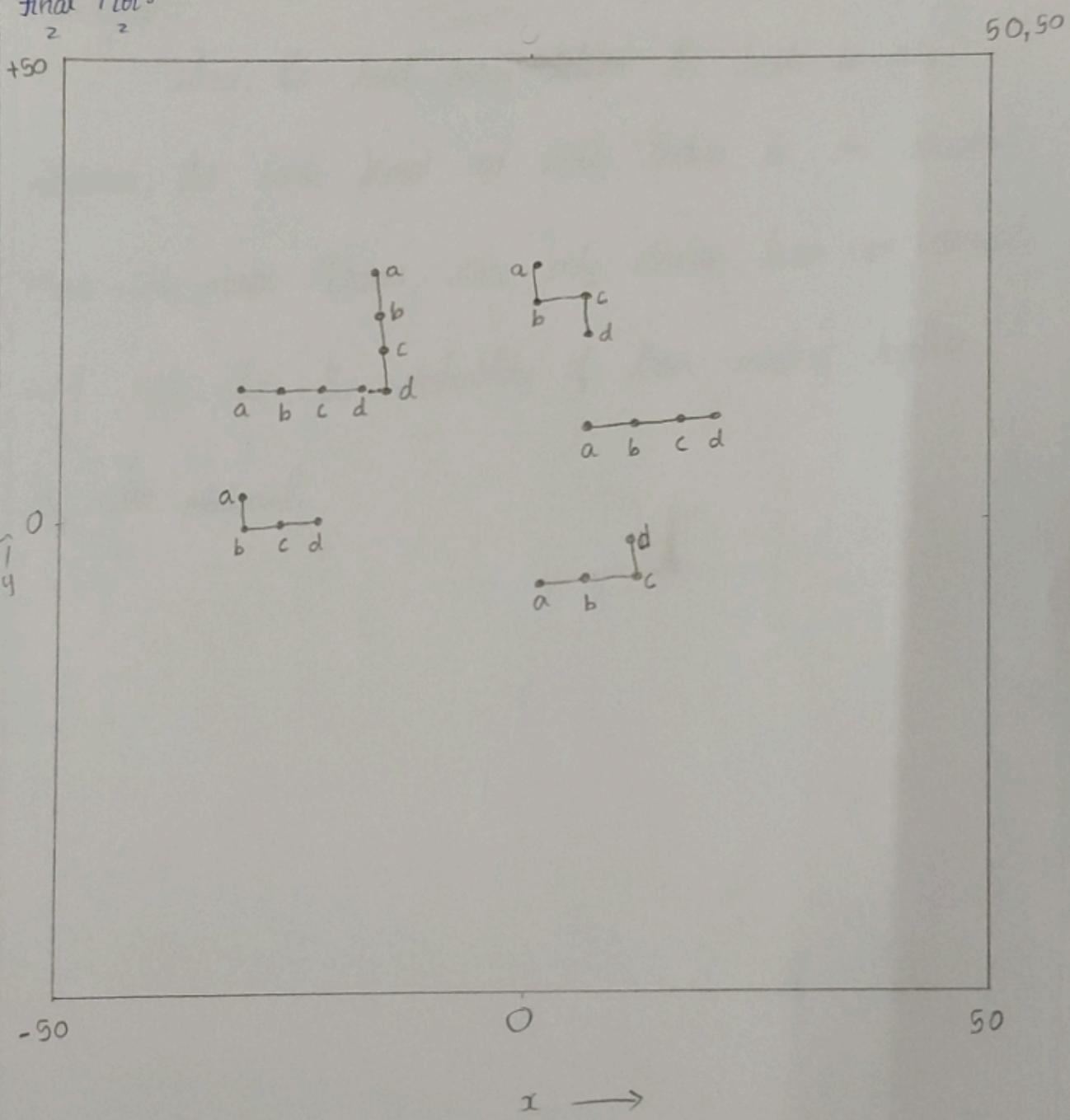
but still move counts as one.

- 5] Similarly, repeat for  $10^6$  trials.

1) Conditions:

- \* One unit lattice length =  $a=5$
- \* Boundaries =  $[-50, 50]$
- \* a bead interact with a bead only. Similarly for b, c, d.
- \* Bond energy = -1

Final Plot:



Calculations:

$$\text{Total bond interactions} = 1$$

$$\text{Bond Energy} = -1$$

$$\text{Total bond energy} = 1 \times -1 = -1$$

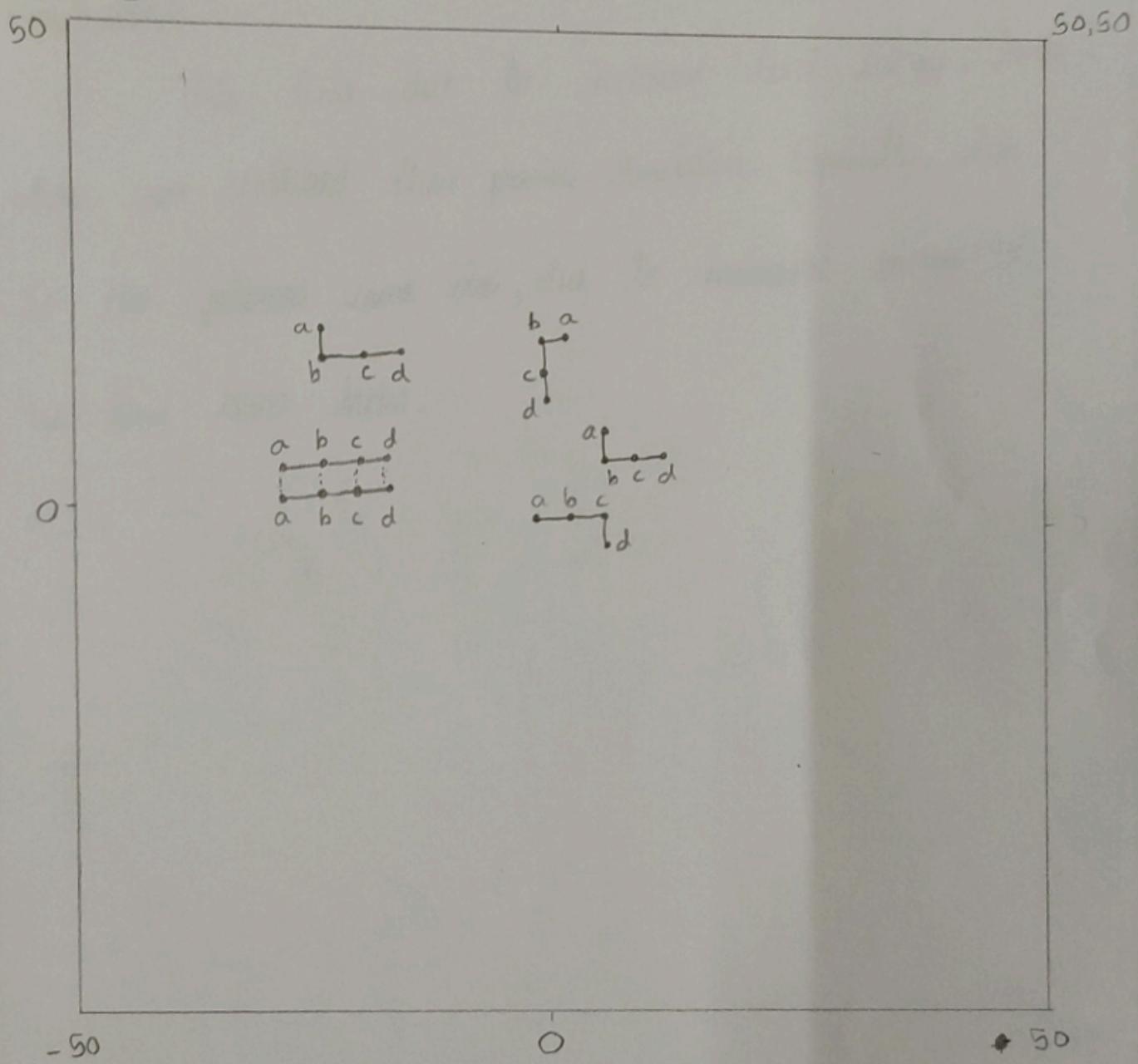
Conclusions:

Since, the bond energy between the beads is very minimal, the bonds formed are easily broken in the successive Monte-Carlo moves. Moreover, since only similar beads can interact with each other, the probability of them meeting together is also minimal.

Conditions:

- \* One unit lattice length =  $\alpha$
- \* Boundaries =  $[-50, 50]$
- \* a bead interact with a bead only. Similarly for b, c, d.
- \* Bond Energ = - $\omega$

Final Plot:



Calculations:

$$\text{Total Bond interactions} = 4$$

$$\text{Bond Energy} = -2$$

$$\text{Total Bond Energy} = 4 \times -2 = -8$$

Conclusion:

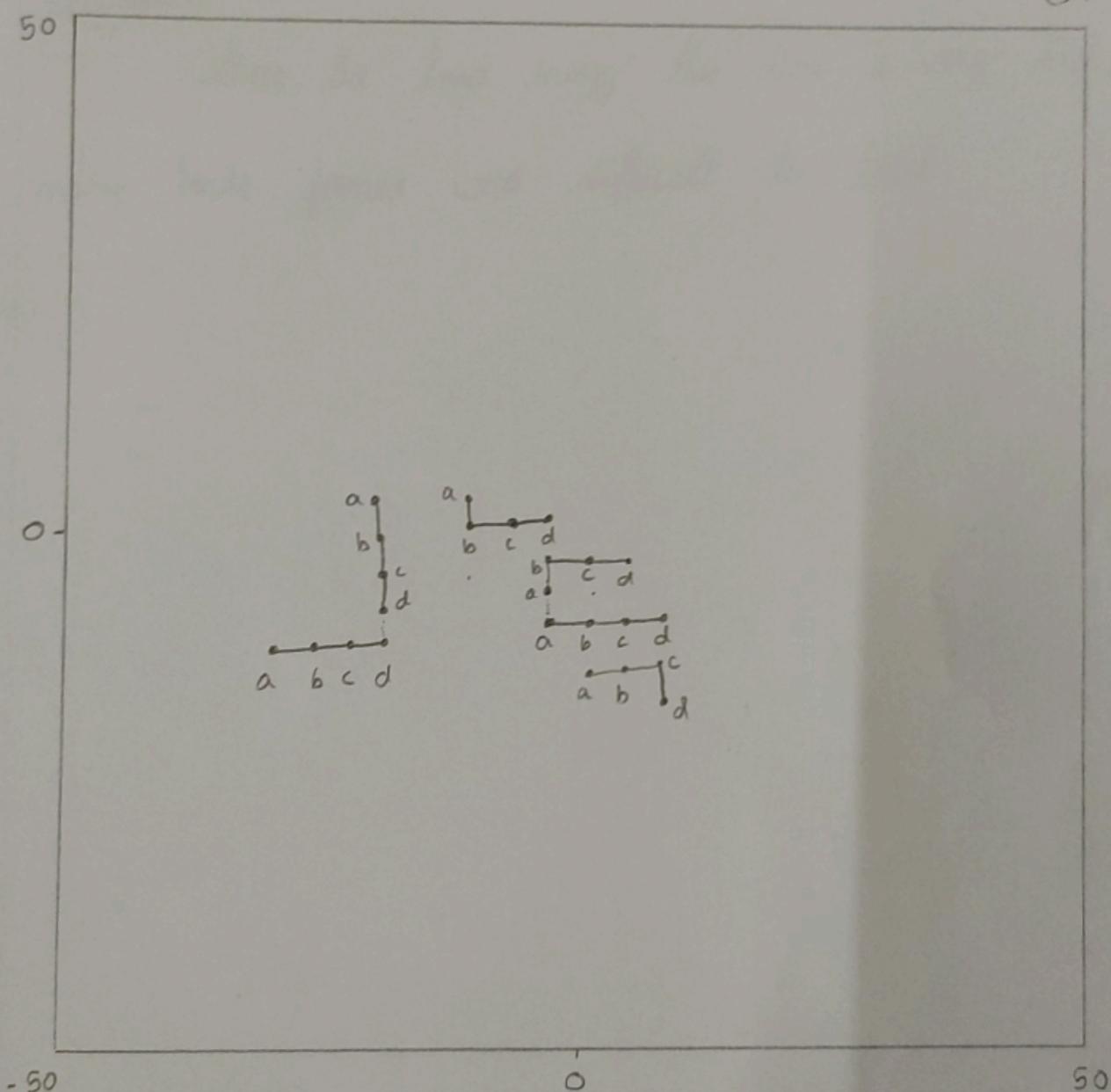
This time due to increased bond energy, bonds were more stabilised than previous simulation. Especially, when the two polymers came close, due to increased energy (-8) the bond never broke.

Conditions:

- \* One unit lattice length = 2.5
- \* Boundaries =  $[-50, 50]$
- \* a bead interact with a bead only. Similarly for b, c, d.
- \* Bond energy = -5

Final Plot:

(50,50)



Calculations:

$$\text{Total Bond Interactions} = 2$$

$$\text{Bond Energy} = -5$$

$$\text{Total Bond Energy} = -10$$

Conclusion:

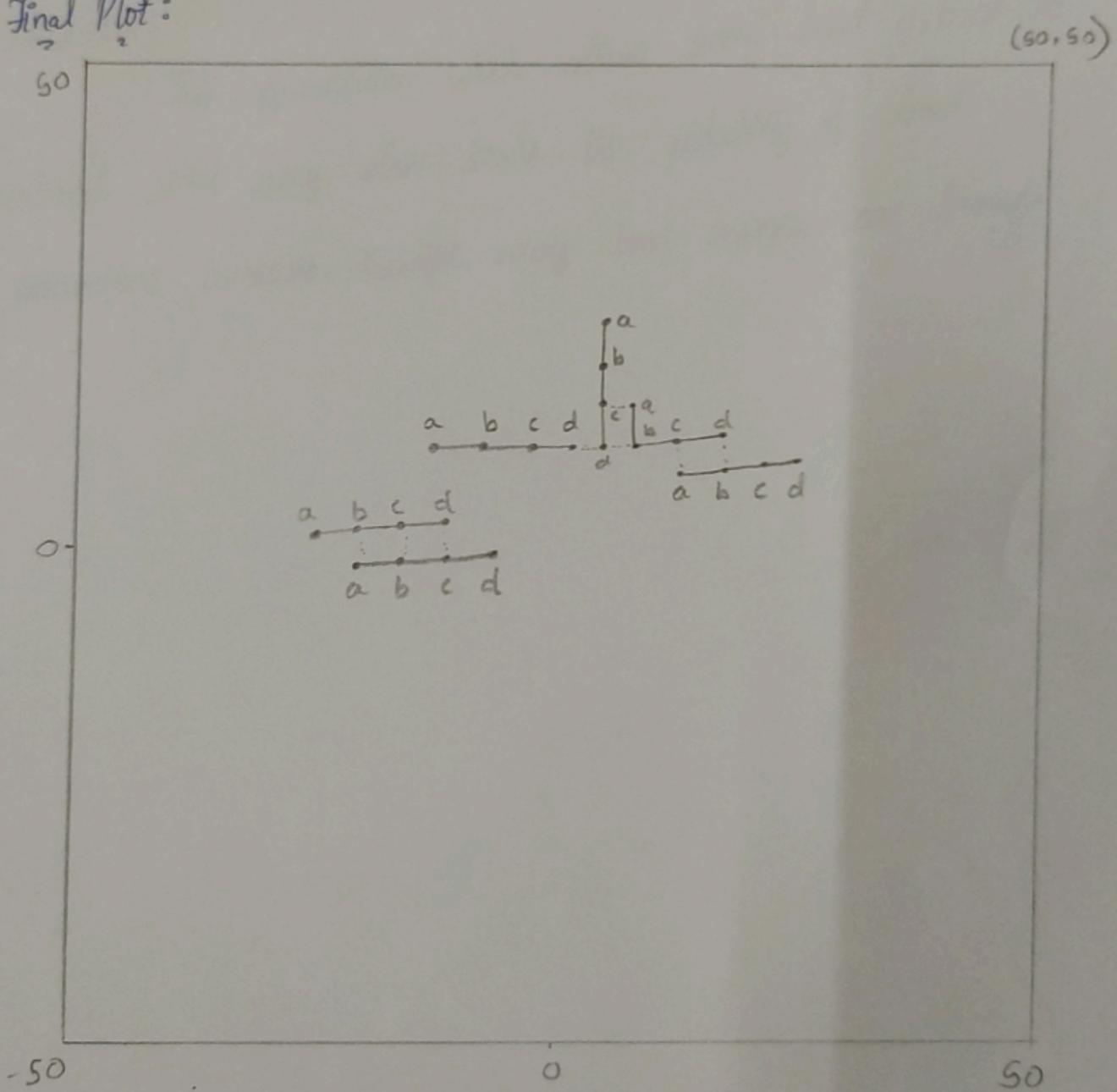
Since, the bond energy this time is very high,  
many bonds formed were difficult to break.

2)

Conditions:

- \* One unit lattice length = 2.5
- + Boundaries =  $[-50, 50]$
- \* a bead can interact with any bead  $[a, b, c, d]$ . similarly  $b, c, d$  beads.
- \* Bond energy = -1

Final Plot:



Calculations:

$$\begin{array}{c} \text{Total Bond interactions} = 8 \\ \hline \quad \quad \quad \quad \end{array}$$

$$\text{Bond Energy} = -1$$

$$\text{Total Bond Energy} = 8 \times -1 = -8$$

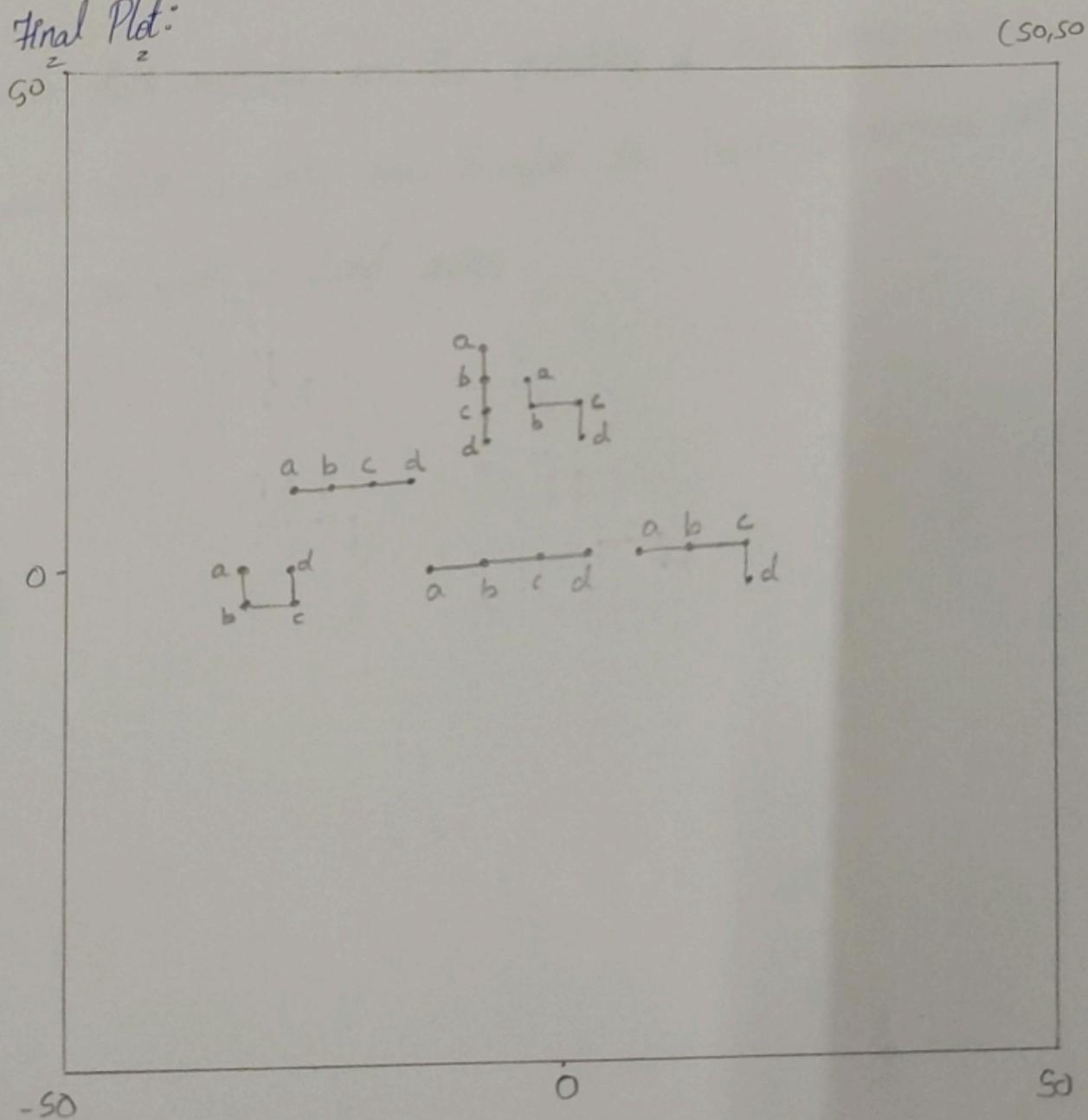
Conclusion:

This simulation which allows every bead a, b, c, d to interact with every other bead, the probability of bond interactions increases. Therefore, many bond energies are formed.

3] Conditions:

- \* One unit lattice length = 2.5
- \* Boundaries =  $[-50, 50]$
- \* Only a and b beads can interact with a and b beads only.
- \* c and d beads no contribution.
- \* Bond energy = -1

Final Plot:



Calculations:

$$\text{Total Bond Interactions} = 0$$

$$\text{Bond Energy} = -1$$

$$\text{Total Bond Energy} = -1 \times 0 = 0$$

Conclusion:

In this simulation, only *a* and *b* beads offer interactions with other molecules, so, the probability of these beads meeting each other is very low. Therefore, the bond interactions are low as well as bond energy.