Homework 4

The Sapling portion will be due before recitation on Tuesday, September 29
The remaining portion will be due in class on Wednesday, September 30

Name: ______________________________ **Andrew ID:** __________________________

Recitation Time: 6:30 7:30 (circle one)

If you worked with other students (which we think is a great idea), please list their names here:
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1) (5 pts) Sapling learning assignment named "Sapling 4". Please see an announcement on Blackboard for instructions on accessing the system.

2) (5 pts) Online Entropy activity

Please go through the materials on the website listed along with this handout in the Blackboard site. Those materials contain questions labeled with a bold **Q.** These questions are reproduced here along with a place for you to fill in your answers.

The reaction coordinate

Q: What is the minimum kick needed to knock the box from the metastable to stable state (kick 1)? (Please give answer to 1 point past the decimal point.)

kick = __________________

Q: What is the minimum kick needed to knock the box from the stable state to the metastable state (kick 2)? (Please give answer to 1 point past the decimal point.)

kick = __________________

Q: Compare your results for the above minimum kicks to the three numbers above the energy landscape. These three numbers give the energy of state 1, the energy at the top of the barrier, and the energy of state 2. What is the relation between these numbers?

The energy landscape

Q: For which aspect ratios is the reaction uphill in energy (energy of state 2 > energy of state 1)? For which aspect ratios is it a downhill reaction?

Aspect ratios in the range: ____________________________

Q: The driving force of a reaction is the magnitude of the energy difference between states 1 and 2. For what aspect ratio is the driving force the greatest? For what aspect ratio is it easiest to knock the box over, i.e. requires the smallest kick1?

Aspect ratios in the range: ______________________________

Population distributions

Q: Try lowering the temperature to 300. Let the simulation run for a while (so that the particles can reach thermal equilibrium). Is the average population on the upper platform larger or smaller than it was at T=700?

circle one: larger smaller

Motion at constant temperature, and exchange of energy with the heat bath

Q: Supposed that the difference in energy between the upper and lower platform in the above diagrams is 5 kJ/mol. When the ball falls from the upper to lower platform, what is the flow of energy (both magnitude and direction) between the ball and the heat bath?

Amount of energy that flows is ______________kJ Direction is *to* *from* *(circle one)* the heat bath

Thermally activated processes

Q: What happens to the number of activated molecules, i.e. balls on the activated platform, as you increase the temperature?

The number of activitated molecules *increases* *decreases* *(circle one)*

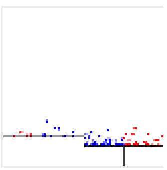
Q: How does this affect the rate of the reaction, i.e. the rate at which balls reach the platform on the right that represents the stable state?

The rate of the reaction *increases* *decreases* *(circle one)*

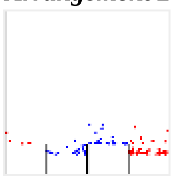
Energy and temperature determine the populations

Set 1

Arrangement 1

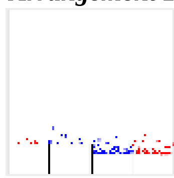


Arrangement 2

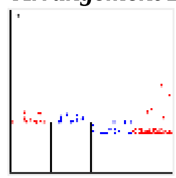


Set 2

Arrangement 1



Arrangement 2



Q: (set 1) At thermal equilibrium, will the populations of the upper and lower energy platforms be the same for both arrangements? (please explain your answer.)

Q: (set 2) At thermal equilibrium, will the ratio of populations between the higher and lower platforms (P_2/P_1) be the same for both arrangements? (please explain your answer.)

Entropy and free energy

Q: Is there a temperature at which the higher-energy state (the total population of the four higher-energy platforms, or the total number of boxes standing up) has a larger population than the lower-energy state (the total population of the two lower-energy platforms, or total number of boxes laying down)?

Mathematical derivation of free energy

Q: Consider a box with dimensions as shown below. Suppose the difference in energy between the box standing up and laying down is ΔE. What is the ratio between the total pollution of boxes standing up versus laying down, $P_{standing\ up}/P_{laying\ down}$, at a given temperature T.