Experiment 7

1 Aim

To plot the distribution number against the energy of state and check if we get an exponentially falling curve

2 Apparatus

Laptop, MS Excel, Plotting Software

3 Theory

3.1 Boltzmann Distribution

In statistical mechanics and mathematics, a Boltzmann distribution is a probability distribution or probability measure that gives the probability that a system will be in a certain state as a function of that state's energy and the temperature of the system.

3.2 Micro State

A micro-state is a description of a system in terms of a dynamical configuration of individual molecules or particles, such that the larger macro system obeys certain constraints. For instance, a system could be described in terms of the occupations of molecular energy states of its particles, or of the momenta and position coordinates of its particles. Suppose we have a system of free particles in which each particle has a unit mass and the system has a total energy of 100 units. Then all possible states are allowed such that the sum of the squares of the momenta of individual particles taken together is 200 units. The particles may be anywhere in space. The configuration of momenta and position of the particles at any particular time is a micro-state

of the system. The constraint here is the constant total energy. The different combinations in which each total can occur are microstates.

3.3 Macro State

A macrostate is defined by the macroscopic properties of the system, such as temperature, pressure, volume, etc. For each macrostate, there are many microstates which result in the same macrostate. The possible totals of the rolls are macrostates.

3.4 Multiplicity

In statistical mechanics, multiplicity refers to the number of microstates corresponding to a particular macrostate of a thermodynamic system. Commonly denoted as Ω , it is related to the configuration entropy of an isolated system via Boltzmann's entropy formula. The number of ways each total can occur is the multiplicity, **W**.

$$S = klog\Omega$$

where S is the entropy and k = 1.38×10^{-23} J / K is Boltzmann's constant.

3.5 Frequency Table

A frequency table is a method of organizing raw data in a compact form by displaying a series of scores in ascending or descending order, together with their frequencies—the number of times each score occurs in the respective data set.

3.6 Degenerate Energy States

States are of equal energy with equal probability of occupation

3.7 Non-Degenerate Energy States

States with the higher probability of occurence being the ground state and one with lower probability is the excited state

3.8 Micro Chart

MicroCharts are miniature versions of actual charts. Win-loss charts are microcharts in which the value of each column is either 1 or -1, often denoting a win or loss. In our case State 1 corresponds to Win(+1) and State 2 corresponds to Loss(-1).

4 Procedure

1. Consider the roll of a pair of dice. For each possible sum of the values on the dice in one roll note the number of ways this sum can occur. Plot the Number of possible ways vs the total sum using any plotting software like python, matlab, excel etc.
2. Take a pair of dice. Roll the pair 36 times and note the values each time. Plot the number of times a total is occuring vs the value of the occured total.
3. Repeat the same procedure using the dice rolls of all members of the team
4. Take one die and roll it 100 times. Note the readings each time. Using the definition of experiment A and B given. Note down the state values of each roll for both experiments.
5. Maintain a count value for each experiment with initial value = 0. For a given roll if the state value is 1 add 1 to the count value. If it is 2 then subtract 1 to the count value.
6. Plot the count value at each roll against the index of the roll. This is called the microchart. Obtain the microchart corresponding to experiment A and B.
7. Collect readings of all the group members.
8. Generate frequency table using the count for Experiment A and B. Now calculate the frequency of occurrence of a given number of molecules in state I.
9. After 25, 50 and 100 moves, calculate p_i, p(I) and draw the frequency bar diagram.

5 Group Members and Contributions

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6 Individual Plots and Setups:

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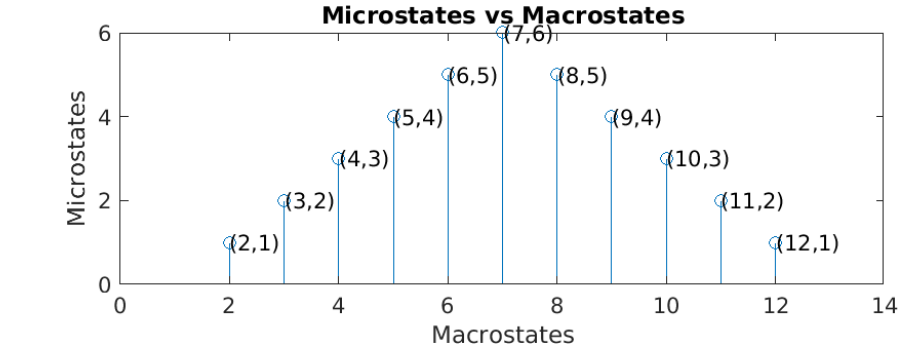
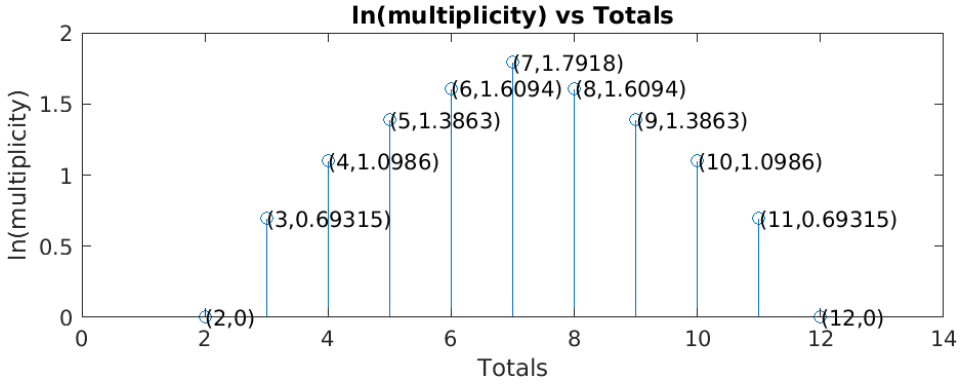
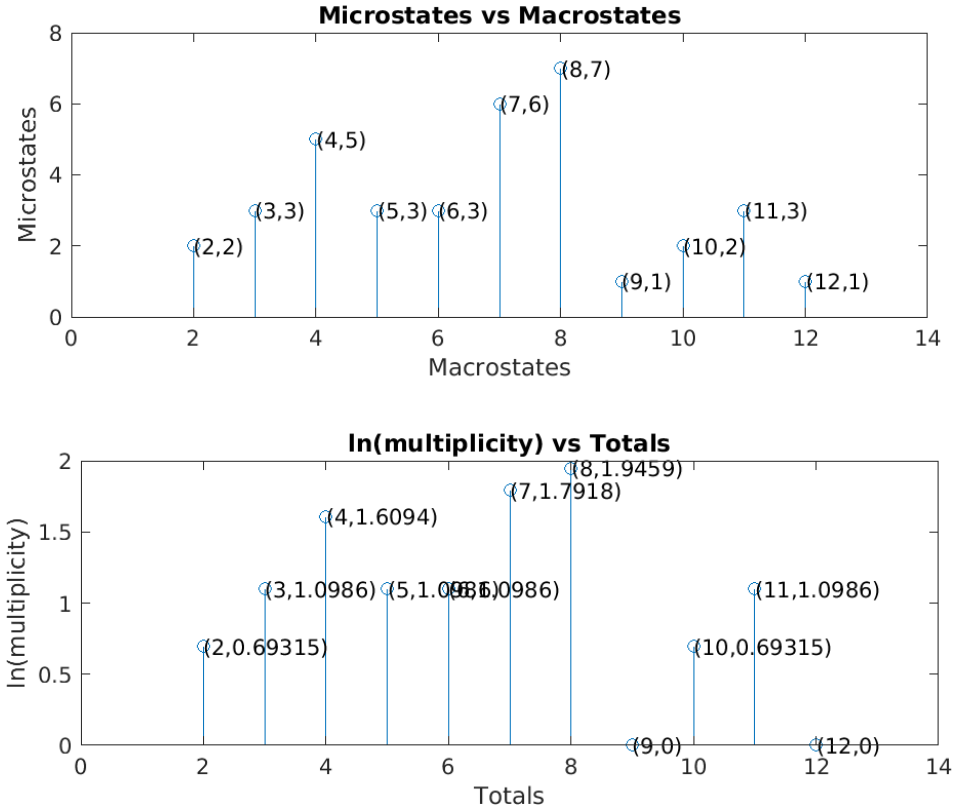
1) a)
Histograms:





b)
Histograms:



Results

	A	B	C	D	E	F
1	Die Roll	Multiplicity W (Expected)	Multiplicity W (Actual)	ln W (Expected)	ln W (Actual)	Probability of Expected Microstates (= W/Omega)
2	2	1	2	0	0.6931	0.055555556
3	3	2	3	0.693147181	1.0986	0.083333333
4	4	3	5	1.098612289	1.6094	0.138888889
5	5	4	3	1.386294361	1.0986	0.083333333
6	6	5	3	1.609437912	1.0986	0.083333333
7	7	6	6	1.791759469	1.7918	0.166666667
8	8	5	7	1.609437912	1.9459	0.194444444
9	9	4	1	1.386294361	0	0.027777778
10	10	3	2	1.098612289	0.6931	0.055555556
11	11	2	3	0.693147181	1.0986	0.083333333
12	12	1	1	0	0	0.027777778

Note: Part 1) c) is done all collaboratively, therefore it is at the end.

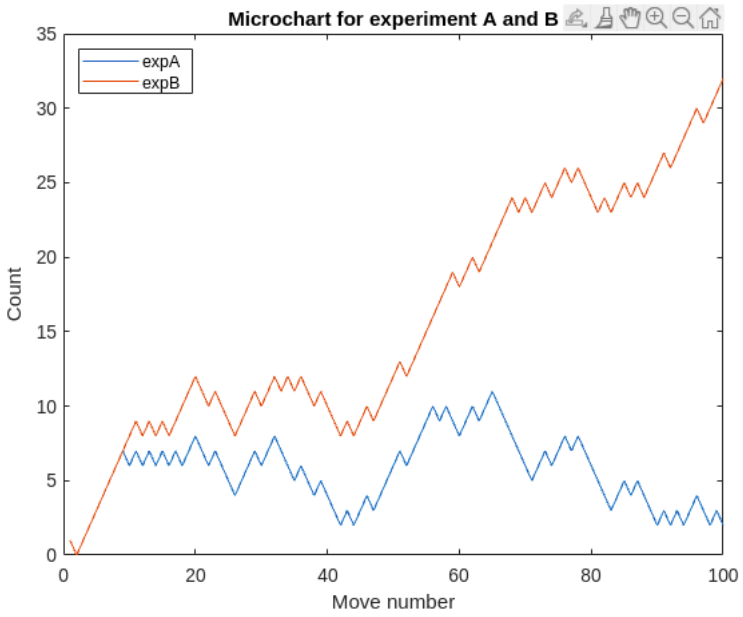
2) a)
Data and Results:

1	Move number	Reading on die	Exp A molecular state	Move number	Exp B molecular state
2	1	3	1	1	1
3	2	5	2	2	2
4	3	1	1	3	1
5	4	2	1	4	1
6	5	1	1	5	1
7	6	1	1	6	1
8	7	2	1	7	1
9	8	3	1	8	1
10	9	3	1	9	1
11	10	4	2	10	1
12	11	3	1	11	1
13	12	5	2	12	2
14	13	2	1	13	1
15	14	6	2	14	2
16	15	1	1	15	1
17	16	5	2	16	2
18	17	3	1	17	1
19	18	4	2	18	1
20	19	1	1	19	1
21	20	2	1	20	1
22	21	5	2	21	2
23	22	6	2	22	2
24	23	2	1	23	1
25	24	5	2	24	2
26	25	6	2	25	2
27	26	6	2	26	2
28	27	1	1	27	1
29	28	1	1	28	1
30	29	2	1	29	1
31	30	6	2	30	2
32	31	1	1	31	1
33	32	3	1	32	1

34	33	6	2	33	2
35	34	4	2	34	1
36	35	5	2	35	2
37	36	2	1	36	1
38	37	5	2	37	2
39	38	6	2	38	2
40	39	1	1	39	1
41	40	5	2	40	2
42	41	6	2	41	2
43	42	5	2	42	2
44	43	2	1	43	1
45	44	5	2	44	2
46	45	1	1	45	1
47	46	3	1	46	1
48	47	6	2	47	2
49	48	2	1	48	1
50	49	2	1	49	1
51	50	1	1	50	1
52	51	1	1	51	1
53	52	5	2	52	2
54	53	2	1	53	1
55	54	2	1	54	1
56	55	3	1	55	1
57	56	1	1	56	1
58	57	4	2	57	1
59	58	1	1	58	1
60	59	4	2	59	1
61	60	5	2	60	2
62	61	1	1	61	1
63	62	3	1	62	1
64	63	5	2	63	2
65	64	3	1	64	1
66	65	1	1	65	1

67	66	4	2	66	1
68	67	4	2	67	1
69	68	4	2	68	1
70	69	6	2	69	2
71	70	4	2	70	1
72	71	6	2	71	2
73	72	1	1	72	1
74	73	1	1	73	1
75	74	5	2	74	2
76	75	3	1	75	1
77	76	1	1	76	1
78	77	6	2	77	2
79	78	3	1	78	1
80	79	5	2	79	2
81	80	5	2	80	2
82	81	6	2	81	2
83	82	4	2	82	1
84	83	5	2	83	2
85	84	3	1	84	1
86	85	2	1	85	1
87	86	6	2	86	2
88	87	3	1	87	1
89	88	6	2	88	2
90	89	4	2	89	1
91	90	4	2	90	1
92	91	1	1	91	1
93	92	6	2	92	2
94	93	3	1	93	1
95	94	4	2	94	1
96	95	3	1	95	1
97	96	2	1	96	1
98	97	6	2	97	2
99	98	4	2	98	1
100	99	1	1	99	1
101	100	4	2	100	1

b)
Microchart:



Results in excel file and code in python are in a folder.

Note: Part 2) c) is done all collaboratively, therefore it is at the end.