

1. Microstates of a Few Oscillators

Open the Excel/Calc shell file provided to you. Make sure you are looking at the sheet tab “#1”. In this problem you will model a system consisting of two atoms (three oscillators each), among which 4 quanta of energy are to be distributed.

- a) Use combinatorics to calculate the number of ways q_1 quanta can be distributed in the first block (column B). In Excel/Calc, the function for factorial is “FACT()” (capital letters are always optional in Excel/Calc). Begin writing a formula with the character “=”. You can refer to cells on your spreadsheet using the notation “A1”, “C3”, “F6”, etc. To do this part you will need to refer to the number of quanta in block 1 and the number of oscillators in block 1. Once you write your formula in cell B8, you can copy it downwards by dragging the small black square in the lower righthand corner of the selected cell. Tip: Excel/Calc will automatically adjust the cell references as your formula is copied to new cells. However, you want the cell reference to the number of oscillators (B1) to stay the same. To do this, write that cell reference as “\$B\$1”. Then copy your formula downwards.
- b) Do the same for the microstates of block 2 in column C. The number of quanta in block 2 is $q_2 = N - q_1$. The total number of quanta N is given in cell B3. Check: Column B read downwards should be the same as column C read upwards. Why?
- c) Write the total number of microstates for blocks 1 and 2 in column D. Hint: Should you add or multiply?
- d) Insert a chart and choose type “XY Scatter Plot”. Use the q_1 values in column A as the x values and the total number of microstates in column D as the y values. What is the most probable number of quanta for block 1 to have? In this case, how many quanta will block 2 have?

2. Statistical Temperature and Specific Heat Capacity

Switch to sheet tab “#2”. Now block 1 has 75 oscillators and block 2 has 50, among which 50 quanta of energy are to be distributed.

- a-d) Repeat steps a-d) from #1. What is the most probable number of quanta for block 1 to have? In this case, how many quanta will block 2 have? For this most probable case, why does $q_1 \neq q_2$ this time?
- e) Entropy is given by $S = k_B \ln \Omega$. Notice that Boltzmann’s constant k_B is defined near the top of the spreadsheet. Fill out the columns for the entropies of the two blocks, S_1 and S_2 . Use the function “LN()” for natural log.
- f) Fill out the column for total entropy. You can use column D or columns E and F to do this.
- g) Create a new XY scatter plot. Use 3 data series to graph S_1 , S_2 , and total S against q_1 on the same plot. At what q_1 is the total entropy a maximum? How does this compare to the q_1 you found in part d) for the maximum number of microstates?
- h) Why does S_2 decrease as q_1 increases? Hint: What happens to q_2 as q_1 increases?
- i) Fill out the columns for temperatures T_1 and T_2 using the definition $T \approx \frac{\Delta E}{\Delta S}$. There are multiple ways to calculate this slope, but for definiteness, use adjacent cells to calculate ΔS . That is, if you are solving for the temperature T_1 at $q_1 = n$, then use $\Delta S_1 = S_1^{(n)} - S_1^{(n-1)}$, the n th value minus the $(n-1)$ th value. Between adjacent cells, the factor ΔE is always one quantum, the energy for which is given by

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$$E_{\text{quantum}} = \hbar \sqrt{\frac{4k_{s,\text{atom}}}{m_{\text{atom}}}}$$

– in the Einstein model. This value is calculated for you near the top of the spreadsheet. Remember that for T_2 , $\Delta E = -E_{\text{quantum}}$.

- j) Plot T_1 and T_2 versus q_1 on the same chart. At which q_1 do the functions cross? How does this compare with the q_1 at which the total entropy S is maximum? Explain.
- k) Using the definition

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$$C_{\text{per atom}} = \frac{\Delta E / N_{\text{atoms}}}{\Delta T}$$

– calculate C in column J. Use the temperatures T_2 for this calculation, and again use adjacent cells to find ΔT . Remember that the number of atoms $N_{\text{atoms}} = N_{\text{oscillators}}/3$ in the Einstein model.

- l) Plot the $C_{\text{per atom}}$ column and the column labeled “ $3k_B$ ” versus T_2 on the same chart. How does the C you calculated compare to the non-quantum value of $3k_B$?