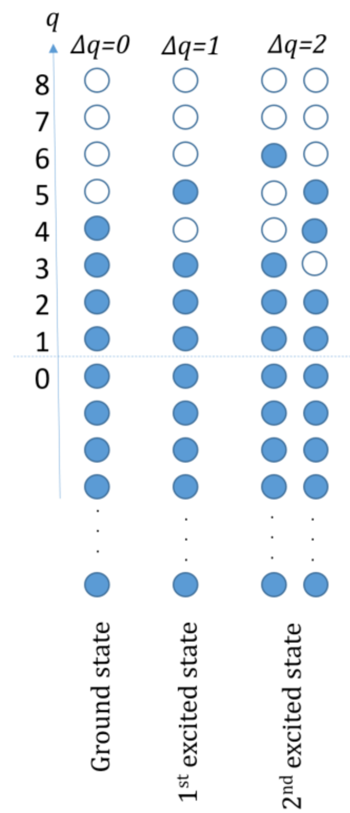
PHYS 410 **Marie Lopez del Puerto**

Project #8: The Fermi-Dirac Distribution[1]

Introduction



Consider an isolated system of N_{total} identical fermions, inside a container where the allowed energy levels are nondegenerate and evenly spaced. For instance, the fermions could be trapped in a one-dimensional harmonic oscillator potential. For simplicity, neglect the fact that fermions can have multiple spin orientations (or assume that they are all forced to have the same spin orientation). Then the energy levels are given by $E_i = q\varepsilon$ and each level is either occupied or unoccupied.

In the ground state, a system of N_{total} fermions would have ground-state energy E_0. Let's look at only the 4 fermions in the highest energy levels. If we set the 0 of energy below where these 4 fermions are as shown in the figure, then we could describe the state of these fermions by the vector (1, 2, 3, 4) with total energy $(1+2+3+4)\varepsilon = 10\varepsilon$. Since this is the ground state, $\Delta E = E - E_0 = 0$, or $\Delta q = 0$.

The first excited state would then be represented by the vector (1, 2, 3, 5) with a total energy of 11ε. Then, $\Delta E = E - E_0 = \varepsilon$, or $\Delta q = 1$.

The second excited state is either (1, 2, 3, 6) or (1, 2, 4, 5), both with total energy 12ε; $\Delta q = 2$. According to the fundamental assumption, all allowed system states with a given energy are equally probable. If the system is in the second excited state, then the probability of levels 1 and 2 being occupied is 1; the probability of levels 3, 4, 5, and 6 being occupied is ½.

For a given energy state (or Δq), we want to find and plot the probability of an energy level being occupied as a function of ε/kT. In the thermodynamic limit, where q is large, the probability of a level being occupied should be given by the Fermi-Dirac distribution.

Algorithm

For a given number of fermions above the zero of energy, N, and maximum number of levels above the ground state, q_{max}, find all possible combinations of q in N (i.e. how many ways can you distribute N electrons in q_{max} levels? These are the microstates).

Calculate the total energy of each microstate.

Find all microstates that have a given energy E.

[1] Adapted from Schroeder 7.16.

The probability that level x is occupied is then given by how many microstates with energy E have a fermion in level x, over the total number of microstates with energy E.

Questions

1. Start with $q_{max} = 8$ and $N = 4$. Make a histogram of energies (i.e. how many levels have each value of total energy). Does the plot have the shape you would expect? If not, explain.
2. Plot the probability of a level being occupied as a function of q for the state with $\Delta q = 3$. Remember that there are many occupied states below q = 1 and empty states above $q = q_{max}$. Check that your results match Fig. 7.8.
3. Repeat Q1 with $q_{max} = 20$ and $N = 10$. Make a histogram of energies (i.e. how many levels have each value of total energy).
4. Plot the probability of a level being occupied as a function of q for the state with $\Delta q = 10$.
5. Estimate the values of μ and T that you would have to plug into the Fermi-Dirac distribution to best fit the graph from Q5. Plot this fit line on top of your plot for Q5.
6. Calculate the entropy of this system for each value of energy up to the 10^{th} excited state. Make a plot of entropy vs. energy.
7. Find the slope of the entropy vs. energy plot near the energy of the 10^{th} excited state to obtain another estimate of the temperature of the system at this point. Check that it is in rough agreement with your answer to Q6.

Write-up

Your write-up should have project number and title, your name and your partner's name if working with a partner, answers to questions: plots or text included in your MATLAB / Jupyter notebook / Mathematica script with appropriate formatting or the appropriate lines of code and printed output. Your write-up should be should be detailed, neat, organized, and easy to follow. Upload a pdf or html file to Canvas under Project #8, due before class time on Friday April 27.