CHEM279
Laura Jones
10.7.2024

HW2

In this assignment, we examined the approximation of electron orbitals via gaussian overlap. In part 1, I was able to roughly attain the values in the output files by using riemann sums to approximate the overlap function. I believe that the discrepancy lies in the fact that I rounded my values, so they were not as accurate as the provided .txt output files. Nonetheless, I feel I learned a great deal about what the area under the curve means in the context of overlapping 1D orbitals.

In part 2, we were to find the overlap for 2 3D orbitals. I feel that my function is incomplete, and I did not understand how to generate the multiple orbitals mentioned in the output txt file. Regardless, I did get values that seem to relate to my results from part 1.