1 The Diatomic Molecule

1. Together in class, we will use Python to solve Schrodinger's equation for the diatomic molecule.

   1. Investigate how the difference in the eigenvalues changes as the atoms move farther apart. You should generate a plot to show the relationship.

   2. Use hypothesis/testing to investigate what affects the magnitude of the diagonal and off-diagonal terms in the Hamiltonian matrix.

2. In class we used an atomic-orbital basis set to solve Schrodinger's equation for a diatomic moleculte. Modify your code to use an infinite-square-well basis set instead (hereafter will be called a "plane wave" basis set).

   1. Investigate the quality of your results as you increase the size of your basis set. Make a plot of the wavefunctions for several choices of N (number of basis functions)

   2. With the results obtained using $N = 100$ considered to be exact, investigate the error in the eigenvalues as the size of the basis set is increased. You should generate a plot with N(number of basis functions) on the horizontal axis and relative error in the eigenvalue on the vertical axis.