1 The Heteronuclear Diatomic Molecule

1. In Sutton on pages 32-33, Schrodinger's equation is solved for the heteronuclear diatomic molecule. However, some of the details were left out. Complete the derivation, filling in all of the necessary steps.

2. By now you should have a working python code for solving the homonuclear diatomic problem. By modifying the depth of one of the potential wells, model a heteronuclear diatomic molecule and use your code to recreate figure 2.4 in the book.

3. So far in Sutton, the size of our basis has been two. In other words, we have expressed the wavefunction as:

$$|\psi\rangle = c_1|1\rangle + c_2|2\rangle \tag{1}$$

where $|1\rangle$ and $|2\rangle$ represent 1s states centered on atom 1 and atom 2 respectively. This was done to make the math easier. A better solution can be obtained by expanding the basis. Let's expand that basis to include $1s$, $2s$, and $2p$ orbitals **for each atom**. That's a total of 6 terms in the expansion. Work through the same math from pages 32-33 in Sutton, but using this basis. Don't solve the eigenvalue problem, just work through the math until you get to the eigenvalue problem.