He Binding Energy Project

Your problem is to calculate the binding energies of the $1s2p^3P_1$ and $1s2p^1P_1$ states of He, using 2$^{nd}$ order perturbation theory. You will write a brief paper, and submit accompanying Mathematica code, calculating the energies of these states. You are free to use the HePertThy2.m code as a base for your work, making sure you explain your changes. Energies should be as good as you can get, but at least 1% or better.

1) Look up the experimental values of these energies, using the NIST tables at http://physics.nist.gov/PhysRefData/ASD/levels_form.html.

2) Explain/derive how you will handle exchange symmetry for your calculation. Explain why we didn’t have to worry about exchange symmetry for the $1s1s$ state.

3) Modify the Mathematica code to calculate the matrix elements you will need:
   \[
   \langle n_1 s n_2 p | \frac{1}{r_{12}} | n_3 s n_4 p \rangle, \langle n_1 s n_2 p | \frac{1}{r_{12}} | n_3 p n_4 d \rangle, \\
   \langle n_1 s n_2 p | \frac{1}{r_{12}} | n_3 p n_4 s \rangle, \langle n_1 s n_2 p | \frac{1}{r_{12}} | n_3 d n_4 p \rangle
   \]
   You will need to handle the angular integrations using the method we went over in class. Include your code for doing that. Get help from Thad if needed. Explain why you don’t have to include $p + p$ states.

4) The first step is to identify a proper unperturbed wavefunction. Since the $1s2p$ state is very close in energy to the $1s3p$ and $1s4p$ states, calculate the Hamiltonian matrix in the basis of these three states. Note that some of the off-diagonal elements are comparable in size to the difference between the diagonal elements. This signals that your proper unperturbed wavefunction will not be simply $1s2p$. Diagonalize the matrix and you will see that the lowest energy level, which we will call “$1s2p$”, is in fact a significant mixture of the $1s2p$ and another state.

5) The superposition state you have just found is the proper unperturbed wavefunction $|0\rangle$ to use. Modify your theory to take into account this superposition state.

6) Now you can use 2$^{nd}$ order perturbation theory to calculate the energies of the $1s2p^3P_1$ and $1s2p^1P_1$ states. Compare to experiment.

You are free to work in groups to do the calculations, but your paper should be your own. Feel free to cite the handout as needed. Your paper can be handwritten if you like, without penalty as long as it is legible. A well-documented Mathematica file would be fine as well. I encourage you to come to office hours for help. Don’t wait to get started.

Due: March 22. Hand in your work by email attachment. If you want to work on it over spring break, you can do that but my availability will be limited. Absolute deadline is 8:30 am April 1.