Hartree-Fock Calculations for Neutron Drops and Oxygen 16

Sean Sweany

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1 Introduction

Here we will be finding the energies of neutron drops using Hartree-Fock calculations. This is an important exercise in that it gives you an understanding of how Hartree-Fock works as well as a code that is easy to change to apply to different situations. Here what we will be doing is after the calculations are completed with the neutron drops I will add in protons so as to find the Hartree-Fock energies for nuclei. Calculations were preformed for a system with 8 neutrons and for oxygen 16 which has both 8 protons and neutrons. The calculations were done in a harmonic oscillator basis with $\omega\hbar = 10$. The nuclear shells being filled were chosen to be 0s, 0p, 1s0d, and 1p0f.

2 Hartree-Fock and Numerical Methods Used

The Hartree-Fock energies for the different states can be written as follows.

$$h_{ab} = \epsilon_{ab}\delta_{ab} + \sum_{j=1}^{N}\sum_{\gamma,\delta}^{States} C^*_{j\gamma}C_{j\delta}V_{AS}$$

Where ϵ is just the single particle energies for the harmonic oscillator which are just on the diagonal of the Hartree-Fock energy matrix. The big nasty thing inside of the bras and kets is the two particle data, this is where coupling between states comes from, however as will later be shown the only states that can even couple are those with all quantum numbers the same

except for n. Now, the other part of this equation is the C's, these two matrices for each element go through all of the γ and δ states and for each matrix element sum up to the total particle number. The resulting matrix is what is know as the density matrix.

To start the code we need three main ingredients, the single particle harmonic oscillator energies, the two body data and the density matrix. Luckily for this project we were given the single particle data and the two body interaction data. So the only thing we need to do was to determine what the density matrix was. So what we do is make a guess as to what the C matrix is. For the first iteration is simply the identity matrix. So with these three thing we go and put every thing in to the equation above and sum over the γ and δ states to get the Hartree-Fock energy matrix. Once this step is completed we put the Hartree-Fock into an eigenvalue/eigenvector solver. Next the matrix of eigenvectors is used as our matrix C. Then we start iterating. The iterations stop once the eigenvalues change very little. However, this happens rather quickly for this code so 30 iterations is more than enough to get good looking energies.

3 Project Parts a, b, c and d

Part a: The first part of the project is to simply find the energies for the system without the two body potential added in. This is a nice test since it just give the normal harmonic oscillator energies.

Table 1: Harmonic Oscillator Energies

State	n	l	Energy (MeV)
0s	0	0	15
0p	0	1	25
0d	0	2	35
1s	1	0	35
0f	0	3	45
1p	1	1	45

The values obtained are all correct and provide a good check that the code is working well.

Part b: First off, to show that the Hartree-Fock energy matrix is diagonal for quantum numbers. First looking at the matrix for part c of this project it is apparent that this is true. There are elements on the diagonal where all n, l, and j are equal. There are also extra diagonals where we have the same l and j values but different values of n. This only happens for the states 0s, 1s and 0p, 1p. It is also worth noting that all of the m values do not affect the energy at all. (I will include the energy matrix for the oxygen 16 data to show this). For the next part we need to show that

$$\epsilon_{nlj} C^{lj}_{nn_3} = \sum_{n_3} h^{lj}_{n_1 n_3} C^{lj}_{nn_3}$$

for Hartree-Fock can be done with a simple argument. First off we know that the Hartree-Fock is a nice matrix so all $h^{lj}_{n_1 n_3}$ are just scalars. We also know that the C matrix is just a matrix of the orthogonal eigenvectors for each iteration. So, what we actually have for the energy ϵ_{nlj} is the following:

$$\epsilon_{nlj} = C^* H C$$

This being where we get rid of the sum and just make everything in terms of vectors and matrices. This then is just a large number of similarity transformations which in turn will produce the eigenvalues for the Hartree-Fock matrix. Looking at it to me it appears to be very similar to Jacobi's method of finding eigenvalues.

Part c and d: Here is the data for the Hartree-Fock calculations with just 8 neutrons. When presenting the data I will only include the corresponding n, l and j terms since m doesn't matter.

Comparing the neutron single particle state data to that for just the harmonic oscillator data we can clearly see that all of the energies are lower for the Hartree-Fock calculations than for the SHO. With the cases for the states below the Fermi level actually being shifted quite a bit. This seems to represent the binding nuclear force between the neutrons which would lower the energy.

The next case is for a system with 8 protons and 8 neutrons. The data is shown below.

For this case we see that we actually have that states which are below the Fermi level are bound. Now, an interesting thing to note is that the energy is always less for neutrons than the protons in the corresponding state, indicating that the neutrons are more tightly bound. I believe this can

Table 2: Hartree-Fock Energies for a system of 8 neutrons

n	l	j	Energy (MeV)
0	0	1/2	0.31
0	1	3/2	14.71
0	1	1/2	16.83
0	2	5/2	28.85
0	2	3/2	31.15
1	0	1/2	29.25
0	3	7/2	41.04
0	3	5/2	43.05
1	1	3/2	40.47
1	1	1/2	41.06

Table 3: Hartree-Fock Energies for Oxygen 16

n	l	j	Proton Energy (MeV)	Neutron Energy (MeV)
0	0	1/2	-40.46	-40.64
0	1	3/2	-11.59	-11.72
0	1	1/2	-6.71	-6.84
0	2	5/2	18.81	18.76
0	2	3/2	22.96	22.92
1	0	1/2	21.07	21.02
0	3	7/2	36.06	36.03
0	3	5/2	39.31	39.28
1	1	3/2	35.16	35.13
1	1	1/2	35.88	35.85

be explained by the coulomb force being repulsive and pushing protons away from each other. However the effect seems to be pretty small and decreases as you go to higher single particle states. Now lets assume that we can accurately obtain the separation energy for ^{17}O and ^{16}O between the $0p_{1/2}$ and $0d_{5/2}$. Looking on NNDC for the neutron separation energy the value is 4.1 MeV, and for protons 13.7 MeV. Looking at the Hartree-Fock data

though for neutrons the separation energy is 25.5 MeV and for the protons it is 25.6 MeV. So the Hartree-Fock calculation doesn't do a very good job at estimating separation energies.