PHY 981 - PROJECT 1B

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The Python code I've written gives you the options to select only neutrons, only protons, or both, as well as the choice to include the two-body part of the Hamiltonian. With the two-body interaction neglected, the remaining Hamiltonian is diagonal and the Hartree-Fock algorithm converges after a single iteration. The output for this calculation is shown below, as an example.

```
 Do you wish to consider protons, neutrons, or both?
n
Neutrons selected
Do you wish to include the two-body interaction?  Y/N
n
Energy eigenvalues initialized
After iteration 1.0 , E=
[ 15.  15.  25.  25.  25.  25.  25.  25.  35.  35.  35.  35.  35.  35.  35.
35.  35.  35.  35.  35.  45.  45.  45.  45.  45.  45.  45.  45.  45.  45.
45.  45.  45.  45.  45.  45.  45.  45.  45.  45.]
diff= 0.0
The calculation converged after 1.0 iterations.
The converged energy eigenvalues are
 [ 15.  15.  25.  25.  25.  25.  25.  25.  35.  35.  35.  35.  35.  35.  35.
35.  35.  35.  35.  35.  45.  45.  45.  45.  45.  45.  45.  45.  45.  45.
45.  45.  45.  45.  45.  45.  45.  45.  45.  45.]
```

The harmonic oscillator part of the interaction is obviously diagonal, because that's how we chose our starting basis. The two body-part is diagonal in l, j, and m because of the orthogonality of the harmonic oscillator states in those variables. Everything else was done in the class notes and I'd rather just be done with this thing than rewrite that all in LaTeX.

Adding now the two-body interaction, the code takes substantially longer to run (I had a hard enough time getting it working; I wasn't about to make it run fast...). Nevertheless, it works. Ignoring all interactions involving protons, we can compute the neutron energy levels and we see that they are different from the harmonic oscillator levels. The degeneracies from the harmonic

oscillator, however, are broken but still visible (2 states with energy 0.3 MeV, 6 with energy 15 MeV, 12 with energy 30MeV, and 20 with energy 42MeV). So the two-body interaction acts to break the degeneracy as well as to change (typically decrease) the single particle energy levels.

Those results are shown here:

```
 The calculation converged after 11.0 iterations.
The converged energy eigenvalues are
[ 0.31029405 0.31029405 14.70873572 14.70873572 14.70874003
14.70874003 16.82953558 16.82953558 28.85066259 28.85066259
28.85066404 28.85066404 28.85066604 28.85066604 29.24695792
29.24695792 31.14975806 31.14975806 31.14975914 31.14975914
40.47253948 40.47253948 40.47254128 40.47254128 41.04486896
41.04486896 41.04486907 41.04486907 41.04487074 41.04487074
41.04487093 41.04487093 41.06195331 41.06195331 43.04670671
43.04670671 43.04670712 43.04670712 43.04670815 43.04670815 ]
```

Finally, we can consider the case in which both protons and neutrons are considered together, which gives a somewhat-realistic model for oxygen-16. With a convergence parameter of $\epsilon = 10^{-5}$ (which was taking long enough, never mind $\epsilon = 10^{-8}$!), the calculation converges after 12 iterations.

```
 The calculation converged after 12.0 iterations.
The converged energy eigenvalues are
[-40.64258498 -40.64258498 -40.46016241 -40.46016241 -11.72008572
-11.72008572 -11.72008034 -11.72008034 -11.58864782 -11.58864782
-11.58864493 -11.58864493 -6.84033381 -6.84033381 -6.71334458
-6.71334458 18.75887277 18.75887277 18.75888858 18.75888858
18.7588964 18.7588964 18.80821476 18.80821476 18.80823187
18.80823187 18.80823695 18.80823695 21.02472815 21.02472815
21.06535441 21.06535441 22.91526071 22.91526071 22.91526186
22.91526186 22.96218943 22.96218943 22.96219115 22.96219115
35.13448887 35.13448887 35.13449125 35.13449125 35.15841727
35.15841727 35.15841746 35.15841746 35.85257224 35.85257224
35.87705735 35.87705735 36.03386505 36.03386505 36.03386528
36.03386528 36.03386568 36.03386568 36.03387313 36.03387313
36.05961649 36.05961649 36.05961723 36.05961723 36.05961839
36.05961839 36.05962509 36.05962509 39.28250074 39.28250074
39.28250186 39.28250186 39.28250312 39.28250312 39.30670735
39.30670735 39.30670827 39.30670827 39.30670858 39.30670858 ]
```

The full results are shown in the attached file `hf.out`.

Interpreting these values, the 16 negative energies correspond to the ground state configuration of the system. So for example, the binding energy of a nucleon in a $p_{\frac{1}{2}}$ shell is bound by approximately 6.7 MeV. Meanwhile, to move a particle to the $d_{\frac{5}{2}}$ shell would take something like 18.8 MeV. Comparing this to experiment, we see some room for improvement:

According to the BNL NNDC database, the ^{16}O single neutron separation energy is 15663.9 keV and the single-proton separation energy is 12127.41 keV. The single-proton separation energy for ^{17}F is 600.27 keV and the single neutron separation energy for ^{17}O is 4143.0801 keV.