PHY981 Project 1

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In this project, I developed a C++ code to perform the required Hartree-Fock calculations. A few of the programming ideas were borrowed from Prof Hjorth-Jensen's example code in python.

The codes can be found at https://github.com/Gartenzwerg/PHY981/blob/master/Project1B/ .(Please be reminded to compile and link with options "-O2 -larmadillo".)

1 Task A: Harmonic Oscillators

The program reads and stores all single-particle states from *spdata.dat*. The relevant neutron states were extracted, and a 40×40 diagonal Hamiltonian matrix in m-scheme was set up. The matrix was then diagonalized with the help of *armadillo*, a linear algebra library.

Results of single-particle energies are as follows.

label	state	Energy [MeV]
1	$0s_{1/2}$	15
2	$0s_{1/2}$	15
3	$0p_{3/2}$	25
4	$0p_{3/2}$	25
5	$0p_{3/2}$	25
6	$0p_{3/2}$	25
7	$0p_{1/2}$	25
8	$0p_{1/2}$	25

2 Task B: Formalisms

Consider two-body matrix elements of the form $\langle n_1 l_1 j_1 m_{j1} n_2 l_2 j_2 m_{j2} | V | n_3 l_3 j_3 m_{j3} n_4 l_4 j_4 m_{j4} \rangle$. We shall show that they are diagonal in ljm_j and is independent of m_j, given that V is a scalar tensor operator.

Since V, a rank-0 tensor operator, cannot connect states with different j or different m_j, we must have $j_1 = j_3$, $j_2 = j_4$, $m_{j1} = m_{j3}$ and $m_{j2} = m_{j4}$ for the non-vanishing matrix elements. Also note that V is a scalar operator and thus has even parity. The difference in l between the *bra* and the *ket* must be even for non-vanishing elements. However, since $j = l \pm \frac{1}{2}$ for nucleons and the j's in the *bra* and the *ket* match, the difference in l must be 0.

Therefore, we can restrict our attention to those of the form $\langle n_1 l j m_j n_2 l' j' m_{j'} | V | n_3 l j m_j n_4 l' j' m_{j'} \rangle$. In fact, better still, we need only look at $\langle n_1 l j n_2 l' j' | V | n_3 l j n_4 l' j' \rangle$, as V is independent of m's. Indeed,

$$\langle n_1 l j n_2 l' j' | V | n_3 l j n_4 l' j' \rangle = \langle n_1 l j m_j n_2 l' j' m_{j'} | V | n_3 l j m_j n_4 l' j' m_{j'} \rangle$$

for any m_j and m'_j. If necessary, we can also express these reduced matrix elements by an average over all m_j and $m_{j'}$ values.

It is obvious from definition that the hamiltonian matrix elements can be written as (I denote by p the new Hartree-Fock states.)

$$h^{lj}_{n_1 n_3} = \delta_{n_3 n_1}(2n_1 + l + 3/2)\hbar\omega + \sum_{p \le \mathrm{F}} \sum_{n_2 n_4} \sum_{l' j' m_{j'}}^{occ} C^{*l'j'}_{n_2 p} C^{l'j'}_{n_4 p} \langle n_1 l j m_j n_2 l' j' m_{j'} | V | n_3 l j m_j n_4 l' j' m_{j'} \rangle.$$

By introducing the reduced matrix elements

$$\langle n_1 l j n_2 l' j' | V | n_3 l j n_4 l' j' \rangle := \frac{1}{(2j+1)(2j'+1)} \sum_{m m'} \langle n_1 l j m n_2 l' j' m' | V | n_3 l j m n_4 l' j' m' \rangle \,,$$

and defining the density matrix elements as

$$\rho^{l'j'}_{n_4 n_2} := \frac{1}{2j'+1} \sum_{p \le \mathrm{F}} C^{*l'j'}_{n_2 p} C^{l'j'}_{n_4 p} \,,$$

we can simplify the hamiltonian

$$h^{lj}_{n_1 n_3} = \delta_{n_3 n_1}(2n_1 + l + 3/2)\hbar\omega + \sum_{n_2 n_4} \sum_{l' j'}^{occ} \langle n_1 l j n_2 l' j' | V | n_3 l j n_4 l' j' \rangle \rho^{l'j'}_{n_4 n_2}.$$

Fianally, it follows straight from definition that the Hartree-Fock equations should read

$$\sum_{n_3} h^{lj}_{n_1 n_3} C^{lj}_{n_3 p} = \epsilon_{plj} C^{lj}_{n_3 p} \,.$$

3 Task C: Hartree-Fock calculations with a two-body potential

I extracted only the neutron-neutron interactions from $two-body.dat$ and constructed the two-body potential matrix accordingly in each iteration. The uncoupled neutron basis was used and the dimension of the matrix is 40×40. However, thanks to the selection rules mentioned in *Task B* and the symmetry of the matrix itself, computations of many of the elements were either safely skipped or largely simplified. The entire program takes merely two seconds to complete the task and outputs correct results.

Below are the Hartree-Fock single-particle energies and comparison with the harmonic oscillator energies.

label	state	E_{HO} [MeV]	E_{HF} [MeV]
1	$0s_{1/2}$	15	0.310294
2	$0s_{1/2}$	15	0.310294
3	$0p_{3/2}$	25	14.7087
4	$0p_{3/2}$	25	14.7087
5	$0p_{3/2}$	25	14.7087
6	$0p_{3/2}$	25	14.7087
7	$0p_{1/2}$	25	16.8295
8	$0p_{1/2}$	25	16.8295

As can be obviously seen, the Hartree-Fock energies are much lower than the harmonic oscillator ones. This agrees with our expectation, as the two-body potential serves to lower the energy levels. It is also critical that the two-body potential lifts the degeneracy in j. The Hartree-Fock energies with a two-body potential have dependence on n, l and j, whereas n and l only suffice to determine the energy levels in the harmonic oscillator model.

It should also be pointed out that the calculations performed are not exact, owing to the facts that 1) the neutron-proton interactions are deliberately excluded, that 2) only a finite subset (of size 40) of the infinite harmonic oscillator basis were used, and that 3) corrections to the two-body potential, three-body interactions, clustering effects, etc. might exist.

4 Task D: ^{16}O

The previous code was modified to perform Hartree-Fock calculations for ^{16}O. Results are listed in the following table. E^{ν}_{HF} and E^{π}_{HF} denote the Hartree-Fock energies for neutrons and protons, respectively.

state	E^{ν}_{HF} [MeV]	E^{π}_{HF} [MeV]
$0s_{1/2}$	-40.6426	-40.4602
$0p_{3/2}$	-11.7201	-11.5886
$0p_{1/2}$	-6.84033	-6.71334
$0d_{5/2}$	18.7589	18.8082

A hint of charge symmetry breaking can be observed. Proton single-particle energies are slightly higher than their neutron counterparts in the corresponding states, because of the Coulomb repulsion.

I would compare $\epsilon_{0p_{1/2}}$ for neutrons or protons with S_n or S_p for ^{16}O, $\epsilon_{0d_{5/2}}$ for neutron with S_n for ^{17}O, and $\epsilon_{0d_{5/2}}$ for proton with S_p for ^{17}F.

state	E^{ν}_{HF} [MeV]	S_n [MeV]	E^{π}_{HF} [MeV]	S_p [MeV]
$0p_{1/2}$	-6.84033	15.7 [^{16}O]	-6.71334	12.1 [^{16}O]
$0d_{5/2}$	18.7589	4.14 [^{17}O]	18.8082	0.600 [^{17}F]

It seems that our naive Hartree-Fock calculations fail to reproduce the actual separation energies. It is no surprise that there is much more to the picture than meets the eye. The Hartree-Fock calculations here are on a single-particle level, in the sense that they make little reference to the whole 16-body problem. Solving for single-particle states and energies using single-particle basis is primitive and limited. Instead, we ought to consider using Slater determinants as our basis and recognizing energy as a functional of Slater determinant.