The Hartree-Fock Algorithm

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Introduction

This project applies the Hartree-Fock algorithm to a system of 8 neutrons confined in a harmonic oscillator potential (eq. 1) with an added nucleon-nucleon interaction. Eight protons are then added to the system to model ^{16}O. The results of the calculation can then be compared to measured separation energies.

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{N} \frac{1}{2} m\omega r_i^2 + \sum_{i<j} \hat{V}_{ij} \tag{1}$$

Using the harmonic oscillator states as our single particle basis, the Hartree-Fock matrix can be written as

$$\hat{h}_{\alpha\beta}^{HF} = \delta_{\alpha,\beta}\epsilon_\alpha + \sum_{\gamma\delta} \rho_{\gamma\delta} \left\langle \alpha\gamma \right| \hat{V} \left| \beta\delta \right\rangle_{AS} \tag{2}$$

where the density matrix ($\rho_{\gamma\delta}$) and the harmonic oscillator energies (ϵ_α)are, respectively,

$$\rho_{\gamma\delta} = \sum_{k=1}^{N} C_{k\gamma} C_{k\delta}^* \tag{3}$$

$$\epsilon_\alpha = \hbar\omega(2n + l + 3/2) \tag{4}$$

The Hartree-Fock algorithm essentially consists of defining some interaction Hamiltonian, a convenient basis in which to expand the HF single particle (s.p.) states and a guess for the initial coefficients of each HF s.p. state. Then we minimize the single particle energies by varying the contribution (coefficients) of the basis states to each HF state. This procedure is implemented by iteratively solving a set of eigenvalue equations until the change in s.p. energies between iterations converges to a user-defined limit

Symmetries

Certain symmetries of the 3D harmonic oscillator and the added nucleon interaction can be utilized in the numerical implementation of the HF algorithm. The single-particle HF

Hamiltonian (eq. 2) is a scalar operator (energy). Therefore, the nucleon interaction $\hat{V}$ must also be a scalar ($L = 0, M = 0$). This imposes conditions on the matrix elements $\langle \alpha\gamma | \hat{V} | \beta\delta \rangle$ according to

$$\langle \xi' j' m' | T_{LM} | \xi j m \rangle = 0 \quad \text{unless} \quad \begin{cases} \triangle(jLj') \\ m + M = m' \end{cases} \tag{5}$$

where

$$\triangle(jLj') \Rightarrow |j - L| \leq j' \leq j + L \tag{6}$$

and $j = l + s$ with s as the spin of the particle (always 1/2 in our case). So, the condition 6 reduces to $j = j'$ and imposes the restriction 7 (since s is always 1/2) in order to have non zero matrix elements $\langle \alpha\gamma | \hat{V} | \beta\delta \rangle$.

$$l_\alpha + l_\gamma = l_\beta + l_\delta \tag{7}$$

Furthermore, the second condition from 5 reduces to 8 with $M = 0$.

$$m_\alpha + m_\gamma = m_\beta + m_\delta \tag{8}$$

Finally, since we are dealing with indistinguishable particles, these restrictions must hold regardless of how we label the states. Therefore, we can fix $l_\alpha = l_\beta$ and $m_\alpha = m_\beta$ so that the HF s.p. Hamiltonian is diagonal in ljm.

Testing without the nucleon interaction

The file `hfHOneutrons.py` contains a version of the code that leaves out the nucleon interaction and runs the Hartree-Fock algorithm for 8 neutrons. The output is contained in the file `HO.out` and gives the harmonic oscillator energies (eq. 4, taking $\hbar\omega = 10$ MeV) and level degeneracies ($g_l = 2l + 1$, $g_s = 2$, $g = g_s g_l$). The results are summarized in Table 1.

$N = 2n + l$	n	l	g	ϵ [MeV]
0	0	0	2	15
1	0	1	6	25
2	0	2	10	35
	1	0	2	35
3	0	3	14	45
	1	1	6	45

Table 1: Harmonic oscillator quantum numbers (nl), degeneracies and energies for the first 40 states.

ϵ	g	Assignment
-18.5136	2	$0s_{1/2}$
1.5706	4	$0p_{3/2}$
7.1960	2	$0p_{1/2}$
22.5123	6	$0d_{5/2}$
24.2719	2	$1s_{1/2}$
27.7574	4	$0d_{3/2}$
36.9189	4	$1p_{3/2}$
37.2630	8	$0f_{7/2}$
38.0082	4	$1p_{1/2}$
41.5403	6	$0f_{5/2}$

Table 2: Neutron drop energies. Levels are labeled by matching occupancy to the familiar WS+s.o. level scheme.

Neutron Drops

The file `hfneutrons.py` is a modified version of the code that reads in only data for the neutron orbitals ($t_z = 1/2$); its output is collected in `HFn.out` and summarized in Table 2. Compared to the harmonic oscillator energies, the most noticable difference when the nucleon interaction is introduced is the re-ordering of the level structure. The HF single particle energies do not have the same degree of degeneracy as the harmonic oscillator levels. The level groupings now reflect the familiar arrangement of a Woods-Saxon potential with spin-orbit coupling (WS + s.o) for the lower levels (the $1p_{3/2}$ appears below the $0f_{7/2}$). The Assignments in Table 2 are made based on the occupancy of each level.

^{16}O Model

The python code `hfnuclei.py` adds 8 protons to model the ^{16}O system; the results are listed in `HFnp.out` and Table 3. Similar to the neutron system, the HF s.p. energies are grouped like the WS + s.o. levels, however, the neutron and proton energies for a particular level are not the same. This is attributed to a difference in the nucleon interaction for particles with different t_z. In other words, the nucleon interaction breaks isospin symmetry.

We can now compare the HF model predictions to their corresponding separation energies (Table 4). The HF predictions for the ^{16}O separation energies differ from experimental results by a factor of 2. This suggests that this simple model is quite a good starting point. However, the discrepancy between prediction and experiment grows much larger for non-closed-shell systems.

ϵ_ν	ϵ_π	g	Assignment
-40.64	-40.46	g	$0s_{1/2}$
-11.72	-11.59	4	$0p_{3/2}$
-6.84	-6.71	2	$0p_{1/2}$
18.76	18.81	6	$0d_{5/2}$
21.02	21.07	2	$1s_{1/2}$
22.92	22.96	4	$0d_{3/2}$
35.13	35.16	4	$1p_{3/2}$
35.85	35.88	2	$1p_{1/2}$
36.03	36.06	8	$0f_{7/2}$
39.28	39.31	6	$0f_{5/2}$

Table 3: Neutron and proton HF s.p. energies labeled based on comparison to the WS + s.o. level scheme.

$\epsilon^\nu_{0p1/2} = 6.84$ MeV	$\epsilon^\pi_{0p1/2} = 6.71$ MeV	$\epsilon^\nu_{0d5/2} = 18.76$ MeV	$\epsilon^\pi_{0d5/2} = 18.81$ MeV
$S_n(^{16}\mathrm{O}) = 15.7$ MeV	$S_p(^{16}\mathrm{O}) = 12.1$ MeV	$S_n(^{17}\mathrm{O}) = 4.14$ MeV	$S_p(^{17}\mathrm{F}) = 0.6$ MeV

Table 4: Comparison of HF s.p. energies to measured separation energies.