

a) 8 neutrons, without interaction:

[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.	45.	45.	45.	45.	45.]

calculation proves correct at this step, energy obeys:

$$E_{h.o.} = (2n + l + 1.5) \cdot \hbar\omega$$

b)

Since the **interaction** given in this problem is **scalar**, it does not have the property to change angular momentum, basically **it's a spherical harmonic** $\sim Y_{00}$ which cannot link 2 different l or j values. Again since the **interaction** given is **spin-independent**, it doesn't involve the quantum number m . The harmonic potential hamiltonian is diagonal on it's own with the Kronecker delta, thus the entire hamiltonian, **$h_0 + V$ is diagonal in ljm** when added together.

In the number representation, we have the many-body energy:

$$E[\Psi] = \sum_{i=1}^A \sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta} \langle \alpha | h | \beta \rangle + \frac{1}{2} \sum_{ij=1}^A \sum_{\alpha\beta\gamma\delta} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS}$$

and for the coefficient C's, we have:

$$\langle i | j \rangle = \delta_{i,j} = \sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta} \langle \alpha | \beta \rangle = \sum_{\alpha} C_{i\alpha}^* C_{i\alpha},$$

within the HF variational method, we sought to minimize the energy, which should converge to the true ground state energy if we've chosen a good set of basis.

Thus we'd want to minimize the below functional, w.r.t. the approximated wave-function (thus the coefficient vector) we choose:

$$F[\Phi^{HF}] = E[\Phi^{HF}] - \sum_{i=1}^A \epsilon_i \sum_{\alpha} C_{i\alpha}^* C_{i\alpha}$$

$$\frac{d}{dC_{i\alpha}^*} \left[E[\Phi^{HF}] - \sum_j \epsilon_j \sum_{\alpha} C_{j\alpha}^* C_{j\alpha} \right] = 0$$

after bringing in explicitly the top expression of E^{HF} , we get:

$$\sum_{\beta} C_{i\beta} \langle \alpha | h | \beta \rangle + \sum_{j=1}^A \sum_{\beta\gamma\delta} C_{j\beta}^* C_{j\delta} C_{i\gamma} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS} = \epsilon_i^{HF} C_{i\alpha}$$

we can now clearly see if we replace the hamiltonian with:

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

we can easily arrive at:

$$\sum_{n_3} h_{n_1 n_3}^{lj} C_{n_3 \bar{n}}^{lj} = \epsilon_{\bar{n} l j} C_{n_3 \bar{n}}^{lj}$$

c) 8 neutrons, with interaction:

Iteration: 14, diff = 6.1687343067e-08 MeV

[0.31029368	0.31029387	14.70873554	14.70873565	14.70873989
	14.70873991	16.82953551	16.82953556	28.85066256	28.85066258
	28.85066401	28.85066404	28.85066601	28.85066603	29.24695785
	29.24695791	31.14975808	31.1497581	31.14975916	31.14975919
	40.47253942	40.47253945	40.47254123	40.47254124	41.04486896
	41.04486898	41.04486907	41.04486909	41.04487074	41.04487076
	41.04487094	41.04487095	41.06195329	41.0619533	43.04670674
	43.04670676	43.04670716	43.04670716	43.04670819	43.04670819]

Compared to no-interaction harmonic oscillator single-particle energies, all of the neutron s.p. energies with interaction are lowered, this is the work of these single particles binding with each other, forming a more stable collective entity, through nuclear forces (no Coulomb for neutron). We could also see the degeneracy for states with the same angular momentum J.

However, all the s.p. energies are positive, which means under the given interaction, this 8-neutron system is not bound.

Starting from 0s, 0p, 1s0d, 1p0f, we can determine the corresponding orbitals (energy from low to high), using also the degeneracy numbers, and also see the detailed shell structure:

0s shell, magic #: 20s_{1/2} 2 states ~0.31 MeV**0p shell, magic #: 2 + (4+2) = 8**0p_{3/2} 4 states ~14.71 MeV0p_{1/2} 2 states ~16.83 MeV**1s0d shell, magic #: 8 + (6+2+4) = 20**0d_{5/2} 6 states ~28.85 MeV1s_{1/2} 2 states ~29.25 MeV0d_{3/2} 4 states ~31.15 MeV**1p0f shell, magic #: 20 + (4+8+2+6) = 40****

**A more precise interaction should show that 1f_{7/2} state has lower energy intruding into the 1s0d shell, thus forming a shell of 28. In my calculation, 1p_{3/2} state has a lower energy.

1p_{3/2} 4 states ~40.47 MeV0f_{7/2} 8 states ~41.04 MeV1p_{1/2} 2 states ~41.06 MeV0f_{5/2} 6 states ~43.05 MeV

c) 8 protons, with interaction:

Iteration: 15, diff = 4.57021918088e-08 MeV

0.47931374	0.47931399	14.82113847	14.82113864	14.82114229
14.82114238	16.92933316	16.92933321	28.90094561	28.90094568
28.90094629	28.90094638	28.90094712	28.90094714	29.30152728
29.30152736	31.19275532	31.19275537	31.19275551	31.19275552
40.51646855	40.51646857	40.51647221	40.51647225	41.07108411
41.07108416	41.07108436	41.07108439	41.07108454	41.0710846
41.07108528	41.07108529	41.1054643	41.1054643	43.06893353
43.06893354	43.06893362	43.06893363	43.06893395	43.06893397

We could use similar analysis as in the above neutron case. The difference is, protons has Coulomb interaction, thus the s.p. energies are higher when you put a bunch of protons that has Coulomb repulsion with each other close together.

d) 8 neutrons + 8 protons, with interaction:

Iteration: 13, diff = 8.92481359926e-07 MeV

-40.64258531	-40.64258519	-40.46016272	-40.46016264	-11.72008582
-11.72008581	-11.72008045	-11.72008042	-11.58864794	-11.5886479
-11.58864506	-11.588645	-6.84033386	-6.84033384	-6.71334463
-6.7133446	18.7588728	18.75887281	18.7588886	18.75888862
18.75889643	18.75889644	18.80821479	18.80821479	18.80823189
18.80823191	18.80823697	18.80823698	21.02472817	21.02472818
21.06535442	21.06535444	22.91526075	22.91526077	22.9152619
22.91526192	22.96218947	22.96218949	22.96219118	22.96219121
35.13448888	35.13448888	35.13449126	35.13449126	35.15841728
35.15841728	35.15841746	35.15841747	35.85257225	35.85257225
35.87705735	35.87705736	36.03386508	36.03386509	36.03386531
36.03386532	36.03386571	36.03386572	36.03387317	36.03387318
36.05961653	36.05961653	36.05961726	36.05961727	36.05961842
36.05961843	36.05962512	36.05962513	39.28250077	39.28250079
39.2825019	39.28250191	39.28250316	39.28250317	39.30670738
39.3067074	39.30670831	39.30670832	39.30670861	39.30670863

It's quite obvious that the first 16 s.p. states are occupied, and have a significant lower energy (all negative) than those s.p. states above occupation level, which tells us **this system is bound under the given interaction**. I'm guessing that the 'twobody.dat' interaction was abstracted from real data, thus only with the full neutron-proton picture, the s.p. energies would be negative and thus showing that they're bound.

Given that we've discovered protons have slightly higher s.p. energy than the neutrons with the orbital quantum numbers, we can interpret these s.p. energy eigenvalues as neutrons first,

protons second within each set of orbital quantum numbers, with a little counting, we can identify the s.p. energies for different proton, neutron orbitals.

Now, we should be comparing:

1. **Proton** separation energy of **O-16** with the **0p_{1/2}** proton energy of our O-16 HF calculation,
2. **Proton** separation energy of **F-16** with the **0d_{5/2}** proton energy of our O-16 HF calculation,
3. **Neutron** separation energy of **O-16** with the **0p_{1/2}** neutron energy of our O-16 HF calculation,
4. **Neutron** separation energy of **O-17** with the **0d_{5/2}** neutron energy of our O-16 HF calculation.

$$BE(^{16}\text{O}) - BE(^{15}\text{O}) \approx \epsilon_{0p_{1/2}}^{\text{HF}},$$

$$BE(^{17}\text{O}) - BE(^{16}\text{O}) \approx \epsilon_{0d_{5/2}}^{\text{HF}},$$

$$BE(^{16}\text{O}) - BE(^{15}\text{N}) \approx \epsilon_{0p_{1/2}}^{\text{HF}}.$$

$$BE(^{17}\text{F}) - BE(^{16}\text{O}) \approx \epsilon_{0d_{5/2}}^{\text{HF}}.$$

comparing with experimental values on the right column (ignore the minus signs):

$$n\epsilon_{0p_{1/2}}^{\text{HF}} \approx -6.84\text{MeV}$$

$$S_n^{\text{exp}}(^{16}\text{O}) \approx 15.664\text{MeV}$$

$$n\epsilon_{0d_{5/2}}^{\text{HF}} \approx 18.76\text{MeV}$$

$$S_n^{\text{exp}}(^{17}\text{O}) \approx 4.143\text{MeV}$$

$$p\epsilon_{0p_{1/2}}^{\text{HF}} \approx -6.71\text{MeV}$$

$$S_p^{\text{exp}}(^{16}\text{O}) \approx 12.127\text{MeV}$$

$$p\epsilon_{0d_{5/2}}^{\text{HF}} \approx 18.81\text{MeV}$$

$$S_p^{\text{exp}}(^{17}\text{F}) \approx 16.801\text{MeV}$$

It's not ideal... except for Fluorine-17's proton separation energy.