Nuclear Shell Model

Introduction to Nuclear Science

Simon Fraser University
SPRING 2011

NUCS 342 — January 26, 2011

Outline

1. Shells in atoms and in nuclei

Outline

1. Shells in atoms and in nuclei
2. The mean-field potential

Outline

1. Shells in atoms and in nuclei
2. The mean-field potential
3. Phenomenological (empirical) shell model

Outline

1. Shells in atoms and in nuclei
2. The mean-field potential
3. Phenomenological (empirical) shell model
4. The spin-orbit splitting

Outline

1. Shells in atoms and in nuclei
2. The mean-field potential
3. Phenomenological (empirical) shell model
4. The spin-orbit splitting
5. Total angular momentum

Outline

1. Shells in atoms and in nuclei
2. The mean-field potential
3. Phenomenological (empirical) shell model
4. The spin-orbit splitting
5. Total angular momentum
6. Modified spectroscopic notation

Outline

Outline

1. Shells in atoms and in nuclei
2. The mean-field potential
3. Phenomenological (empirical) shell model
4. The spin-orbit splitting
5. Total angular momentum
6. Modified spectroscopic notation
7. Extreme single-particle shell model
8. Nuclei near ^{16}O

Why the atomic shell model works well in Hydrogen?

- A hydrogen atom is a two-body system consisting of an electron and proton. A motion of such system can be described fully and accurately by a translational motion of the centre of mass of the system and orbital motion around the centre of mass.
- Since proton is $\sim$1836 times heavier then electron the centre of mass coincides with good accuracy with the centre of the proton.
- Nucleus is a point-like source of long-range electromagnetic force.
- Electromagnetic interactions are well understood, in particular, the Schrödinger equation for Coulomb potential has been solved analytically.

Why the same can not be done in nuclei?

- A nucleus is a many-body systems of interacting particles. There are no analytic solutions of the Schrödinger equations for such system, also often only approximate solutions can be obtained.
- In a nucleus there is no dominant centre of the long-range force. Rather than that, the force is short range and there are many pairs of interacting nucleons.
- The nuclear force is still poorly understood.
- Recent results indicate that nucleon-nucleon interactions are modified in the presence of a third nucleon (the three-body force)
- There are two types of particles (protons and neutrons).

Then why and how does the shell model work for nuclei?

- Interaction between nucleons in nuclei averages out and results in a potential which depends on position but does not depend on time. This potential is often referred to as the "nuclear mean field".
- A nucleus, therefore, is an example of a self-organizing system in which the nuclear potential emerges from a large number of nucleon-nucleon interactions.
- There are some similarities between self-organization of nucleons in nuclei and electrons in multi-electron atoms, with one significant difference though, namely, that in multi-electron atoms the electromagnetic potential between the nucleus and an electron dominates the potential between electron-electron interactions. There is no equivalent dominating potential in a nucleus.

Two-body interactions

- Note that the nucleon-nucleon interaction has a two-body character (there are two nucleons involved).
- If we would like to describe this fact in terms of the potential energy of these interaction we would need to use $V_{i,j}$ with i representing one of the nucleons and j representing the other one.
- The total energy would be

$$E = \sum_{i=1}^{n} T_i + \sum_{i>j}^{n} \sum_{j=1}^{n} V_{i,j} \tag{1}$$

with the second sum running over $i > j$ to avoid double-counting of the interaction energies.

The mean field potential

- The mean field potential attempts to replace the two-body interaction of Eq. 1 with a potential V_i which depends only on the position of a single nucleon. If this is successful many things become simple:

$$E = \sum_{i=1}^{n} T_i + \sum_{i=1}^{n} V_i = \sum_{i=1}^{n} (T_i + V_i) = \sum_{i=1}^{n} E_i \tag{2}$$

  where E_i, T_i and V_i are single-particle total, kinetic and potential energies, respectively.

- This is especially convenient for solving the Schrödinger equation since in case of Eq. 2 it separates into a set of independent Schrödinger equations for each nucleon, while in case of Eq. 1 all these equations are coupled.

Residual interactions

- With a tiny bit of simple algebra it can be shown

$$
\begin{aligned}
E &= \sum_{i=1}^{n} T_i + \sum_{i>j}^{n}\sum_{j=1}^{n} V_{i,j} = \sum_{i=1}^{n} T_i + \sum_{i=1}^{n} V_i - \sum_{i=1}^{n} V_i + \sum_{i>j}^{n}\sum_{j=1}^{n} V_{i,j} \\
&= \sum_{i=1}^{n}(T_i + V_i) + (\sum_{i>j}^{n}\sum_{j=1}^{n} V_{i,j} - \sum_{i=1}^{n} V_i) = E_{sm} + E_{res} \qquad (3)
\end{aligned}
$$

- The E_{sm} represent the shell-model energy specified by Eq. 2 while

$$
E_{res} = (\sum_{i>j}^{n}\sum_{j=1}^{n} V_{i,j} - \sum_{i=1}^{n} V_i) \qquad (4)
$$

is the energy of the residual interactions "left out" by the shell model.

- The shell model works well when the residual interaction are small.

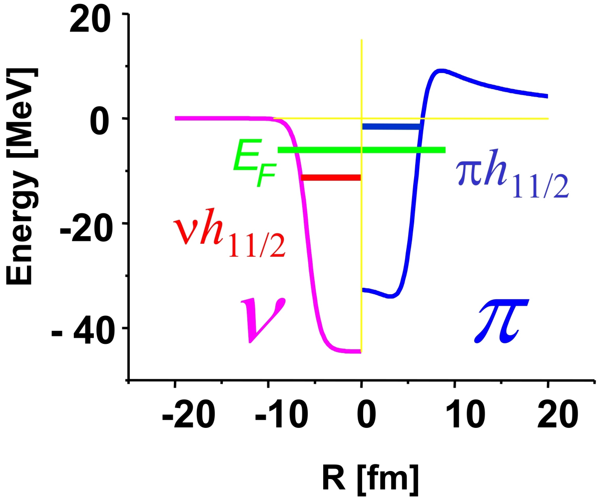
Calculation of the mean-field potential

- Mean field potentials are calculated for nucleon in nuclei and for electrons in multi-electron atoms or in molecules using very similar methods (but very different interactions).
- These methods take advantage of the fact that the ground-state solution of the Schrödinger equation has the lowest energy available for the system.
- These methods seek a density distribution for nucleons or electrons which minimizes the sum of kinetic and potential energy in the Schrödinger equation for the system.
- These methods were initially know as the Hartree or Hartree-Fock methods, self-consistent mean field methods, and are presently know as the density functional methods.
- An underlying assumption in these methods is a proportionality between the mean-field potential and density distribution in the system of interest.

Phenomenological shell model

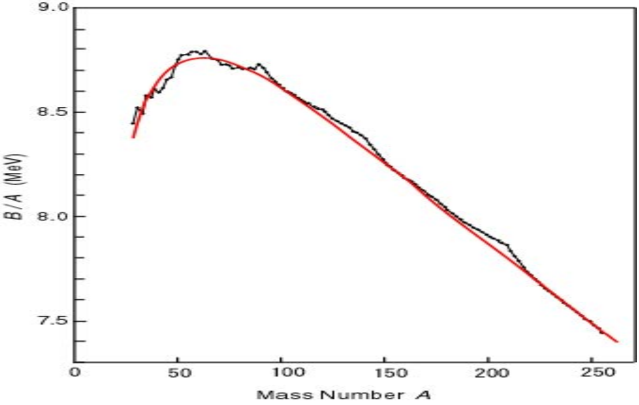
- While above arguments explain why the shell model works for nuclei the historical development of the shell model follow a different path.
- The nuclear shell model was proposed to explain a collection of experimental data which indicated existence of nuclear shells in analogy to the atomic shell model.
- When proposing this model the scientists recognized the difference in the radial equation between the atomic and the nuclear shell model.
- In particular the saturation property of the nuclear force (known from the liquid drop model) called for a potential flat in the centre.
- Scattering and reaction experiments called for diffused surface.
- Early approximation of the nuclear potential were in form of a potential well, modified harmonic oscillator (flat bottom) or later the Wood-Saxon potential (proportional to Fermi density distribution).

Phenomenological shell-model potential



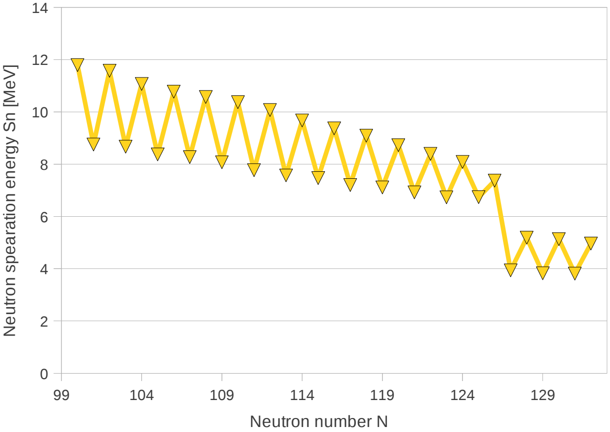
Experimental evidence for closed nuclear shells

- Binding energies deviate from the liquid drop model with increased binding at N or Z at the "magic" numbers of 2, 8, 20, 28, 50, 126,



Experimental evidence for closed nuclear shells

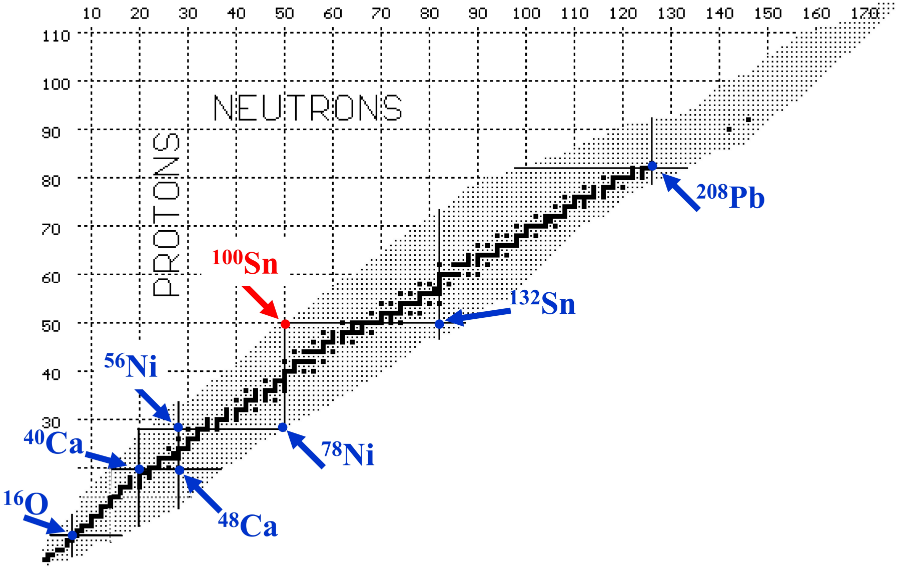
- Neutron and proton separation energies show steps at the “magic” numbers of 2, 8, 20, 28, 50, 126,



Experimental evidence for closed nuclear shells

- Number of stable isotopes/isotones is significantly higher for nuclei with the proton/neutron number equal to the magic number.
- Nucleon capture cross sections are high for nuclei with one nucleon shy from the magic number (single vacancy in a closed shell), but significantly lower for nuclei with number of nucleons equal to the magic number (at the closed shell).
- Energy of the first excited state for nuclei with the proton or the neutron number equal to the magic number are significantly higher than for other nuclei.
- Excitation probabilities of the first excited state are low for nuclei with the proton or neutron number equal to the magic number.
- Quadrupole moments vanish for nuclei with proton or neutron number equal to the magic number.

Doubly magic nuclei

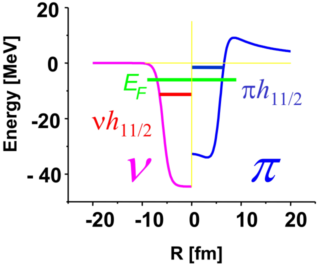


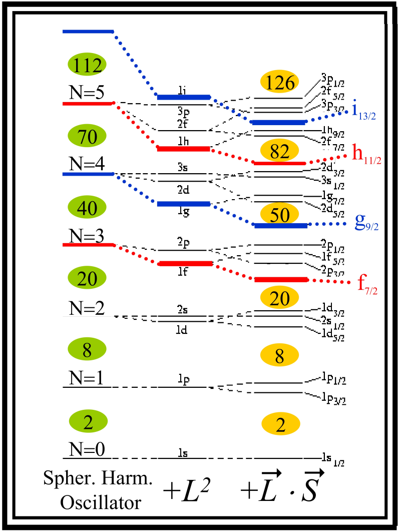
The confusion

- A serious confusion arose in early comparisons of nuclear shell model predictions with data.
- The data clearly pointed out to nuclear magic numbers at 2, 8, 20, 28, 50, 126.
- But nuclear shell model with a flat bottom potential gave the shell gaps which explain the magic numbers at 2, 8, 20, 40, 70, 112.
- Therefore, while the first three magic numbers were in agreement with the data the consecutive higher ones were not.
- The models was wrong, but not completely wrong.
- An important piece was missing!

The spin-orbit splitting

$$H_{SM} = V(r) + V_{LS}(r)\, \vec{L} \cdot \vec{S}$$





The spin-orbit term

- The spin-orbit term in nuclei reduces the energy of states with spin oriented parallel to the orbital angular momentum while increasing the energy of states with spin oriented opposite to the orbital angular momentum.
- This is different to the result of spin-orbit interaction in atoms where states with spin oriented opposite to the orbital angular momentum are lower in energy.
- The spin-orbit interaction in atoms is understood from the electromagnetic interaction of the magnetic moment of an electron with the magnetic field resulting from orbiting a charged nucleus.
- The spin-orbit interaction in nuclei results from the spin-orbit part of the nuclear force (see Lecture 5, slide 27).

The spin-orbit term

- The nuclear potential with the spin-orbit term is

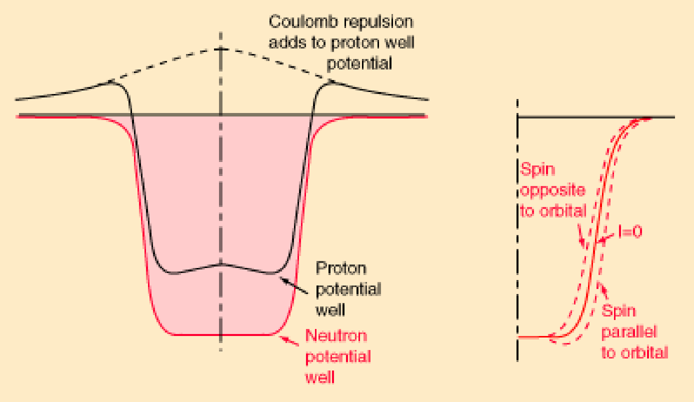
$$V(r, \vec{L}.\vec{S}) = V(r) + V_{LS}(r)\vec{L} \cdot \vec{S} \quad (5)$$

- The radial part $V(r)$ is still the flat bottom well with diffuse surface (the Wood-Saxon potential), while the V_{LS} is often taken as negative derivative of $V(r)$ with respect to r

$$V_{LS}(r) = -\frac{dV(r)}{dr}. \quad (6)$$

- For a flat bottom well with diffuse surface the derivative is peaked at the surface.
- The spin-orbit term makes the nuclear potential well wider for nucleons with spin parallel to the orbital angular momentum and less wide for nucleons with spin opposite to the orbital angular momentum.
- Wider well results in states of lower energies.

The spin-orbit term



Total angular momentum

- Total angular momentum is vector resulting from the coupling of the orbital and spin angular momentum

$$\vec{J} = \vec{L} + \vec{S} \tag{7}$$

- The total angular momentum is quantized, the total angular momentum quantum number is

$$j = \begin{cases} l + \frac{1}{2} & \vec{l} \text{ parallel to } \vec{s} \\ l - \frac{1}{2} & \vec{l} \text{ opposite to } \vec{s} \end{cases} \tag{8}$$

- Without the spin-orbit term the energy of a state does not depend on the total angular momentum $\vec{j}$ or the j quantum number.

- However, with the spin-orbit term it does.

The magnitude of the spin-orbit splitting

- The magnitude of the spin-orbit splitting

$$V_{L,S}(r,\vec{L}.\vec{S}) = V_{LS}(r)\vec{L}\cdot\vec{S} = -\frac{dV(r)}{dr}\vec{L}\cdot\vec{S} \qquad (9)$$

  depends on the total angular momentum $\vec{J}$ of the orbital of interest.

- The magnitude of the $\vec{L}\cdot\vec{S}$ term can be computed following the fact that the square of the total, orbital, and spin angular momenta are defined by the corresponding quantum numbers

$$\begin{aligned}\vec{J}^2 &= (\vec{L}+\vec{S})^2 = \vec{L}^2 + 2\vec{L}\cdot\vec{S} + \vec{S}^2 \\ \vec{L}\cdot\vec{S} &= \frac{1}{2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right) \\ \vec{L}\cdot\vec{S} &= \frac{1}{2}\left(j(j+1) - l(l+1) - s(s+1)\right) \qquad (10)\end{aligned}$$

The magnitude of the spin-orbit splitting

- Since

$$\vec{L}\cdot\vec{S} = \frac{1}{2}\left(j(j+1) - l(l+1) - s(s+1)\right) \tag{11}$$

and

$$j = \begin{cases} l+\frac{1}{2} & \vec{l} \text{ parallel to } \vec{s} \\ l-\frac{1}{2} & \vec{l} \text{ opposite to } \vec{s} \end{cases} \tag{12}$$

then

$$\vec{L}\cdot\vec{S} = \begin{cases} sl = \frac{1}{2}l & \vec{l} \text{ parallel to } \vec{s} \\ -s(l+1) = -\frac{1}{2}(l+1) & \vec{l} \text{ opposite to } \vec{s} \end{cases} \tag{13}$$

Modified spectroscopic notation

- So far we used the orbital angular momentum quantum number to label the state according to the spectroscopic notation.
- As a consequence we had the $l = 0$ s states, the $l = 1$ p, $l = 2$ d states etc.
- The modified spectroscopic notation adds as a subscript the total momentum quantum number to indicate the coupling between the orbital and spin angular momentum.
- Thus we have $p_{1/2}$ and $p_{3/2}$ states of $l = 1$, $d_{5/2}$ or $d_{3/2}$ states of $l = 2$, etc.
- Note that we have only $s_{1/2}$ since for the $l = 0$ (no orbital angular momentum) there can not be parallel or opposite coupling.
- Each state of total angular momentum j has $2j + 1$ substates of the same energy which differ by the azimuthal (magnetic) quantum number m_j which runs from $-j$ up to $+j$.

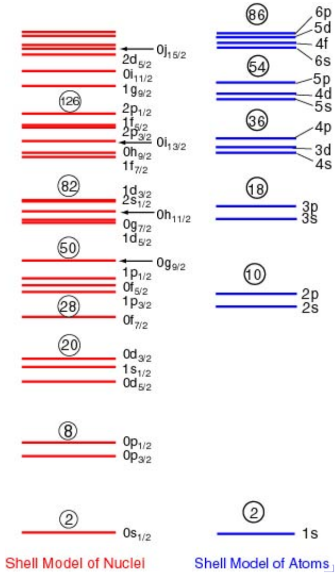
The parity of single-particle orbitals

- Single particle orbitals are also assigned the parity quantum number π.
- The parity is a multiplicative quantum number. The total parity of a system is a product of the parities of all subsystems.
- The parity for a shell model state is defined by the product of the parity of the radial wave function, parity of the spherical harmonic, the parity of the spin wave function and intrinsic parity of a nucleon.
- The parity of radial function, the spin function, and intrinsic parity of a nucleon are all positive.
- Thus, the parity of a single-particle orbital is fully defined by the parity of the spherical harmonics and is $\pi_l = (-1)^l$.
- Parities are significant as they can be measured and compare with model predictions.

Extreme single-particle shell model

- The greatest success of the shell model is in reproducing properties of odd-mass nuclei around doubly-magic cores.
- The model correctly predicts excitation energies, spin/parities, magnetic and quadrupole moments for the ground state and low-energy excited states.
- The model reproduces these properties assuming that a single nucleon is placed in an orbit above a closed shell or that a single nucleon is removed from an orbit below a closed shell.
- Applications near doubly-magic nuclei are often referred to as extreme single-particle shell model since the model space includes a single particle or a single hole (vacancy) outside a closed-shell core.
- The success of the extreme single-particle shell model is a consequence of the fact that the residual interactions between a single valence particle or hole with the closed shell core is small.

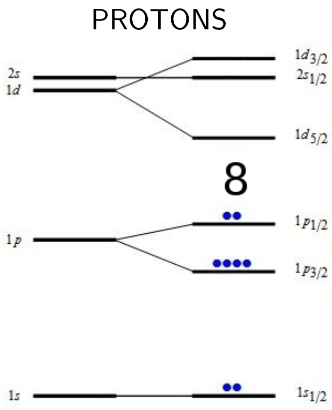
Nuclear vs. Atomic shell model

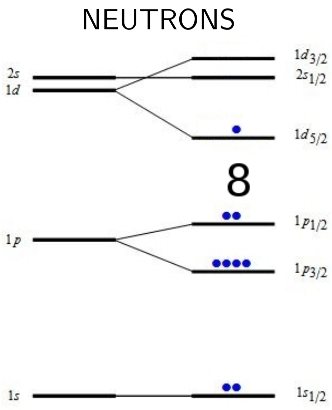


Nuclei near ^{16}O

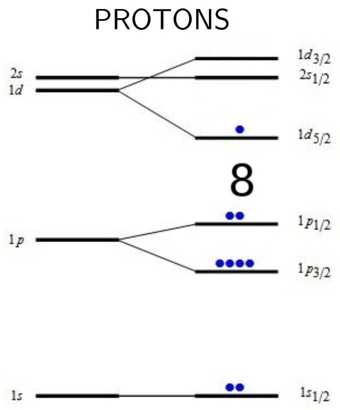
- Let us apply the extreme single-particle shell model to predict spin, parities and excitation energies near the doubly-magic ^{16}O.
- For the reasons to be discussed in the next lecture the spin and parity of the ^{16}O core is 0^+.
- The orbitals above the $N = Z = 8$ shell gaps are positive-parity $d_{5/2}$ and $s_{1/2}$ states. Therefore, we expect for ^{17}O and ^{17}F the ground state of positive parity and spin of $5/2$ and the first excited state of positive parity and spin of $1/2$. This is indeed the case, see Fig. 6.7 in your text book or this link.
- The orbitals below the $N = Z = 8$ shell gaps are negative-parity $p_{3/2}$ and $p_{1/2}$ states. Therefore, we expect for ^{15}O and ^{15}N the ground state of negative parity and spin of $1/2$ and the first excited state of negative parity and spin of $3/2$. This the case for the ground state but not for the first excited state this link.

Ground state in ^{17}O

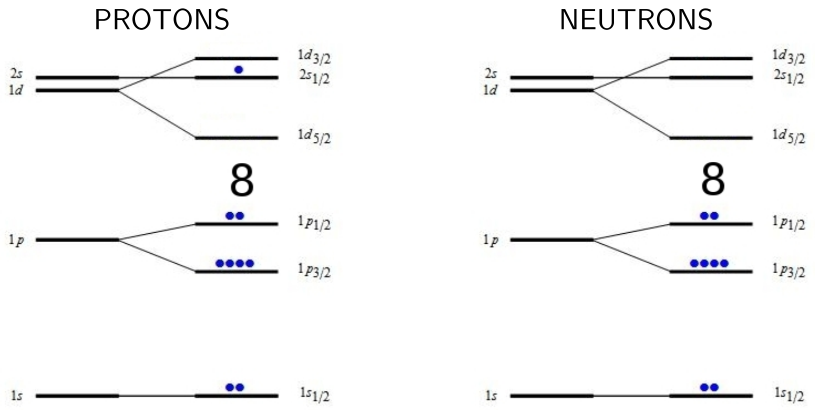




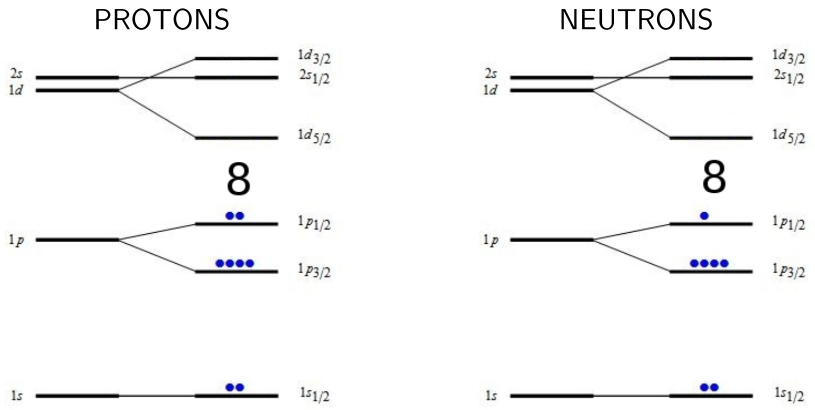
Ground state in ^{17}F



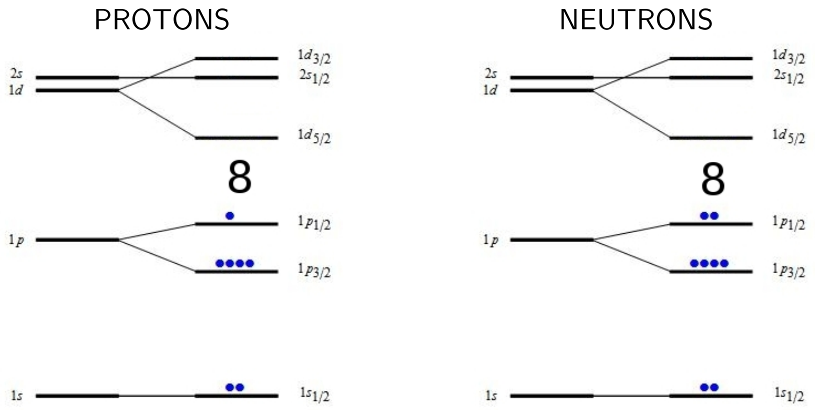
Excited state in ^{17}F



Ground state in ^{15}O



Ground state in ^{15}N



Nuclei near ^{16}O

- If we look closer into excited states near ^{16}O we will see negative-parity states of spin $1/2$ and $3/2$ in ^{17}O and ^{17}F as well as positive-parity states of spin $3/2$ and $5/2$ in ^{15}O and ^{15}N.
- For these states to be explained multi-nucleon configurations have to be considered, including the residual interactions.
- This is going to be done in the next lecture.
- For now we observe that even the extreme single-particle shell model breaks pretty quickly.
- The reason is that the residual interactions are significant and can lead to energy gains comparable to the energies of the shell gap.
- In such a case it may be energetically favoured to promote a nucleon across a shell gap to gain energy from residual interaction despite of the energy increase associated with going into a higher-energy single-particle state.

Cross-gap excitation in ^{17}O