Multinucleon configurations

Introduction to Nuclear Science

Simon Fraser University
Spring 2011

NUCS 342 — January 28, 2011

Outline

1. Beyond the extreme single-particle shell model

Outline

1. Beyond the extreme single-particle shell model
2. Hund's rules

Outline

1. Beyond the extreme single-particle shell model
2. Hund's rules
3. Two-nucleon configurations

Outline

Outline

1. Beyond the extreme single-particle shell model
2. Hund's rules
3. Two-nucleon configurations
4. Contact interactions
5. Pairing

Outline

1. Beyond the extreme single-particle shell model
2. Hund's rules
3. Two-nucleon configurations
4. Contact interactions
5. Pairing
6. The p-n scheme

Beyond the extreme single-particle shell model

- The extreme single-particle shell model considered so far assumed an inert spherical core and a single particle or hole in an orbital outside this core.
- The properties of this single particle/hole define the properties of the ground state and low-energy excited states.
- This model has very limited applicability and can be only expected to work in immediate vicinity of the major shell closures, in nuclei as well as in atoms.
- However, even in the immediate vicinity of the closed shells we observed a break down of the nuclear extreme shell model power to predict the structure of excited states.
- The discrepancies between data and predictions results from neglecting residual interactions. The breakdown of the model indicates that the residual interactions can not be neglected.

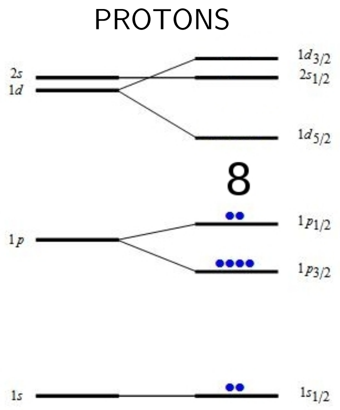
Beyond the extreme single-particle shell model

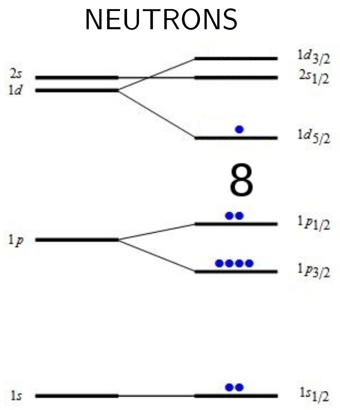
- The residual interaction are key to understanding of nuclear structure.
- All application of the shell model beyond the the extreme single-particle shell model relay on a three step procedure:
  1. First, the one-body Schrödinger equation with a selected nuclear potential is solved and single-particle orbitals are computed.
  2. Next, a configuration space is defined. In this step a choice is made to select "active" and "inert" orbitals. This is a crucial step which determines the computational complexity of the calculations.
  3. Last, the two-body residual interactions are computed within the configuration space defined in the previous step and the final solutions including energies and wave functions are obtained. These solutions are typically complex mixtures of configurations defined in the second step.

Choice of the configuration space for ^{17}O

- In the extreme single-particle shell model for ^{17}O we assumed all proton and neutron orbitals below $N = 8$ as a part of the inert core.
- We also assumed a single neutron in the configuration space consisting of the $d_{5/2}$, $s_{1/2}$ and $d_{3/2}$ orbital (so called *sd*-configuration space).
- This choice results in 3 configurations: $\nu d_{5/2}$, $\nu s_{1/2}$ and $\nu d_{3/2}$.
- Since there are no residual interactions in the extreme single-particle shell model the energy of each of this configuration is defined by the solution of the one-body Schrödinger equation.
- The spin-orbit splitting results in the lowest energy for the $\nu d_{5/2}$, intermediate energy $\nu s_{1/2}$ and the highest energy of the $\nu d_{3/2}$.
- In this configuration space there is the ground state and only two excited states, all positive parity. This is unrealistic and in disagreement with the data.

Choice of the configuration space



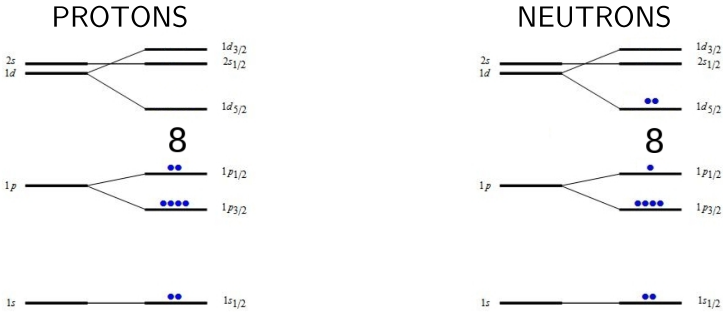


Choice of the configuration space for ^{17}O

- The data indicates a presence of low-energy negative-parity excited states in ^{17}O.
- We discussed a possibility of cross-gap excitation in this nucleus.
- This can prompt us to choose the configuration space differently. For example we can assume all protons and six neutrons in the $s_{1/2}$ and $p_{3/2}$ orbitals as a part of the core.
- This choice results in four active orbitals: $\nu p_{1/2}$, $\nu d_{5/2}$, $\nu s_{1/2}$ and $\nu d_{3/2}$ and three active neutrons. The number of configurations is given by all possible distributions of the three active neutrons between the four active orbitals.
- Neglecting corrections resulting from the fact that only two neutrons can occupy $\nu p_{1/2}$ or $\nu s_{1/2}$ orbitals the number of configurations is $\sim 4^3 = 64$.

Choice of the configuration space: ^{17}O

- The configuration space involving $\nu p_{1/2}$ explains the negative parity states in the excitation spectrum of ^{17}O.
- These are the states with a single neutron in the $p_{1/2}$ orbital and two neutrons above the $N = 8$ shell gap.
- Proper choice of residual interactions should reproduce excitation energy of these states.



Choice of the configuration space for ^{17}O

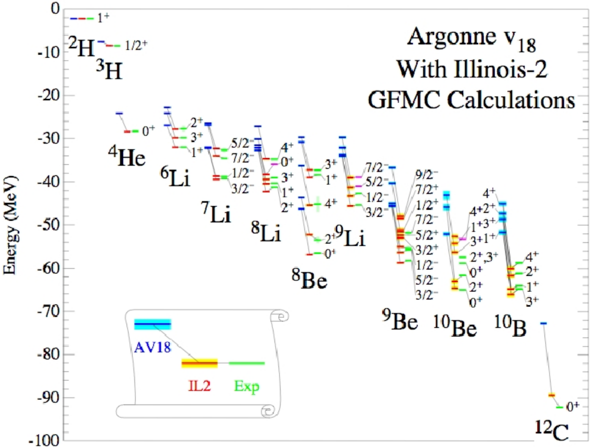
- But we could go further, and consider only the lowest energy neutron $s_{1/2}$ state as a part of the inert core.
- This choice results in five active orbitals: $\nu p_{3/2}$, $\nu p_{1/2}$, $\nu d_{5/2}$, $\nu s_{1/2}$ and $\nu d_{3/2}$ and seven active neutrons. The number of configurations is given by all possible distributions of the seven active neutrons between the five active orbitals!
- Neglecting corrections resulting from restrictions o the number of neutrons in a single orbital the number of configurations is $\sim 7^5{=}16807$!
- And think about what would happen if we allow to break the proton core! The number of configuration would quickly grow further.
- Partial simplification comes from separation of the states according to parity. But this is a reduction by a factor of 2 in the presence of exponential growth.

Configuration space and residual interactions

- On the top of the growing number of configuration, the choice of the residual interaction depends on the choice of active orbitals.
- There are two strategy in dealing with the choice of residual interactions
  1. The empirical shell model relies on a fits of the interactions to selected experimental data. Empirical shell model predictions can be very accurate in limited regions near the fitting points, but usually diverge rapidly when used away from the fitting points.
  2. The ab-initio shell model attempts to derive the residual interactions from the known properties of the nuclear force. The difficulty in this approach results from the hard core in the nucleon-nucleon interactions which leads to computational divergences (infinite energies). Many breakthroughs in this field have been accomplished recently and the ab-initio method are currently a fast developing field. While accuracy of predictions for a single nucleus may not be as good as these given by the empirical models, the global properties are explained in a controlled and systematic way.

The leading edge

- One of the most important recent developments are the no-core ab-initio shell model calculations for light nuclei. So far these can only be done up to ^{12}C but indicate a need for a three-body effective force.



Multi-electron configurations in atoms

- Before we dig deep into multi-nucleon configurations let us step back and look into multi-electron atoms.
- Hund's rules proposed in 1927 identify electron configurations of the lowest energy in case of a number of electrons outside a closed shell. The rules are
  1. The state of the lowest energy has the maximum alignment of individual electron spins (the largest multiplicity) thus the largest total spin $\vec{S}$.
  2. Fulfilling the first rule, the state of the lowest energy is the one with the maximum alignment of individual electron orbital angular momenta, thus the largest total orbital angular momentum $\vec{L}$.
  3. Fulfilling the two above rules the state of the lowest energy for less than a half-filled shell is that of the smallest total angular momentum while for a more than a half-full shell the one with the highest total angular momentum. The total angular momentum is $\vec{J} = \vec{L} + \vec{S}$.

Understanding the Hund's rules

- Two observations explain the first two Hund's rules:
  1. electrons repel each other
  2. electrons obey Pauli's principle.
- Let us consider the simplest two-electron configuration with both particles in the same orbital.
- The maximum spin implies spin triplet coupling which is symmetric under exchange of particles. Since the whole wave function has to be antisymmetric (Pauli's principle) the symmetric spin part implies anti-symmetric spacial part.
- The anti-symmetric spacial part implies that electrons are never in the same place or on average are far from one another. This is a preferred configuration due to electrostatic repulsion.

Understanding the Hund's rules

- On the contrary to rule one, the anti-symmetric spin singlet coupling implies a symmetric spatial part with a probability of electrons being at the same place. This is the configuration of higher energy due to the electrostatic repulsion.
- A similar argument can be used to explain the second rule. Indeed, if electrons have a maximum alignment of the orbital angular momentum they orbit in the same direction and can stay away from each other without crossing their paths. This is a preferred configuration taking into account the electrostatic repulsion.
- On the contrary, a minimum alignment of the orbital angular momenta implies that electrons are orbiting in the opposite directions, thus often cross each other. At the point of crossing there is a strong electromagnetic repulsion which results in a higher energy of such a state.

The $\vec{L}\vec{S}$ and $\vec{J}\vec{J}$ coupling

- Hund's rule imply the $\vec{L}\vec{S}$ coupling in multi-electron atoms. This means that the spin of electrons couple first to the total spin $\vec{S}$, next the orbital angular momenta of electrons couple to the total angular momentum $\vec{L}$ and last the total spin $\vec{S}$ and the total orbital angular momentum $\vec{L}$ couples to the total angular momentum $\vec{J}$.
- This is not what happens in nuclei. Due to the spin-orbit splitting the spin of a nucleon $\vec{s}$ couples first to its orbital angular momentum $\vec{l}$ forming the individual total angular momentum $\vec{j}$, then the individual total angular momenta $\vec{j}$ couple to the total angular momentum $\vec{J}$.
- Despite of this difference there are similarities and understanding of Hund's rules is relevant.

Relevance of the Hund's rules to the nuclear case

- The relevance of the Hund's rules to the nuclear case comes from the fact that nucleons are fermions, they obey Pauli's principle and arguments based on the spin coupling and antisymmetrization of the wave function are valid.
- The important difference is that the electromagnetic force between electrons is repulsive, but the residual interactions between nucleons in nuclei are attractive.
- From that difference follows the fact that in nuclei the state with anti-symmetric spin wave function (the singlet spin 0 state) and symmetric spacial wave functions are strongly favoured for two-nucleon configuration.
- As a consequence all nuclei with even number of protons and even number of neutrons have the ground state of spin zero and positive parity.

Angular momentum coupling in two-nucleon configuration

- Let us explore the coupling of angular momentum of two identical nucleons in the same orbital.
- This is the simplest multi-nucleon configuration beyond the extreme single particle shell model.
- Of the key importance of the shell model extension is a recognition of the way the total angular momentum couples in such a configuration.
- Since total angular momenta $\vec{j_1} = \vec{j_2} = \vec{j}$ are vectors, any value between 0 and $2\vec{j}$ is in principle possible.
- But the consequence of the quantization of the total angular momentum as well as the Pauli principle is that only even spins are allowed in such configurations.
- One way to show it is to analyze the coupling using the M-scheme.

The M-scheme for identical nucleons in the same orbital

Table 5.1 *m scheme for the configuration* $|(7/2)^2 J\rangle^*$

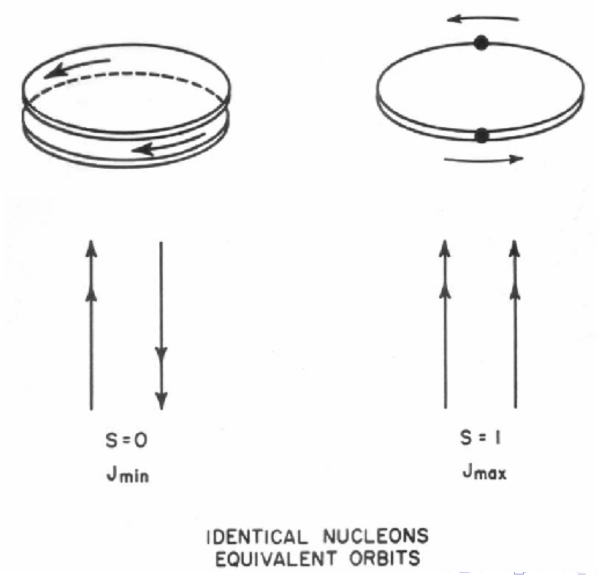
$j_1 = 7/2$ m_1	$j_2 = 7/2$ m_2	M	J
7/2	5/2	6	
7/2	3/2	5	
7/2	1/2	4	
7/2	−1/2	3	6
7/2	−3/2	2	
7/2	−5/2	1	
7/2	−7/2	0	
5/2	3/2	4	
5/2	1/2	3	
5/2	−1/2	2	4
5/2	−3/2	1	
5/2	−5/2	0	
3/2	1/2	2	
3/2	−1/2	1	2
3/2	−3/2	0	
1/2	−1/2	0	0

* Only positive total M values are shown. The table is symmetric for $M < 0$.

Angular momentum coupling in two-nucleon configuration

- The M-scheme shows that only even integer spin states are allowed from coupling of two nucleons of the same type occupying the same state.
- The maximum total angular momentum in configuration with two nucleons in an orbital with total angular momentum of j is $2j - 1$. The minimum is 0.
- Coupling to different even integer spins implies different mutual orientation of total angular momenta of the individual nucleons.
- In a semi-classical analogy the plane of the orbit for a nucleon is perpendicular to the vector of the orbital angular momentum.
- Therefore states coupled to different value of the total angular momentum represent various degree of overlap of the probability distribution for individual nucleons.

Angular momentum coupling in two-nucleon configuration

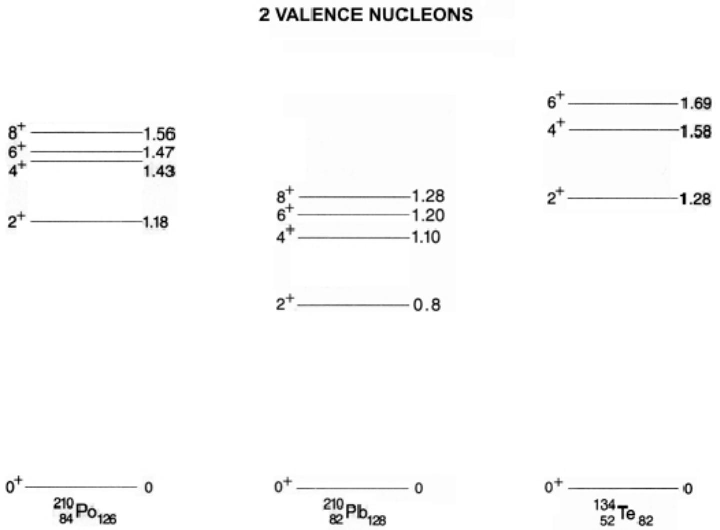


Angular momentum coupling in two-nucleon configuration

- Let us analyze an example of two nucleons in the $g_{7/2}$ orbit.
- The M-scheme depends on the total angular momentum only, therefore the M-scheme for the $g_{7/2}$ is the same as for the $f_{7/2}$ we investigated already.
- The M scheme we investigated implies that the total angular momenta from the coupling are 0^+, 2^+, 4^+ and 6^+.
- In the absence of the residual interactions all these states would have the same energy, equal to twice the energy of the $g_{7/2}$ state. That would be a prediction of the extreme single particle shell model.
- But in nature they do not! Let us look into the data. $^{134}_{82}\mathrm{Te}_{52}$ has a configuration of two protons in the $g_{7/2}$ shell outside a doubly-magic $^{132}\mathrm{Sn}$ core.

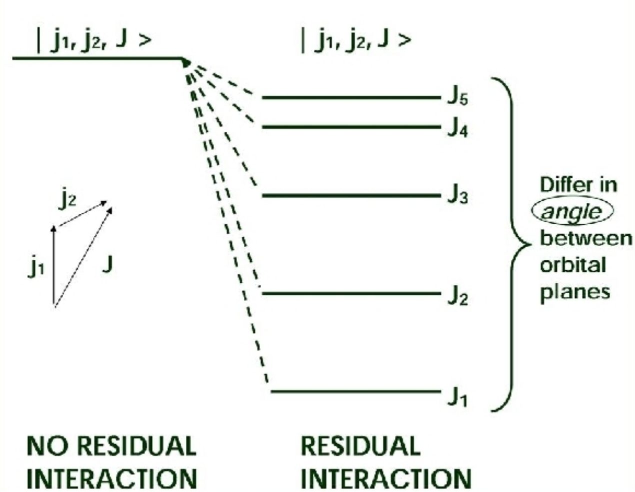
Low-energy excitations in $^{134}_{82}\mathrm{Te}_{52}$

Two-nucleon configurations near doubly-magic nuclei



The pattern

For same nucleons in a single orbit $J_1 = 0^+$, $J_2 = 2^+$, $J_3 = 4^+$, etc.



Contact (delta) interactions

- The pattern we see is that for same type of nucleons in the same orbital the energies of states resulting from the coupling are ordered according to spin, with state of spin 0^+ being the lowest in energy.
- Moreover, the gap between the 0^+ ground state and the first excited 2^+ state is larger than between the 2^+ state and the 4^+ state etc.
- Truly, it can be shown that the energies of the states are correlated with the effective angle between individual total angular momenta of the nucleons.
- This can be easily explain by a residual interactions called contact (or delta) interaction.
- To explain the observe excitation pattern the nuclear residual contact interaction has to be attractive.

Contact (delta) interactions

- Contact interaction assume that the nucleons interact only when they are at the same position.
- This is consistent with the short range of nuclear force, which is a good thing.
- The name delta interactions come from a mathematical operator which is used to incorporate the contact interaction into the Schrödinger equation. This operator is called the Dirac delta operator and in three dimensions it is

$$\delta(\vec{r_1} - \vec{r_2}) = \begin{cases} 1 & \text{for } \vec{r_1} = \vec{r_2} \\ 0 & \text{for } \vec{r_1} \neq \vec{r_2} \end{cases} \tag{1}$$

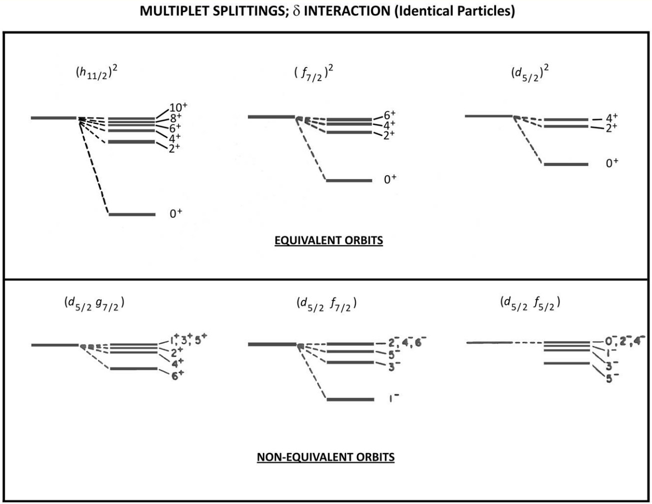
- The contact interactions can be then represented as

$$V_{res}(\vec{r_1}, \vec{r_2}) = -V_R \delta(\vec{r_1} - \vec{r_2}) \tag{2}$$

Extension to other two-nucleon configurations

- Contact interactions extend applications of the shell model to two-nucleon configurations in the same orbit. That is good!
- Truly application of contact interactions is broader, they work reasonably well for two nucleons in different orbits as well.
- For two nucleons in different orbits or two nucleons of different type in the same orbit all couplings of the total angular momenta from $\vec{j_1} - \vec{j_2}$ to $\vec{j_1} + \vec{j_2}$ are allowed since there is no restriction from the Pauli principle.
- The energy shifts of the levels due to the residual interactions depend on the spatial overlap of the wave functions of the interacting nucleons. Large overlap implies a large energy shift down.

Contact interactions in two-nucleon configuration



Energy shifts for a δ-function residual interaction for identical nucleons in several different orbit combinations

Finite range interactions

- If everything looks good there must be something terribly wrong going on.
- Indeed, let us examine the impact of the Heisenberg principle

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \tag{3}$$

on the contact interactions.

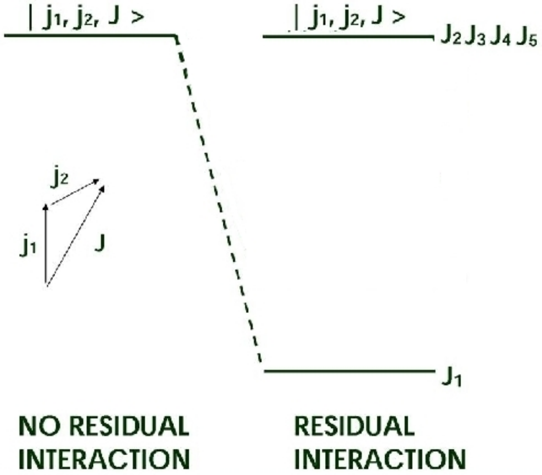
- On the contact $\Delta x = 0$ and this implies $\Delta p_x = \infty$.
- This is clearly not right.
- To correct that deficiency finite range interactions have been developed which interact on the short range but not on contact.
- While the details of the calculations with the finite-range interactions differ from that done with contact interactions, the gross patterns in energy spectra are the same.

Pairing interactions

- The computational overhead of calculations with contact forces is significant and increases rapidly with increasing number of orbitals in the configuration space and number of active nucleons.
- To handle this situation another set of residual interactions called pairing interactions has been developed.
- Pairing interactions lowers in energy a state of two nucleons of the same type in the same orbital coupled to 0^+ but does not impact any other couplings.
- One can look at the pairing interactions as a "poor man" approximation to the contact δ interaction.
- But residual pairing interactions explain a lot of important observations. For example, the fact that nuclei with even number of protons and neutrons have a ground state of spin 0 and positive parity.

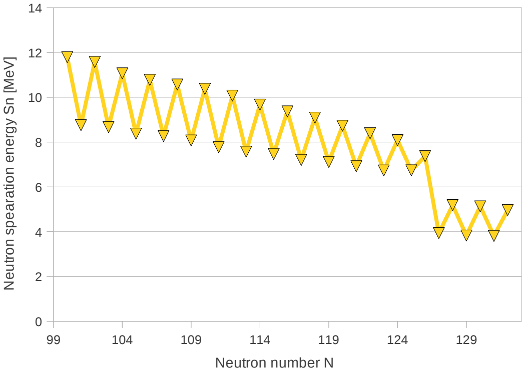
Pairing interactions

For pairing interactions $J_1 = 0^+$, any other couplings are not effected.



Pairing interactions

- Pairing interactions explains staggering in binding energies between nuclei with even or odd number of nucleons.
- For the odd nucleon, there is no pairing interactions and no lowering of a pair in energy, thus the energy is larger.



The p-n interaction

- So the nucleons of the same kind form pairs of spin/parity 0^+ which are shifted lower in energy, thus favoured.
- What about the proton-neutron interactions?
- Data suggest a significant role of this interactions. Proton-neutron residual interactions results in configuration mixing and leads towards deformation of nuclear shapes.
- Note that a state of spin 0 has a spherical symmetry, thus pairing of like nucleons drives towards spherical shapes.
- For that reason doubly- and semi-magic nuclei with only one type of valence nucleons have spherical shapes.

Excitation energy of the first excited state near $Z = 50$

Energy of the first excited 2_1^+ state is a measure of shape deformation (large energy-small deformation, small energy - large deformation).