PC 4421 Lecture 1: Nuclei and Nuclear Forces

Nuclei and Binding Forces

A nucleus is a bound system composed of one to about three hundred strongly-interacting fermions of two distinct types, protons and neutrons. The forces between these nucleons consist of strong nuclear forces and, for protons, Coulomb electrostatic repulsion. The number of nucleons is too small for statistical approaches to be any more than a rough approximation and the strength of the binding forces is too large for perturbative approaches to be useful. The nucleus is a complex and difficult system to study. Modelling is often used; in a particular model the aim is to describe a subset of the observed phenomena within a simplified context incorporating a subset of the available degrees of freedom. This modelling also has a distinct interpretation within quantum mechanics (see later) which is essential to describe the system.

Nuclear Sizes

Within the context of the nucleus, what is meant by size depends on how the spatial extent is being measured. This might result in a dimension associated with either the charge or the matter distribution within the nucleus. Measurements of either distribution generally result in a simple parameterisation, $r=r_oA^{1/3}$, where A is the number of nucleons and r_o is a constant

Charge distributions are easily measured by electromagnetic probes such as electron scattering:

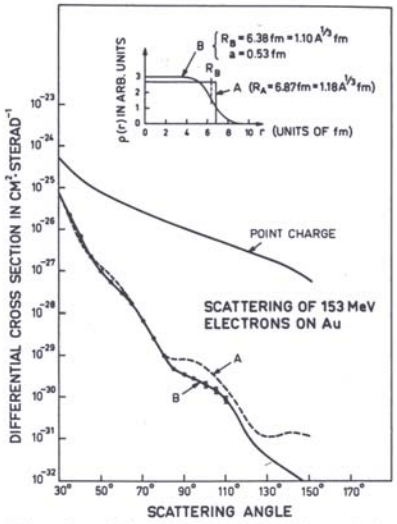


Figure 2-1 The experimental data and the theoretical analysis are taken from B. Hahn, D. G. Ravenhall, and R. Hofstadter, *Phys. Rev.* **101**, 1131 (1956); D. R. Yennie, D. G. Ravenhall, and R. N. Wilson, *Phys. Rev.* **95**, 500 (1954); R. Herman and R. Hofstadter, *High Energy Electron Scattering Tables*, Stanford Univ. Press, Stanford, California, 1960. We wish to thank G. Jacob for help in the preparation of the figure.

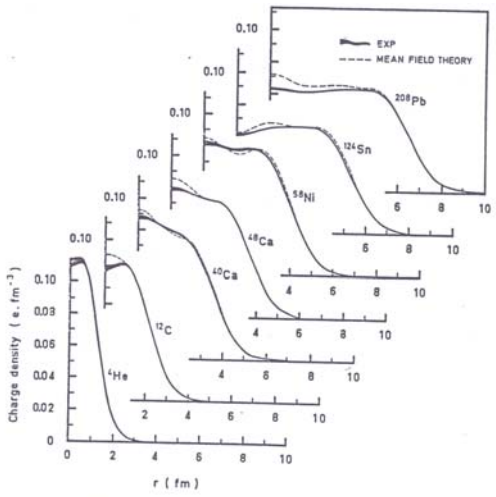


Fig. 7 – Nuclear ground state charge distributions[33])

Nuclear effects on atomic electrons can cause shifts in the spectral lines from which differences in nuclear radii can be obtained (isotope shifts). The energies of X-rays in atoms formed with muons instead of electrons can also be sensitive to the charge radius.

In general, measurements yield a value for r_0 between 1.2 and 1.25 fm.

Matter distributions are generally measured by probes which interact with the strong nuclear force in processes such as nuclear scattering, α decay and in X-rays from pionic atoms. For nuclei close to stability, it is found that the difference between matter and charge radii is of the order of 0.1 fm. Along the line of stability, nuclei have more neutrons than protons, but the Coulomb repulsion between protons and the proton-neutron attraction tend to pull the protons out to give similar radii. Away from stability, on the neutron-rich side, neutrons may become so weakly bound that they wander outside the rest of the nucleus in HALO nuclei. For example, ^{11}Li has a spatial extent which is very similar to a ^{208}Pb nucleus!

Nuclear Masses

Nuclei, within the drip lines, are bound systems: $m_{nucleus} < Nm_{neutron} + Zm_{proton}$.
Nuclear mass has contributions from the nucleons, and both the nuclear and electrostatic forces within the system. *See second and third year nuclear courses and revise the liquid drop model of nuclear masses.*

Angular Momentum and Parity

Nucleons are fermions and have a half-integer intrinsic spin. In addition, they move inside the nucleus relative to the centre of mass and therefore can generate orbital angular momentum.
In quantum mechanics, the orbital angular momentum eigenfunctions satisfy the following eigenvalue equations:

$$\hat{L}^2 Y_{\ell m_\ell} = \ell(\ell+1)\hbar^2 Y_{\ell m_\ell} \text{ and } \hat{L}_z Y_{\ell m_\ell} = m_\ell \hbar Y_{\ell m_\ell} \text{ where } -\ell \le m_\ell \le \ell .$$

So the total angular momentum and its projection on one axis have definite values. In such a situation, ℓ and m are said to be good quantum numbers and turn out to be integers only
The intrinsic spin is also characterised by similar eigenvalue equations:

$$S^2 \mathrm{X}_{sm_s} = s(s+1)\hbar^2 \mathrm{X}_{sm_s} \text{ and } \hat{S}_z \mathrm{X}_{sm_s} = m_s \hbar \mathrm{X}_{sm_s} \text{ where } -s \le m_s \le s .$$

In general, the quantum numbers, s and m_s, can be integer or half-integer. In the case of nucleons, $s=½$.

Coupling these two angular momenta vectorially will give the total nucleon angular momentum:

$$\mathbf{j}=\boldsymbol{\ell} \otimes \mathbf{s}$$ (The symbol $\otimes$ should be read as "coupled to").

The resulting coupled representation has eigenvalue equations:

$$\hat{J}^2 \varphi_{j\ell} = j(j+1)\hbar^2 \varphi_{j\ell} \text{ and } \hat{J}_z \varphi_{j\ell} = m\hbar \varphi_{j\ell} \text{ where } -j \le m \le j .$$

Here the coupled wavefunction is constructed using Clebsch-Gordan coefficients:

$$\varphi_{j\ell} = \sum_{m_\ell m_s} < l m_\ell s m_s \mid j m > Y_{\ell m_\ell} \mathrm{X}_{sm_s}$$

The total nucleon angular momenta themselves couple to give the total spin of the nucleus as a whole, ***J***. *See third year quantum mechanics and revise how to add two angular momenta together.*

The angular momentum is generated by the individual components of the nucleus, the nucleons. It is sometimes useful to think about angular momentum being generated in more macroscopic or liquid-drop pictures. For example, orbits of individual nucleons can fluctuate and sum together in such a way as to generate a non-spherical matter distribution which appears to rotate in space. The angular momentum can be usefully thought of as being generated by the rotation of the deformed nuclear shape as a whole (see the second half of this course), but it is still in reality being generated by the individual nucleons themselves. The rotational angular momentum cannot be larger than that generated by the nucleons themselves i.e. $\mathbf{R} \le \sum \mathbf{j}$. Here the summation sign means "coupled together" all the individual nucleon momenta, **j**. Often rotational bands can undergo an abrupt disruption to the usual rotational I(I+1) sequence when the individual nucleon angular momentum in a particular configuration is exhausted, a so-called band termination. In order to generate more angular momentum, the nucleons must be redistributed in a configuration with more available angular momentum, for example, by exciting one into a single-particle orbital with a higher j.

In a similar fashion, the parity of a nuclear state is the product of all the individual single-nucleon parities.

Electromagnetic Properties

Both nucleons have an individual magnetic moment and move inside the nucleus, and protons also carry charge. A nucleus therefore has an internal distribution of both charge and current and can be expected to be characterised by electromagnetic moments. These can interact with both real applied fields and with the electromagnetic vacuum in γ decay.

Electromagnetic Multipole Moments

The electric or magnetic fields associated with any arbitrary charge or current distribution can be described as the sum of a series of multipoles each with a characteristic spatial dependence:

E= charge (L=0) *term in $1/r^2$ + dipole (L=1) * term in $1/r^3$ + quadrupole (L=2) * term in $1/r^4$+…..
M= dipole moment * term in $1/r^3$ + quadrupole moment * term in $1/r^4$+…..

For magnetic fields the magnetic monopole either does not exist or it is extremely rare, so the first term in the expansion does not exist.
For simple distributions the series terminate abruptly. For example, a sphere of charge just had an electric monopole term, a circular current loop purely a magnetic dipole term. Small distortions from sphericity introduce higher-order multipoles. The first evidence for non-spherical nuclear shapes came from the observation of anomalously large electric quadrupole moments.

Each multipole has an operator, $\hat{O}$, associated with it that has a definite parity, i.e. a characteristic behaviour under the transformation **r**→-**r**. Electric moments have parity $(-1)^L$; magnetic moments have parity $(-1)^{L+1}$.

Excited States

Rearrangement of the internal structure of a nucleus will generate states of motion with more energy than the minimum the system can accommodate. These excited states are characterised by their excitation energy and spin-parity, as well as other, often only approximately, good quantum numbers. This rearrangement can easily visualised as changes in individual nucleon motion, but can also be viewed as changes in bulk motion of the nucleus such as rotation and surface vibration, *see second half of this course.*

Transition probabilities, decay rates, reaction cross sections, spectroscopic factors and other things.

Remember that this is an introductory course so there's plenty of more stuff to learn about!

Forces between Nucleons

(a) Nuclei exist, despite the electrostatic repulsion between protons. There must be an ***attractive force stronger than electromagnetic forces,*** at distances corresponding to the separation of nucleons in the nucleus, to hold the system together. This is the ***strong nuclear force.***

(b) Nuclei have small radii, r=1 to 10fm and atomic/molecular phenomena do not need large nuclear corrections suggesting that the nuclear force is a relatively ***short-range force***

(c) Measurements of the energy needed to rip out a nucleon from a nucleus as a function of the number of nucleons in the nucleus, i.e. the binding energy per nucleon, rise rapidly up to A~10-20 and then level off at approximately 7.5 MeV/nucleon.

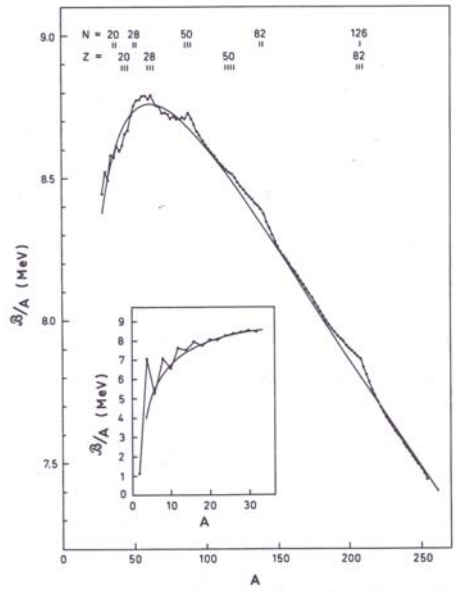


Figure 2-4 The experimental binding energies are taken from the compilation by J. H. E. Mattauch, W. Thiele, and A. H. Wapstra, *Nuclear Phys.* **67**, 1 (1965). The smooth curve represents the semi-empirical mass formula, Eq. (2-12), with the constants given by A. E. S. Green and N. A. Engler, *Phys. Rev.* **91**, 40 (1953).

If we assume that a nucleon interacts with ALL the other nucleons in the nucleus then there should be A(A-1)/2 pairs of nuclei. Since the binding energy increases with the number of interactions BE ~ A(A-1)/2. Then BE/A would be linear, which it is but only roughly up to around A~10.
The binding energy curve suggests that nucleons only interact with their nearest neighbours. The range of the force must be less than the size of a mass-10 nucleus, which is around $1.2 \times 10^{1/3} =$ 2.6 fm. This property is described as ***saturation of the nuclear force.*** It means that nucleons appear to bind rather like they were Velcro© covered balls.

(d) In the situation where the binding force saturates, the volume of a nucleus is proportional to the number of nucleons. The nuclear density in the interior should be pretty constant, in agreement with experimental measurements. Nucleons do not get squashed or overlap or coalesce. So something must prevent this squashing. ***The nuclear force has a hard repulsive core at small distances less than the size of a nucleon ~0.5 fm.*** *At least this is true at temperature and densities in normal nuclei. At very high energies and densities expect breakdown of individual nucleons into a quark-gluon soup….see Nuclear Reactions course.*

(e) The energy levels of *mirror nuclei* are very similar after correction of the different Coulomb energies. These nuclei are the same, but all protons are turned into neutrons and visa versa. All n-n pairs become p-p pairs; all p-p pairs become n-n. The n-p pairs become p-n, so there is no difference between the two mirrors in terms of p-n. The similarity of experimental energy levels and masses (after small corrections for Coulomb forces and the proton/neutron mass difference) suggest that the n-n and p-p forces have to be very similar in strength. ***Nuclear forces are said to be charge symmetric***

(f) You cannot say from mirror nuclei anything about n-n and p-p forces compared to n-p forces. But if you gradually change the individual nucleon types, one by one, into the other you generate a series of nuclei with the same mass, but a range different numbers of protons and neutrons. To make a fair comparison for the strong interactions, you can again correct for the Coulomb effects and the difference in the proton and neutron masses.

For example, the 0^+ ground states of ^{30}Si and ^{30}S, and an excited 0^+ state in ^{30}P are at a very similar mass-energy. The 2^+ states of ^{30}Si and ^{30}S also have an *isobaric analogue* in ^{30}P, as do other levels. Transition probabilities and reaction rates based on strong interactions involving these states also show similarities.

Consider what changes in going between $^{30}_{14}\mathrm{Si}_{16}$ and $^{30}_{15}\mathrm{P}_{15}$. A neutron turns into a proton. In terms

of the forces, initially there are 15 n-n and 14 n-p pairs. Finally there are 14 p-p and 15 n-p pairs. We already know that the n-n and p-p forces are similar. So the experimental similarity of the ^{30}Si level scheme with a subset of states in the ^{30}P level scheme must imply that the n-p force must also be of similar strength. ***Nuclear forces display charge independence.*** *There are other states in ^{30}P which are not isobaric analogue states, they must be somehow different in nature. These can be understood using so called isospin formalism, which will come later given time.*

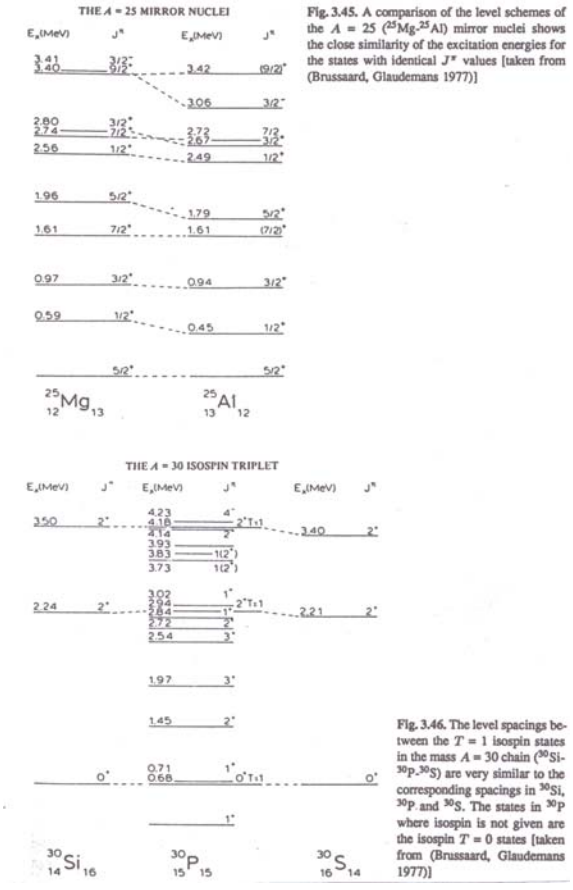


Fig. 3.45. A comparison of the level schemes of the $A = 25$ (^{25}Mg-^{25}Al) mirror nuclei shows the close similarity of the excitation energies for the states with identical J^π values [taken from (Brussaard, Glaudemans 1977)]

Fig. 3.46. The level spacings between the $T = 1$ isospin states in the mass $A = 30$ chain (^{30}Si-^{30}P-^{30}S) are very similar to the corresponding spacings in ^{30}Si, ^{30}P and ^{30}S. The states in ^{30}P where isospin is not given are the isospin $T = 0$ states [taken from (Brussaard, Glaudemans 1977)]

Now we know something about nuclear forces. If you knew something about nucleon-nucleon scattering you could confirm these points and learn more about spin dependence and other features (*see Nuclear Reactions and recommended texts*).

Naively we should be able to use this force in the Schrodinger equation and start calculating the wavefunctions of nuclei. This would be analogous to how atoms are understood, where electrons are put into a potential governed by the Coulomb force.

A single proton, ^{1}H, or neutron, are the simplest nuclei with only one nucleon. Excited states involve internal excitation of the quarks inside the protons and neutrons so here you need a particle physics course.

The next simplest bound nucleus is ^{2}H, the deuterium nucleus or the deuteron. So we can take the proton-neutron force and try to calculate its properties.

PC 4421 Lecture 2: The Deuteron

Experimental Data

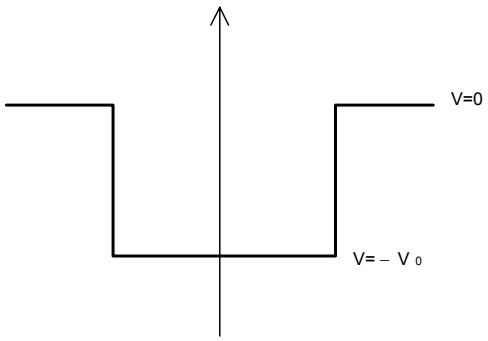
Photodisintegration of the deuteron: γ + d → p + n
Threshold energy for photon is 2.224(2) MeV. Detailed analysis of reaction products suggests that the deuteron ground-state spin-parity is 1^+. Electron scattering measures the separation of p-n to be 2.1 fm. No bound excited states are observed (unbound resonances in proton-neutron scattering are seen).

Deductions

The binding energy of the deuteron is 2.224(2) MeV i.e. BE per nucleon is only 1.112 MeV. Combined with the lack of excited states, this suggests that the binding is very weak.

Calculation

From what we know about nuclear forces, can we deduce a form for the potential between n and p in the deuteron, solve the Schrodinger equation for it and therefore describe and understand its nuclear structure? We know that nucleons act a bit like solid balls held together with Velcro©. The force should be zero a long way away, and then when they come close they stick together and bind, reducing their potential energy. If we choose to ignore the hard repulsive core the potential looks like a simple square well. Second year quantum then gives the answers, so ignoring the hard core makes life easy at this stage and we can look at the calculation compared to experimental results and see how good this approximation is.



Schrodinger equation:

$$\left[-\frac{\hbar^2}{2m_p}\nabla_p^2-\frac{\hbar^2}{2m_n}\nabla_n^2+V_{pn}(r_p,r_n)\right]\Psi=E\Psi$$

Transform to centre of mass frame:

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2+V(r)\right]\varphi=E\varphi$$

where *r* is the separation, μ reduced mass.
Assume solution of the form:

$$\varphi=\frac{u(r)}{r}Y(\theta,\phi)$$

Substitute and separate the variables *see S3 Mathematical Physics and Quantum courses.*

Simplification: the force on the nucleon is (for now anyway) directed towards the other nucleon. In the CM frame it is always towards the centre of mass. This is the definition of a *CENTRAL POTENTIAL*. For example, force that the Earth experiences is always towards the Sun and the CM is on the line joining the Earth and Sun. In classical physics, motion in a central potential is always characterised by orbital angular momentum conservation.

In quantum mechanics, the wavefunction is an eigenfunction of the orbital angular momentum operator and ℓ is a good quantum number. So the angular equation formed after separation must have solutions which are angular momentum eigenfunctions. Such functions $Y_{\ell m}$ are the spherical harmonics, which have parity $(-1)^{\ell}$. You need to remember that Y_{00} is actually spherically symmetric and has no angular dependence, others you might need to look up or expect to be given. The angular equation resulting from the separation turns out to look like:

$$\hat{L}^2 Y_{\ell m}(\theta,\phi) = \ell(\ell+1) Y_{\ell m}(\theta,\phi)$$

The radial equation is

$$-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2} + \left[V(r) + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1)\right]u(r) = Eu(r)$$

where:

$$V(r) = -V_o \qquad 0 < r < R$$
$$= 0 \qquad elsewhere$$

The second term in the square brackets is known as the *centrifugal term,* and works in the opposite sense to the binding potential, *V(r)*, implying that the most bound state should have ℓ=0.

Written with this way, E<0 are bound states and E>0 are unbound. Just consider the ground state for now, and assume it is bound:

$$-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2} + V(r)u(r) = -|E|\,u(r)$$

For r>R: $-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2} = -|E|\,u(r)$ with solutions $u = Ce^{k_2 r} + De^{-k_2 r}$ where $k_2 = \sqrt{\frac{2\mu|E|}{\hbar^2}}$

and since we require $u(r) \longrightarrow 0$ as $r \longrightarrow \infty$, $C=0$.

For r<R: $-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2} = (V_0 - |E|)u(r)$ with solutions $u = A\sin k_1 r + B\cos k_1 r$ where

$$k_1 = \sqrt{\frac{2\mu(V_0 - |E|)}{\hbar^2}}$$

Since wavefunction is actually u(r)/r we need B=0 to keep wavefunction finite as $r \longrightarrow 0$.

At the boundary between these two regions we need both *u(r)* and *du(r)/dr* to be nice continuous functions otherwise we run into trouble (see note at end), so match them at r=R:

$$De^{-k_2 R} = A\sin k_1 R$$
$$-Dk_2 e^{-k_2 R} = Ak_1 \cos k_1 R$$

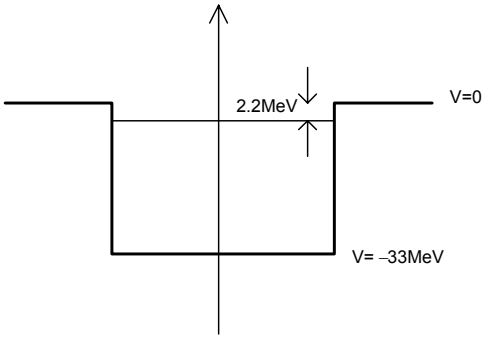
and dividing these equations gives: $-k_2 = k_1 \cot k_1 R$

This is the final equation for the ground-state of the deuteron. It is a relationship between μ ~ 931.5 / 2 MeV |*E*|, which is the magnitude of the binding energy which we know to be 2.224 MeV, and *R,* the separation of the proton and neutron which is also known to be 2.1 fm. The only unknown is the depth of the potential, V_0. This can be solved numerically to show that V_0 ~ 33 MeV.

Hint: Divide both sides by k_1 and rewrite equation in the form $\tan bx = -x$, solve by plotting y=tanbx and y=-x on the same graph and find intersection. Or use some other fancy numerical method!

Inferences:

The binding energy of the deuteron, 2.224 MeV, is small in comparison with the well depth, 33 MeV



Also since we now can find k_1 and k_2 , the wavefunction is fully defined, apart from the constants *A* and *D* which can be found by requiring a normalised wavefunction. Then we can calculate the properties of the deuteron. For example, electromagnetic multipole moments.

Electric Quadrupole Moment of the Deuteron

The electric quadrupole moment is given by:

$$\langle Q \rangle = \int \rho_E \left(3z^2 - r^2\right) dV \quad classically$$
$$= Ze \int \varphi^* \left(3z^2 - r^2\right) \varphi \; dV \quad quantum$$

Substitute in the wavefunction and integrate. Or notice that the wavefunction is spherically symmetric since the ground state has ℓ=0. This would just give a spherically symmetric charge density, which would give an electric field outside the nucleus which is identical to that of a point charge. Since the multipole expansion of a field looks like this, $\mathbf{E} = a\mathbf{E}_{\text{point charge}} + b\mathbf{E}_{\text{dipole}} + c\mathbf{E}_{\text{quadrupole}} + d\mathbf{E}_{\text{octupole}} + \ldots\ldots$, it is obvious that the quadrupole moment is actually zero for the calculated wavefunction.

When the actual deuteron quadrupole moment was measured it caused a huge stir as it indicated that nuclear physics was not going to be as easy as that of other systems like atoms. The observed moment is 0.00288(2) barns. So what are we missing?

We require a non-spherical component with positive parity to get a non-zero quadrupole moment i.e. a small component proportional to Y_{2m} i.e. ℓ=2. The wavefunction has to look something like: $\varphi = a\varphi_{\ell=0} + b\varphi_{\ell=2}$, in other words the orbital angular momentum is not precisely conserved!

The nuclear force must have a small non-central or tensor component

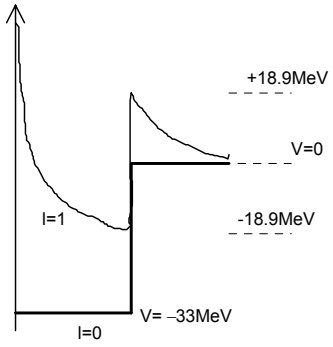
Excited States of the Deuteron

Add in the centrifugal term to the 33 MeV deep square well:

For ℓ=1 at r=R $\dfrac{\hbar^2\ell(\ell+1)}{2\mu R^2}=\dfrac{197\times1\times2}{2\times465\times2.1^2}=18.9$ MeV.

[Always work in units of distance in fm, energy in MeV, mass in MeV/c^2, momentum in MeV/c and use $\hbar c$=197 MeV.fm, then things will turn out in nice units. Practise it and get the answer above. You might sometimes need to also use $e^2/4\pi\varepsilon_o=\hbar c/137$, if electronic charge is in the formula (not needed here!).]

The combined potential for ℓ=1 is a sum of the square potential and a $1/r^2$ potential. Compared to the ℓ=0 potential it looks something like this:



It is much shallower than for ℓ=0 and is narrower. Recall from simple quantum mechanics that shallower wells result in states with higher energy. Here the state goes up and over the top and becomes an unbound ℓ=1 state, or resonance, which can be seen in p-n scattering.

Spin Coupling in the Deuteron

Reminder: two nucleons each with ℓ=0, have intrinsic spins s_1 and $s_2=\frac{1}{2}\hbar$. The two intrinsic spins couple vectorially to give a total intrinsic spin $\mathbf{S}=\mathbf{s_1}\otimes\mathbf{s_2}$, the results of which are either $S=s_1+s_2$, s_1+s_2-1, s_1+s_2-2,……,$|s_1-s_2|$. In other words, S=0 or 1 for the combined ℓ=0 nucleon system. The S=0 has one substates with S_z=0 and is therefore known as a *singlet state.* The S=1 has three substates with S_z=+1, 0 and −1 and is known as a *triplet state.*

Ground state of n+p is ℓ=0 and is known experimentally to have a spin-parity of 1^+. In other words the ground state is a spin triplet state and spins of the two nucleons must be coupled "parallel" to get this total angular momentum i.e. S=1.

The other coupling of spins, the singlet state S=0, results in an ℓ=0, $I=0^+$ state. But where is this? It is found as an unbound resonance in pn scattering and not as a bound excited state of the deuteron.
Our simple approach so far would say that both singlet and triplet states would have the same energy.
We have no terms which depend on spin in our potential between two nucleons.

The difference in energies suggests that ***nuclear forces depend on the spin orientations.***

Summary so far:

What we did:

(a) Got info about nuclear forces from simple observables like radii, binding energies etc.
(b) Guessed a potential for the n-p system on the basis of this info

(c) Calculated the wavefunction of the deuteron
(d) Inferred more things about nuclear forces

What we now know about nuclear forces:

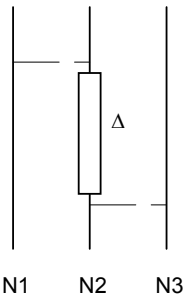
(a) Lowest order attractive central potential depending on nucleon separation
(b) Charge symmetric: n-n same strength as p-p
(c) Charge independent: all n-n, p-p and n-p are the same strength
(d) Repulsive hard core at small distances
(e) Spin dependence of the form $V_s(r)\mathbf{s_1.s_2}$
(f) Small non-central, "tensor" component

You can also learn more from scattering experiments e.g. depends on relative momentum of nucleons.
Go on and refine method: use the force to calculate a potential, solve Schrodinger equation, and calculate wavefunctions, energies and other properties with progressively more sophisticated forces. So far the BEST formulations of the nucleon-nucleon force can calculate up to mass-10 nuclei to a reasonable comparison with experimental information. [S. Peiper and R. Ringo, Argonne National Lab]

Complications:

The many-body problem leads to complexity: ^{6}Li composed of three protons and three neutrons takes 40hours processing on desktop PC, but ^{10}Be, with four protons and six neutrons, takes 9000 hours on a large farm of parallel processors.

There are complicated in-medium effects such as three-body forces. To illustrate what a three-body force is, imagine the system made up of the Earth, the Moon and a satellite, and you have the problem of calculating the motion of the satellite. You could separate the force on the satellite into that due to the Earth and that due to the Moon and sum the two. But the presence of the Moon causes tidal bulges on the Earth, which affect the force between the Earth and the satellite. Three-body effects are modifications to two-body forces due to the presence of a third body. In a nucleus, the force between two nucleons, N_1 and N_2, is modified by the presence of a third, N_3. Before N_1 and N_2 interact, N_2 is excited into a delta resonance. N_1 actually interacts with a Δ not a nucleon. The interaction of a delta with a third nucleon is different from that between two nucleons as the delta resonance has a different spin to the nucleon ground state and therefore exerts different forces.



Three-body effects are difficult to isolate experimentally. They can only really be inferred from the comparison of experiment with calculations with and without them. For example, the calculations referred to above suggest that ^{4}He is under bound by 4 MeV in calculations without three-body effects; the mass-10 species are under bound by 20 MeV!

So this approach to nuclear structure is DIFFICULT. How long would calculations for ^{238}U take and what computer would you do it on? Would the current parameterisations of the nucleon-nucleon force, developed for light nuclei, actually work? So we need to look for another approach, namely MEAN-FIELD THEORIES.

Note on the Boundary Conditions:

If the radial wavefunction is not continuous at the boundary, the probability density changes abruptly at the edge of the well.

At the boundary point both Schrodinger equations hold; the one with $V=0$ and the one with $V=-V_0$. This can only be possible it d^2u/dr^2 itself is zero. Hence du/dr is continuous at the boundary.

PC 4421 Lecture 3: Mean Field Theories and the Fermi Gas

The Mean Field and Hartree-Foch Methods

Generalising the deuteron Schrodinger equation to a system with *i* nucleons gives a complicated equation for the nucleus:

$$\hat{H}\,\Psi = \left[-\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i>j} V_{ij} \right] \Psi = E\,\Psi$$

This includes a kinetic energy term for each nucleon and two-body forces between pairs of nucleons V_{ij}, but ignores three-body and higher effects. We saw that solving such equations is difficult, complicated and time consuming. We're going to try a different route using an approximation. This isn't a very good one, so we'll need to pack it up at a later date!

The mean-field approximation suggests that we imagine that all the two-body interactions that a nucleon experiences due to all the other nucleons in the nucleus can be replaced to a good approximation by an equivalent average or mean-field potential *U(r)*. The Hamiltonian above can now be written:

$$\hat{H} = \sum_i \left[-\frac{\hbar^2}{2m}\nabla_i^2 + U(r_i) \right] + \sum_{i>j} V_{ij} - \sum_i U(r_i)$$

Here the term in brackets is the *mean-field problem for an individual nucleon* and the last two terms are known together as the *residual interaction*. If the mean-field approximation is a good one, then the residual interaction is small and if it is very good you can neglect it. If you do neglect it then all you have to do is solve the independent-particle Schrodinger equation for each individual nucleon:

$$\hat{H}_i\,\varphi_i = \left[-\frac{\hbar^2}{2m}\nabla_i^2 + U(r_i) \right] \varphi_i = E_i \varphi_i$$

Then the energy of the nucleus as a whole is a sum of the individual nucleon energies, $E=\Sigma E_i$. If this is not entirely obvious to you, then take a Hamiltonian, $H=\Sigma H_i$, and a wavefunction $\Phi=\Pi\varphi_i$ (where the Π means multiply all the φ_i together) and substitute these into the Schrodinger equation $H\,\Phi=E\,\Phi$. It should separate out into individual equations, $H_i\,\varphi_i = E_i\,\varphi_i$, if $E=\Sigma E_i$.
Realistically we need to be able to take the residual interaction into account as a secondary effect. It might not necessarily a small perturbation though, but if it were small perturbation theory might be one way you could consider doing it.

This is somewhat similar to how you might deal with a many-electron atom. The parallel here is that the central Coulomb potential is rather like *U(r)*, with electrons moving in this potential. You can solve the Schrodinger equation for one electron. Fill up the resulting electron orbits according to the Pauli Principle, adding up their energies to give the overall atomic energy. But then the Coulomb repulsion between electrons (a non-central force!) may need to be taken into account as a correction to the simple calculation. The difference in the nuclear situation is that there is no defined centre; nucleons orbit around the centre of mass of the system. Also the nuclear force itself has non-central components to it, so the average mean-field potential itself is only an approximation and residual nucleon-nucleon interactions need to be taken into account as a correction to the "simple" calculation.

If you know the wavefunction of an individual nucleon, φ_j, you can find the probability of it being at a particular point in space. Given the force between two nucleons, V_{ij}, then you use this to *calculate* the average force on one nucleon, *i,* due to all the others*:*

$$U(r_i) = \sum_{j \neq i} \int V_{ij}(r_i - r_j)\rho(r_j)\, dV = \sum_{j \neq i} \int \varphi^* V_{ij}(r_i - r_j)\varphi\, dV$$

But you don't know the wavefunctions without solving the Schrodinger equation, and to do that you need to know what *U(r)* is to do it!

What you can try to do is adopt the HARTREE method. This was actually developed first in atomic physics when the electron-electron repulsion is taken into account. The steps are as follows:

(a) Make a damn good guess at what *U(r)* is.
(b) Solve the Schrodinger equation to get the first approximation to the nucleon wavefunctions, φ_i.
(c) Use these wavefunctions, φ_i, to calculate an improved *U(r).*
(d) Solve the Schrodinger equation to get a second approximation to the nucleon wavefunctions, φ_i
(e) Repeat these steps and hopefully you'll get a better and better solution. The changes between successive solutions should get progressively less and less, a process known as convergence. But convergence isn't guaranteed!

There are several variations to this approach. HARTREE-FOCH (HF) methods use properly antisymmetrised wavefunctions needed for fermions. *We'll talk more on antisymmetrisation later, if there's time, it can be wrapped up with isospin.* HARTREE-FOCH-BOGOLUBOV (HFB) methods incorporate pairing correlations between nucleons which scatter nucleon pairs between different orbits. This all ends up being difficult stuff and the preserve of nuclear theorists.

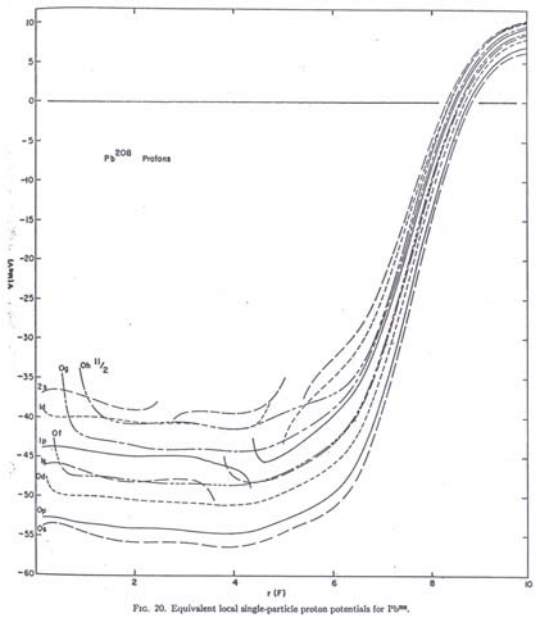


FIG. 20. Equivalent local single-particle proton potentials for Pb^{208}.

The picture on the left shows HF potentials which have been generated for protons in ^{208}Pb. They depend on how the nucleon is orbitting, but in general they follow the form of the matter density distribution.

Often people will just choose a convenient mathematical form for the mean-field potential, usually something which looks about right compared to the nucleon density distribution or something which is easy to deal with mathematically*;* there'll be some examples later on. That's fine, but you pay the price in the end as the mean field you have will not be as good an approximation as the full HF method. You have to play close attention to the effect of the much larger residual interaction as a consequence

.

To get a feel for orders of magnitude and so on, kick off with the very simplest potential that you could imagine. What's the easiest method for confining nucleons to a small region of space? Stick them in a box which is the same size as the nucleus i.e. a three-dimensional infinite square well or perhaps a three-dimensional infinite spherical well. Even though this is a gross approximation, run with it for a while and see what comes out the end. We're also going to assume we can treat the whole thing statistically!

Fermions in a Box; the Fermi Gas Model

The Fermi gas model is pretty crude. It assumes that all the nuclear forces do is confine nucleons to a certain region of space which we're referring to as a box. Once confined, we assume that they no longer interact with each other. Pretty far from the truth, but it will give some useful estimates of various quantities

When putting things in a box, statistical mechanics will be able to tell you about the density of states. For a particle in a box, you know that the number of states with a wave number between *k* and *k+dk* is given by $Vk^2/2\pi^2$. Remember the wave number is related to the momentum by the de Broglie relationship, $p=\hbar k$,and that this expression is correct for spinless particles in a box of volume *V*. Surprisingly it is independent of the shape of the box *(see Mandl's Statistical Physics)* even though you will probably remember deriving it for a square box.

For neutrons with spin-½ there are two spin substates so add a factor of 2 and convert into momentum, *p*:

$$dN = 2 \times \frac{4\pi V}{h^3} p^2 dp$$

For low excitation/temperature, they fill levels according to the Pauli principle, up to a certain level known as the Fermi level. Writing this mathematically you can find the momentum of the highest level filled, p_F:

$$N = \int_{bottom}^{top} dN = \frac{8\pi V}{h^3} \int_0^{p_F} p^2 dp = \frac{8\pi V}{h^3} \frac{p_F^3}{3}$$

where the momentum at the Fermi level is given by

$$p_F = \sqrt[3]{\frac{3h^3 N}{8\pi V}} = 315.1 \left(\frac{N}{A} \right)^{1/3}$$

in units of MeV/c. This last step uses $\hbar c$=197MeV.fm, $V = \frac{4}{3}\pi r^3$ and $r = r_0 A^{1/3}$ with $r_0 = 1.2$ fm.

Converting from momentum to energy will turn the Fermi momentum into the energy of the highest energy nucleon in the box, in units of MeV:

$$E_F^{\upsilon} = 52.84 \left(\frac{N}{A} \right)^{2/3}$$

Doing the same exercise for protons gets you:

$$E_F^{\pi} = 52.91 \left(\frac{Z}{A} \right)^{2/3}$$

This represents the kinetic energy of the most energetic nucleon in the nucleus. [NB: Since the nucleus is just a box, the potential energy in this model is the same for all nucleons and can be taken as zero.]

A better representation of nucleon energies might be the average nucleon energy which is given by:

$$\frac{\int \frac{p^2}{2m} p^2 dp}{\int p^2 dp} = \frac{3}{5} E_F$$

For light nuclei along the line of stability, N≈Z, and so N/A=Z/A=1/2 which gives E_F ~ 33 MeV and the average nucleon energy of around 20 MeV.

This is an important and useful result:

(a) The nucleon velocity is approximately 20% of c, but the situation is not terribly relativistic as the average energy of 20 MeV is a lot less than the rest mass-energy of a nucleon, 938MeV. We can safely use non-relativistic approaches as a reasonable approximation.
(b) Knowing both *r* and *v* you can estimate the orbital period of a nucleon orbit to be 10^{-21} to 10^{-22} seconds this is extremely important in justifying the collective models of the nucleus. For example, if macroscopic bulk rotation is to make any sense the nucleon orbital frequency has to be much faster than the rotational frequencies, otherwise nuclear shape would be meaningless. Luckily they are as you'll see in the second half of the course.

Adding up the energies of protons and neutrons gives you the total kinetic energy in the nucleus:

$$\text{total KE} = Z \times \frac{3}{5} E_F^{\pi} + N \times \frac{3}{5} E_F^{\nu} = 31.9 \left\{ \frac{Z^{5/3} + N^{5/3}}{A^{2/3}} \right\}$$

For the deuteron find that E_F ~33 MeV and the binding energy per nucleon is 1.112 MeV. This model gives a well depth close to our previous estimate. The total KE in the deuteron is around 40 MeV.

In heavier nuclei there are more nucleons so you would expect the Fermi energy to be higher. But adding nucleons increases the size of the box, lowering the energy levels. You find that the Fermi energy along N=Z stays the same at ~33 MeV.

For more neutron-rich nuclei, the neutron Fermi surface is higher up than that for protons. This is the origin of β decay; a neutron at the Fermi surface can turn into a proton and fall down to the proton Fermi surface at a lower overall energy. Except that you increase the Coulomb electrostatic energy in doing so. The liquid drop mass formula handles all these contributions, and notably has the symmetry term which is proportional to $(N-Z)^2/A$.The Fermi gas model can justify this form for the symmetry energy.

Hint: write $N-Z=\varepsilon$ such that $N=\frac{1}{2}(A+\varepsilon)$ and $Z=\frac{1}{2}(A-\varepsilon)$. Substitute into the formula for the total kinetic energy and expand in terms of ε. Thus show that the total kinetic energy of nucleons has the form $A+5(N-Z)^2/9A$, which is the same as the liquid drop formula apart from the Coulomb and pairing terms.

Summary of Fermi Gas Model

In the Fermi Gas Model we have:

(a) Non-interacting Fermions in a nuclear size box.
(b) Apply Pauli principle and use density of states to count the nucleons.
(c) Use thermodynamic averaging.
(d) Get simple estimates of nucleon speeds and energies, and total KE in the nucleus.
(e) Actually get many other estimates of other properties from this model, such as level densities.

BUT: ***Nuclei are NOT boxes; the potential isn't an infinite square well.***
Nucleons DO interact with each other.
Do you expect thermodynamic averaging to work in nuclei, how great are the fluctuations?

We're going to work on the first question for a while; you can get a surprisingly long way without calculating and just knowing that the potential is central. I'll tell you how residual interactions can be treated to get over the second part. And we'll not use an approach based on statistical mechanics.

PC 4421 Lecture 4: Central Mean-Field Potential

Averaging procedure of the mean field suggests that the majority of the force on a nucleon is directed towards the centre of mass of the nuclear system. The average mean-field potential is therefore both spherically symmetric and central in character. In other words, $U = U(r)$ only and it does not depend on direction i.e. θ and Φ. The potential also needs to be realistic and would therefore have to have the following limiting characteristics:

$$U(r) \to 0 \text{ as } r \to \infty \text{ and as } r \to 0$$

with no nasty discontinuities anywhere. It probably also follows the density distribution if the nuclear force is short ranged.

The Hamiltonian for a single particle alone is:

$$\hat{H}_i = -\frac{\hbar^2}{2m}\nabla_i^2 + U(r_i)$$

The full nuclear Hamiltonian is then $\hat{H} = \sum_i \hat{H}_i$.

The solution to the single-particle eigenvalue equation can be written as:

$$\psi_i = \frac{R_{n\ell}(r)}{r} Y_{\ell,m}(\theta,\phi)$$

where $Y_{\ell,m}$ are spherical harmonics, as the potential is central and therefore ℓ is conserved. Remember that ℓ is an integer, $\ell \geq 0$ and m takes integral values according to $-\ell \leq m \leq \ell$. The parity associated with the spherical harmonic is $(-1)^{\ell}$.

[Note in passing: the full nuclear wavefunction can be constructed from the single-particle wavefunctions by forming an appropriately antisymmetrised product wavefunction since nucleons are fermions. This needs some care; Slater determinants are one example.]

The radial equation turns out to be:

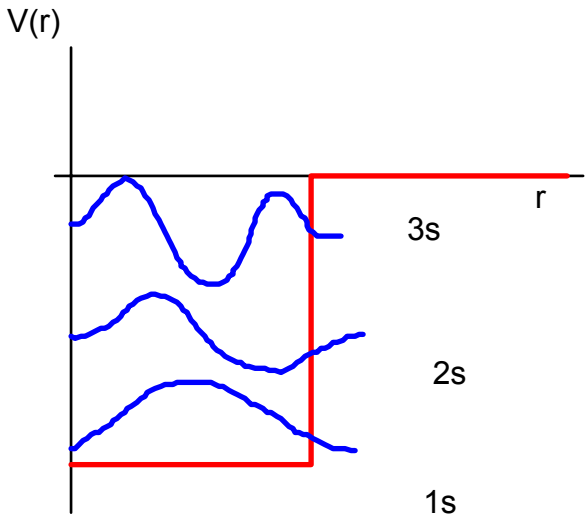
$$-\frac{\hbar^2}{2m}\frac{d^2R_{n\ell}}{dr^2} + \left[U(r) + \frac{\hbar^2}{2mr^2}\ell(\ell+1)\right]R_{n\ell} = E_{n\ell}R_{n\ell}$$

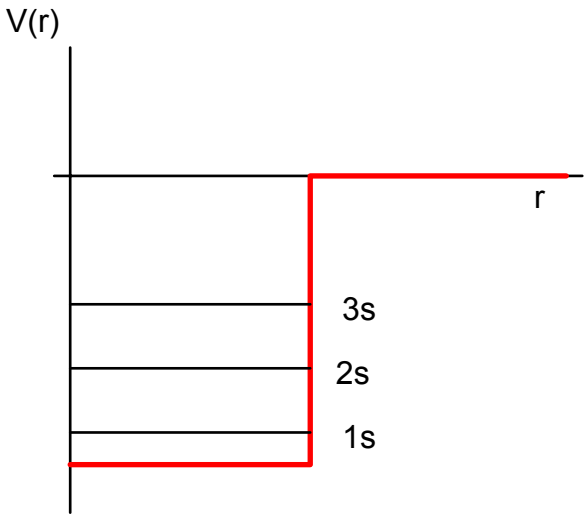
The related quantum numbers are *n* which is the principle quantum number and is the number of turning points, other than 0 and ∞, in the radial wavefunction.

You can already make some guesses as to what might come out of detailed calculations. The qualitative form of the radial wavefunction, R_{nl}, can be found just by sketching them in the particular potential bearing in mind the following conclusions which arise from simple quantum mechanics:

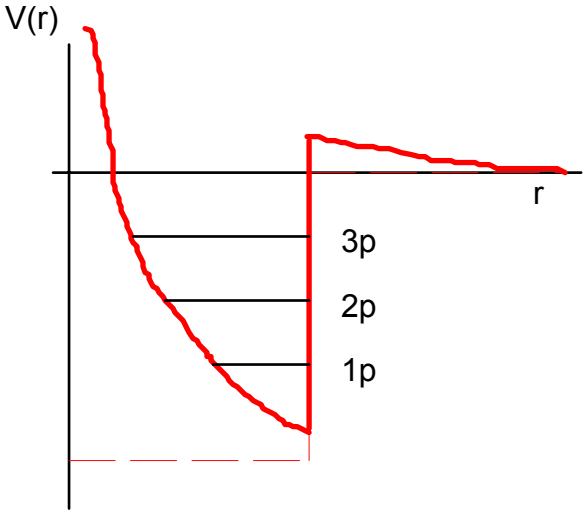
(a) Eigenfunctions are standing waves which "fit" into the potential well.
(b) Eigenfunctions need to be normalisable, so generally they tend to zero at large distances.
(c) For bound states, eigenfunctions tend to zero outside of the region of the binding potential.
(d) To keep the overall wavefunction finite at the origin, $R_{nl} \to 0$ as $r \to 0$.
(e) For de Broglie waves, $\lambda = h/p$; shorter wavelengths have higher momentum and therefore energy.

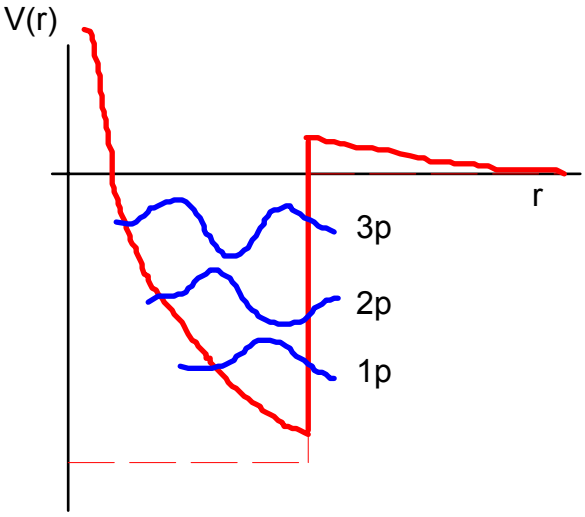
For example, take a finite-square well and think about how standing waves might fit into it.
For ℓ=0, sketch bound radial wavefunctions which fit the potential according to (a) to (d). Then sort them into ascending energy using (e).





ℓ=1 has the centrifugal term added to the square well:





The centrifugal term narrows the potential. For the same number of turning points i.e. a particular n, the wavelength in the narrower potential for ℓ=1 is smaller than for ℓ=0. Therefore the energy of a particular p state is higher than the s state with the same *n*. It is easy to have potentials where, for example, the 2s state is at a similar energy as the 1d state.

Remember for later on, that each of the ℓ=0 or s orbitals is a single state with m_ℓ=0. The ℓ=1 or p orbitals have substates with m_ℓ=+1, 0 and −1. In general, each ℓ orbital has (2ℓ+1) substates with m_ℓ running in integer steps from m_ℓ=ℓ to m_ℓ=−ℓ.

This is about as far as you can get without actually specifying the radial shape of the distribution.

Realistic single-particle potentials

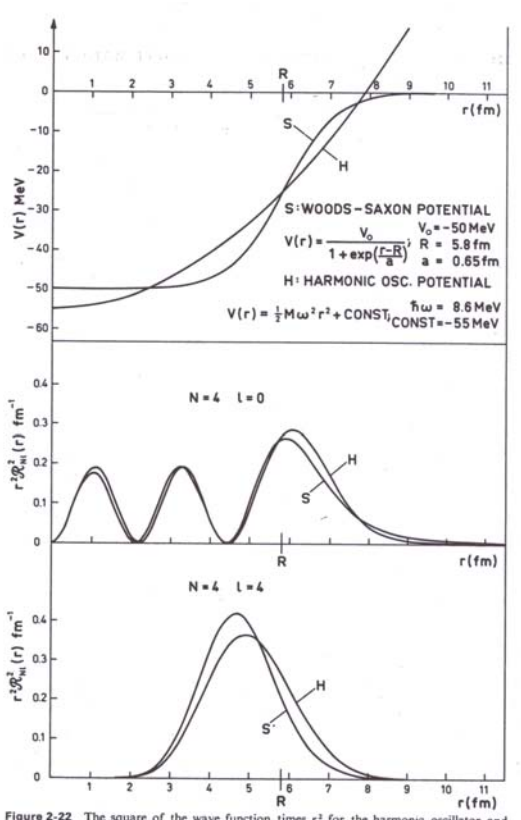


Figure 2-22 The square of the wave function times r^2 for the harmonic oscillator and the Woods-Saxon potential are plotted in units of fm^{-1}.

A nucleon in the interior of the nucleus is surrounded by similar numbers of nearest nucleons on all sides, since we know that the nuclear density in the interior is fairly constant. It is pulled equally in all directions with the result that the net force on it is zero. The potential energy in the interior is therefore constant; remember from mechanics that **F**=−grad V. Outside the nucleus, along way from the surface there is also no force and thus a constant potential.

A finite square-well potential would be a good approximation, except the change at the surface is too abrupt. A *Woods-Saxon* (WS) potential is a good approximation and looks very much like the measured matter distributions and calculated HF mean-field potentials. A big disadvantage is that only numerical solutions to the eigenvalue problem exist.

A simple harmonic oscillator (SHO) potential is also sometimes used for the sole reason that it has nice analytic solutions that can be written down as a mathematical expression. It doesn't look like the matter distribution; it is not flat in the middle, and it goes off to ∞ at large *r*. The latter is not too much bother as the eigenfunctions fall off rapidly with *r*, actually as $e^{-\alpha r^2}$. In other words, the probability of finding a nucleon at large distances where things go wrong is not tvery high. You can approximately correct it by adding a term $-D\ell^2$. This reduces the potential progressively for increasing ℓ, which sample larger and larger radii. With this addition the potential is referred to as a modified harmonic oscillator (MHO) well. Turns out to give a reasonable description if $\omega=41A^{-1/3}$ MeV; a result which can be proved by matching the radius produced by the modified oscillator to $r_0A^{1/3}$. Don't use the MHO potential if tails of wavefunctions are important though; it will get the eigenfunctions at large radii wrong.

Use these potentials, and add a Coulomb term for protons and you can get a reasonable description for nuclei that are near stability or proton rich. If you build up a large neutron excess and approach the neutron drip line things can alter drastically; the loosely bound neutrons can drift out to large radii, spreading out the density distribution making the surface much more diffuse.

Harmonic Oscillator Levels

For a 1D oscillator, $H=-m\omega x^2/2$ and simple quantum mechanics will lead to the conclusion that the energy levels are equally spaced and have energies $E=\hbar\omega(n_x+½)$ where n_x is an integer and the constant term is known as the zero-point energy (*see second-year quantum mechanics).*

In a 3D, harmonic oscillator the Hamiltonian becomes $H=-m\omega r^2/2=-m\omega(x^2+y^2+z^2)/2$. A separable solution of the Schrodinger equation can be used, $\Psi=X(x)Y(y)Z(z)$, which yields three equations each identical to the 1D problem. It is not surprising that the eigenvalues are the sum of three 1D eigenvalues, one for each direction, $E=\hbar\omega(n_x+n_y+n_z+3/2)$ where N is the total number of phonons in the system.

Referring to the diagram below, the N=0 level is just a single state. The N=1 level is actually three degenerate states which correspond to (n_x, n_y, n_z)=(1,0,0), (0,1,0) and (0,0,1). Similarly the N=2 level is made up of (2,0,0), (0,2,0), (0,0,2), (0,1,1), (1,0,1) and (1,1,0). *Make sure that you can verify the following degeneracies of different levels: N=3 is ten-fold, N=4 is fifteen-fold, N=5 is twenty-one-fold and N=6 is twenty-eight-fold degenerate.*

Calculated single-particle levels:

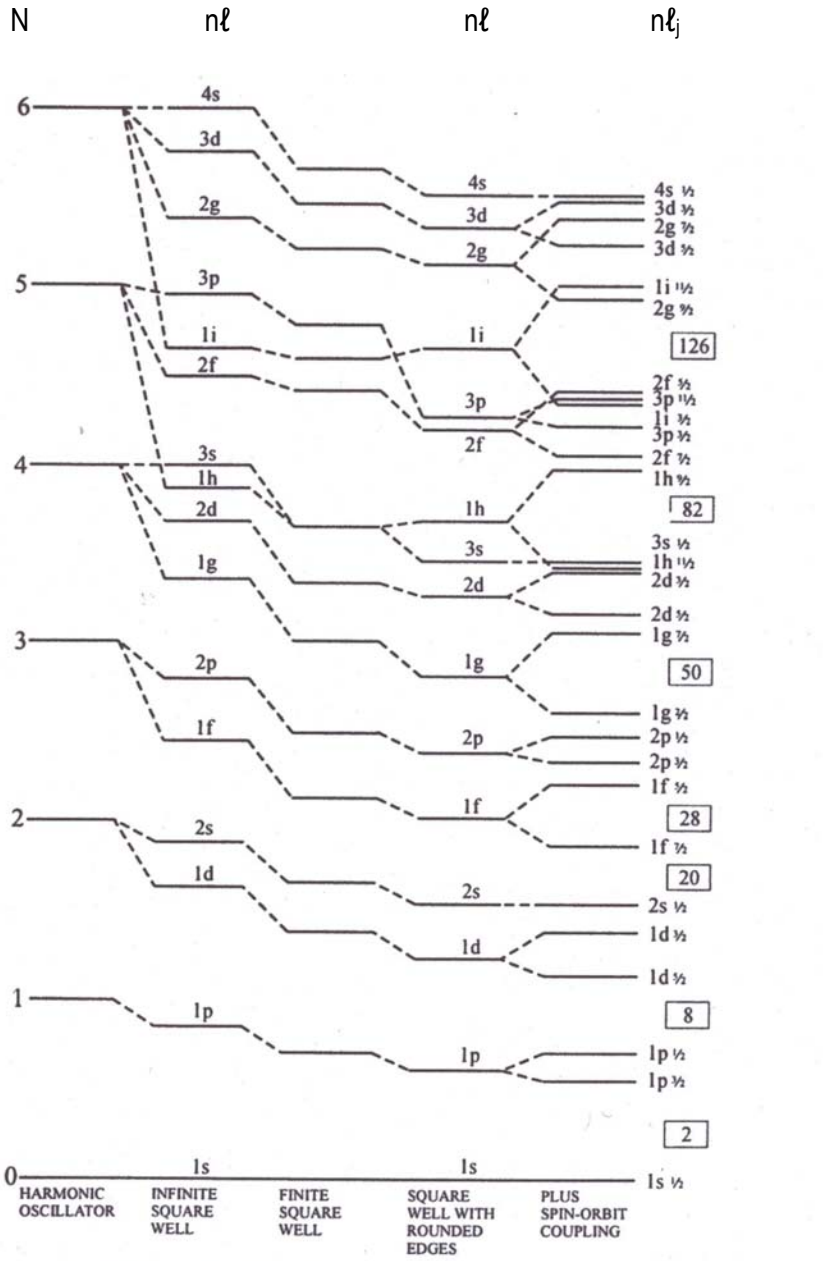


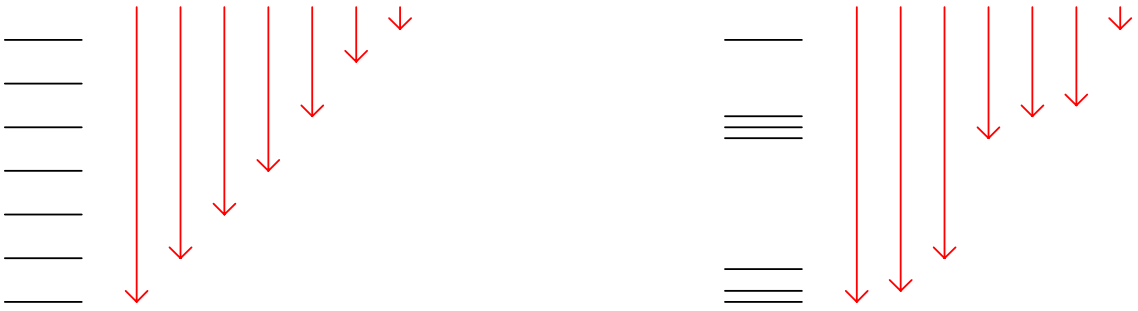
Fig. 17.6 Order of energy levels according to the independent-particle model with various assumptions for the shape of the nuclear potential (Feld 1953).

WARNING: these level orderings are qualitative only; especially for N>3, where level ordering is different for protons and neutrons. Level order depends on the mass *see later*. It also depends on what orbitals the nucleons of the other type are sitting in! But this diagram can act as a reasonable guide.

The 3D oscillator described above is spherically symmetric since the same frequency, ω, applies to each of the three directions, *x, y,* and *z*. It is therefore a central potential and the states of motion should be described with particular ℓ values. We should be able to work out the ℓ quantum numbers of the states if we remember that each ℓ is $(2\ell+1)$ degenerate.
The N=0 level has a degeneracy of one, so if ℓ is a good quantum number then ℓ has to be zero in order match with the one-fold degeneracy. The N=1 level has three states so should correspond to ℓ=1 i.e. m=1, 0 and -1 states. The N=2 has six states which cannot be reproduced with a single integer ℓ value. These six states are actually formed out of five ℓ=2, 1d states and one ℓ=0, 2s state. *Verify that the degeneracies are reproduced if the following harmonic oscillator levels are composed of these orbitals:*
N=3 (1f,2p), N=4 (1g,2d,3s), N=5 (1h,2f,3p) and N=6 (1i,2g,3d,4s).

When the $-D\ell^2$ correction term is put in these different ℓ values split to give a level ordering similar to the square wells shown in the diagram. (Notice that there are different groups of levels or *shells* which have alternate in parity.) The harmonic oscillator is a rather special case without this splitting which leads to a situation with high degeneracy.
Remember that in addition to the m_ℓ-substates of the ℓ levels, which leads to a $(2\ell+1)$-degeneracy, any nucleon placed in these orbitals has intrinsic spin also. There are also two possible intrinsic spin orientations, so each ℓ orbital can be filled with $2(2\ell+1)$ nucleons according to the Pauli Principle. Gaps in the energy level sequence corresponding to filled shells with the following numbers of nucleons: 2, 8, 20, 40, 70 and 112. *Double check these numbers for yourselves.* The Woods-Saxon potential gives very similar orderings as the modified harmonic oscillator potential.

So is this all correct? The experimental signature is the clumping of levels and the gaps between shells. Imagine equally spaced levels, the energy needed to remove nucleons varies smoothly with mass number. Clumped levels give jumps in the separation energy as a function of mass number:



Experimental evidence is available from the following sources:

- variation of nucleon separation energies
- variation of two-nucleon separation energies
- isotopic abundances
- alpha-particle energies
- neutron capture cross sections
- nuclear radii

All of these point to a sequence of gaps at the following nucleon numbers, these are the so-called *magic numbers*:

2, 8, 20, 28, 50, 82, 126 you need to remember these numbers!

So the predictions of the potentials so far are ALL WRONG!

PC 4421 Lecture 5: The Spin-Orbit Interaction

Before the Second World War nuclear physics concentrated on establishing the constituents of nuclei, nuclear masses and radioactive decay leading to semi-empirical mass formulae. In the 1940s fission and neutron capture reactions where studied in great detail in association with the Manhattan Project. These were fairly well understood in terms of a liquid droplet model for the nucleus and with Bohr's hypothesis of the compound nucleus in nuclear reactions. There were also two strong objections to single-particle models of the nucleus that we are studying here:

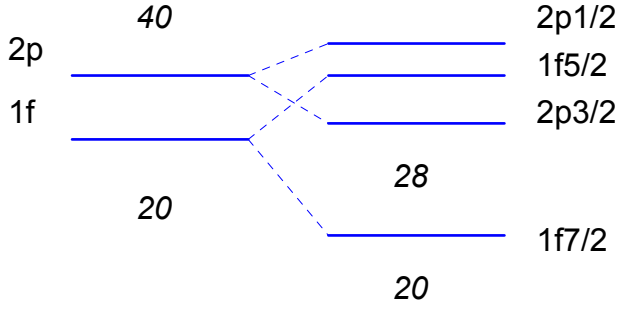
1. How can a nucleon, which interacts with the rest of the nucleus by a strong interaction, maintain a distinct orbital motion in such dense matter without colliding with other nucleons and must be continually changing its state of motion?
2. Any reasonable guess at the nuclear potential results in the wrong magic numbers.

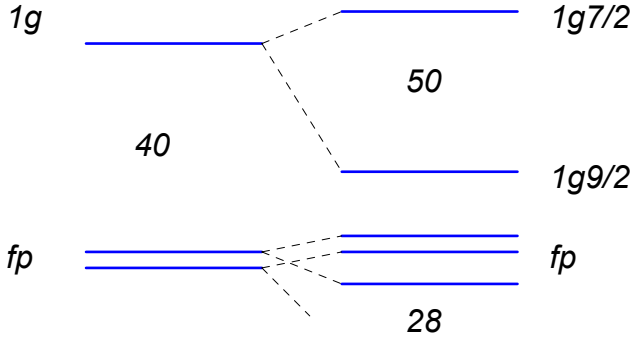
Pauli indicated the answer to the first issue. According to the exclusion principle, states in the single-particle level scheme can only be occupied by two nucleons, each in a different intrinsic spin orientation. So the single-particle levels are filled up to the Fermi level. We know that the wells are approximately 30-40 MeV deep. We also know that the energy associated with the strong interaction binding of one nucleon is approximately 7-8 MeV. According to the Pauli principle, if a nucleon is to change its state of motion, it must jump from the initial level to another level which needs to be empty of nucleons, i.e. one above the Fermi surface. Only nucleons within about 7-8 MeV of the Fermi surface can reach empty states via a strong interaction scattering. The majority are deeper down and therefore cannot scatter at all. As a result distinct nucleon orbitals are a viable entity. In fact, not all such scatterings yield as much as 7-8 MeV. Also in order to scatter between the two orbits, various conservation principles and selection rules must be considered, so the scattering is even less than you'd first imagine.

In order to answer the second objection, Maria Meyer and H. Jensen where both independently asking themselves the same question: "What is the simplest, reasonable alteration that can be made to a single-particle potential in order to reproduce the observed magic numbers?" They both can up with the same answer in the late 1940s and shared a Nobel Prize. This revision made single-particle models of the nucleus viable and practically every aspect of nuclear structure and reactions use such descriptions in some way. This was revolutionary stuff. They both decided to add a spin-dependent term, not a stupid thing to start thinking about as the nucleon-nucleon force is spin dependent.

Remember that for each ℓ there are two different couplings when intrinsic spin is added, $\mathbf{J}=\boldsymbol{\ell} \otimes \mathbf{s}$ and the associated quantum number is given by angular momentum coupling rules, $j=\ell \pm \frac{1}{2}$. For example, the 1g states result in $1g_{9/2}$ and $1g_{7/2}$ states with degeneracies of 10 and 8 respectively. The 1f states result in $1f_{7/2}$ and $1f_{5/2,}$ with degeneracies of 8 and 6 respectively.

If we split the two 1f orbitals, bringing the parallel spin coupling lower, a gap in the scheme is created at nucleon number 28. Similarly lowering the $1g_{9/2}$ with respect to the $1g_{7/2}$ will create a gap at nucleon number 50.





We want to add in an extra term in the Hamiltonian which favours $j_>$ (= ℓ+½) energetically over $j_<$ (ℓ-½),
A quick look at the level scheme shows that this splitting also needs to be bigger for larger ℓ.
If you make a term which looks like $-V_{\ell s}(r)\hat{\ell}.\hat{s}$ what does it do?

$$j^2 = (\underline{\ell} + \underline{s})^2 = \ell^2 + s^2 + 2\underline{\ell}.\underline{s}$$

$$\underline{\ell}.\underline{s} = \frac{1}{2}(j^2 - \ell^2 - s^2)$$

Replacing the operators by their eigenvalues gives

$$\underline{\ell}.\underline{s} = \frac{\hbar^2}{2}(j(j+1) - \ell(\ell+1) - s(s+1))$$

Putting in some numbers to this formula for particular cases gives the right kind of dependencies, as shown in the table.

	ℓ.s	**Δ(ℓ.s)**
$g_{7/2}$	$-5\hbar^2/2$	$9\hbar^2/2$
$g_{9/2}$	$+2\hbar^2$	
$f_{5/2}$	$-2\hbar^2$	$7\hbar^2/2$
$f_{7/2}$	$+3\hbar^2/2$	
$p_{1/2}$	$-\hbar^2$	$3\hbar^2/2$
$p_{3/2}$	$+\hbar^2/2$	

What about the radial dependence of the spin-orbit force?
The Thomas form is often used:

$$V_{so} = -V_{\ell s}\frac{1}{r}\frac{\partial V(r)}{\partial r}\underline{\ell}.\underline{s}$$

Notice that in a typical potential such as a WS well, the *V(r)*, only has a large gradient at the surface. The spin-orbit term is therefore only strong near the surface of the nucleus. This is in line with our previous discussions about why the potential is constant and there are no resultant forces in the interior of the nucleus.
And the strength of the spin-orbit force?
We want something to shift spin-orbit partners across harmonic oscillator shells so $V_{\ell s}$ will be of the order of $41A^{-1/3}$. Usually it is treated as an empirical parameter and fitted to known single-particle energies in particular nuclear mass regions.

Before the spin-orbit term was introduced the single-particle shells alternated in parity. Now, for orbitals with large ℓ, the spin-orbit coupling can shift high-j states from one shell so that they intrude on the next shell down. For example, the $h_{11/2}$ originally in the N=5 negative-parity oscillator shell moves down to join the positive-parity N=4 orbitals in the formation of the gap at particle number 82. Similarly the $i_{13/2}$ moves from N=6 to N=5 in the formation of the gap at 126. These so-called intruder or unique-parity states (as opposed to normal-parity orbitals) become very important in nuclear structure for several reasons:

(i) They have large values of j and therefore are useful to generate states with very large angular momentum.
(ii) They have opposite parity to the single-particle levels around them and are useful to generate negative-parity states at low excitation energy.
(iii) They have high ℓ values and therefore very eccentric orbitals (remember what spherical harmonics look like, look up some pictures for high ℓ). They orbit in very non-spherical paths and can be responsible for pulling the rest of the nucleus away from a spherical shape.
(iv) They have a very high degeneracy. As we'll see later, this means that they are very important if you try to do a liquid-drop model but correct it for shell effects *Strutinsky shell correction.* So they are important for determining the shape and stability of nuclei, for example the so-called superheavies.

(v) Remember the residual interactions: $H = H_{\text{mean field}} + H_{\text{residual interactions}}$

We've ignored the residual interactions so far. Our mean-field eigenfunctions are only approximate. In reality, the real eigenfunctions are different. However, we can, if we want to, express each real eigenfunctions as a summation of terms from basis set formed by the mean-field eigenfunctions. The mean-field eigenfunctions are said to be "mixed" by the residual interaction. If the effect of the residual interaction is small, the sum will be dominated by just one of the original mean-field eigenfunctions and the real eigenfunctions are said to be relatively pure. If the effects are large, then the resulting real eigenfunctions are complex sums of the mean-field ones. It turns out that since most interactions conserve parity, only eigenfunctions with the same parity mix. Another useful result is that mean-field eigenfunctions only mix strongly with others that are close in energy. We'll see all these results quantitatively later on.

For unique-parity orbitals, other orbitals with the same parity are far away in energy and so the single-particle wavefunctions associated with these orbits remain very pure. So they are states for which the wavefunctions are relatively uncomplicated and easy to deal with.

Mass Dependency, Protons and Detailed Ordering

Remember that for states in a potential well the energies of the states depend on the width of the well. The smaller the well, the smaller the wavelengths of standing waves that you can fit into the well and consequently the energies will be higher. Adding nucleons to the nucleus will make it bigger, so levels should fall in energy with increasing mass.

For an infinite square well, the level energies are proportional to the square of the width of the well, $E \sim 1/R^2$. For a nucleus $R=r_o A^{1/3}$, so you might expect an $A^{-2/3}$ dependence of the energy levels. This looks about right in calculations shown in this diagram. Notice also that there are some slight rearrangements of the ordering of levels with different ℓ values. So make sure you use a diagram specific to the mass region you are interested in.

For protons you need to add in a Coulomb potential, so that can lead to slight differences between neutron and proton single-particle orderings.

In addition, residual interactions can play a huge role in the detailed ordering of levels. The interaction can be between the valence nucleon and the rest of the nucleus, called the core. So level ordering sometimes depends on what levels are filled below it in energy. The residual interaction can also be between one type of valence nucleon and the other. For example, in the fp-shell from Ca to Ni the $\pi f_{7/2}$ orbital fills. This has a very large interaction with the $\nu f_{5/2}$ orbital, basically because the radial wavefunctions have very similar shapes (identical other than any Coulomb effects). As the $\pi f_{7/2}$ fills it interacts more and more strongly, pushing the $\nu f_{5/2}$ orbital down in energy. The level ordering in Ca isotopes with N>28 is $p_{3/2}$, $p_{1/2}$, $f_{5/2}$ and in Ni it has become is $p_{3/2}$, $f_{5/2}$, $p_{1/2}$. This is a surprising effect that has only recently been uncovered, and it and similar ones in other mass regions can lead to spectacular changes in nuclear structure which are being actively studied.

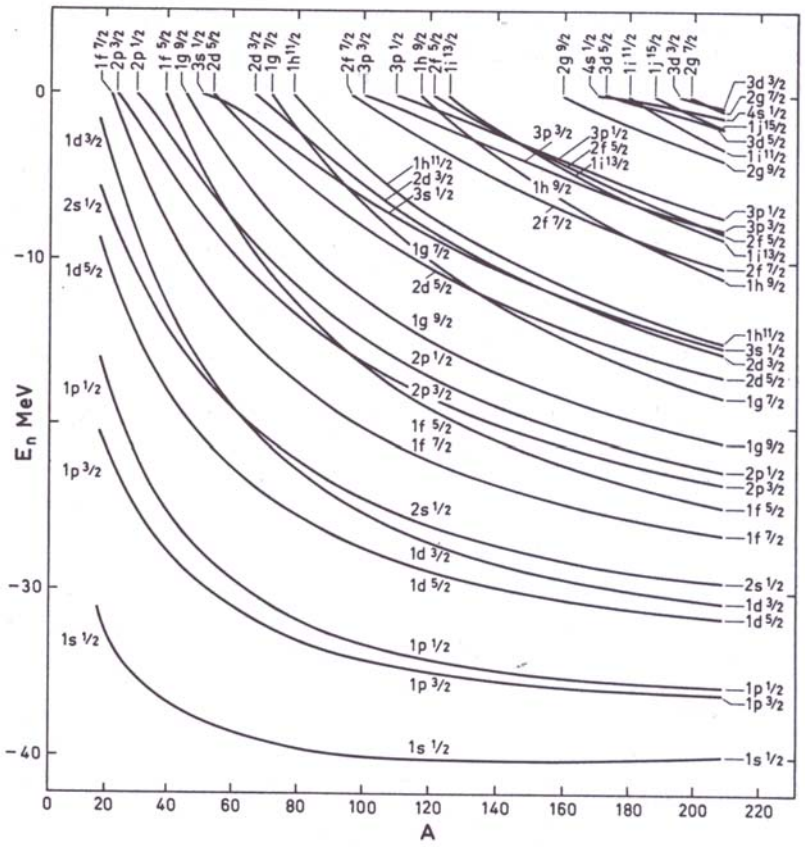


Figure 2-30 Energies of neutron orbits calculated by C. J. Veje (private communication).

PC 4421 Lecture 6: Independent-Particle Models

Quick Recap

We have been assuming the mean-field approximation, where any nucleon moves in a mean one-body central mean-field potential which is the result of its interactions with all the other nucleons in the nucleus. We have been writing the nuclear Hamiltonian as a sum over the single-nucleon Hamiltonians so that $H_{nucleus}=\Sigma H_{nucleons}$. Writing the overall nuclear wavefunction as a suitable combination of single-particle eigenfunctions, the Schrodinger equation for the whole nucleus can be separated out into individual single-particle equations where $E_{nucleus}= \Sigma E_{nucleons}$. These individual single-particle equations can be written as:

$$\hat{H}_i = \left[-\frac{\hbar^2}{2m}\nabla_i^2 + U(r_i) + V_{Coulomb}(r_i) \right] + \left[\sum_{j>i} V_{ij}(r_{ij}) - U(r_i) \right]$$

Here the Coulomb term is only used for the protons. The first term is a one-body potential i.e. it depends only on the coordinates of the nucleon of interest. The second term is the residual interaction which is two-body in nature as it depends on the coordinates of the nucleon of interest and the coordinates of other nucleons that it interacts with. We have so far chosen to ignore (at our peril) the residual interaction, the term in the second square brackets. We have guessed simple forms for $U(r_i)$ and have seen the necessity to include a spin-orbit coupling term in it.

Now we need to think about exactly how we start to understand the states in a nucleus as a whole, rather than the orbitals of the individual nucleons inside it.

Filling a Single-j Shell

It will be useful to first consider putting nucleons into a single-*j* orbital and work out what spins and parities we can have for different numbers of nucleons. We'll find some simplifications and then go on to think about the states of the nucleus overall. As a concrete example, think about putting nucleons of the same type into an $f_{5/2}$ orbital, let's say they are all neutrons.

An empty orbital: $\nu f_{5/2}^{0}$

With no nucleons in an orbital, there is nothing to generate angular momentum so the spin-parity has to be $J^{\pi}=0^{+}$.

Single neutrons: $\nu f_{5/2}^{1}$

The nucleon has spin-parity $5/2^{-}$, and since it is the only one that is also the overall spin-parity of the configuration, $J^{\pi}=5/2^{-}$.

Two neutrons: $\nu f_{5/2}^{2}$

You might think that you couple the two angular momenta and that gives you the possible overall angular momentum for the configuration: $J^{\pi}=5/2^{-} \times 5/2^{-}= 5, 4, 3, 2, 1, 0^{+}$. This would be the right answer if the two nucleons where distinguishable, such as in the case of a proton and a neutron in the $f_{5/2}$ orbital. The problem here is that we have two neutrons and they are indistinguishable. The number of available spins is reduced to $J^{\pi}=4, 2, 0^{+}$.

To see why, we use what is called an M-scheme, and look in detail at the possible substates that can be formed; remember that when combining angular momenta the projection quantum numbers just add, $M=m_1+m_2$. In doing so, we need to carefully consider indistinguishablility and the Pauli exclusion principle.

For example, the $J^\pi=5^+$ state would require the existence of an M=5 substate. This can only be formed by $M= m_1+m_2=5/2 + 5/2$. Such a state is forbidden by the Pauli exclusion principle; both neutrons would be in the same state. As a result the $J^\pi=5^+$ state doesn't exist. Let's look in detail at the possible combinations of m_1 and m_2:

m_1	m_2	M	
5/2	5/2	5	violates Pauli
	3/2	4	☺
	1/2	3	☺
	−1/2	2	☺
	−3/2	1	☺
	−5/2	0	☺

m_1	m_2	M	
3/2	5/2	4	not distinct
	3/2	3	violates Pauli
	1/2	2	☺
	−1/2	1	☺
	−3/2	0	☺
	−5/2	−1	☺

Notice that only one of the two combinations (5/2,3/2) and (3/2,5/2) is allowed; the neutrons are identical and cannot be distinguished so these two sets of labels refer to the same state. Now you have the hang of it, for the rest of the combinations we can just write down those that are possible:

m_1	m_2	M
1/2	−1/2	0
	−3/2	−1
	−5/2	−2
−1/2	−3/2	−2
	−5/2	−3
−3/2	−5/2	−4

Having got the possible M substates, we can now construct the J states from them. For example, the highest allowed M is 4, indicating the highest allowed J is also 4. This state requires M=4, 3, 2, 1, 0, −1, −2, −3 and −4 substates.
Crossing these off the possible M states, we see that we have used the only available M=3 and −3 substates so that J=3 cannot exist.
The highest M left is 2, so we use M=2, 1, 0, −1, −2 to make a J=2.
The only remaining substate is M=0. So there is a J=0 state, but there are no J=1 states.
To summarise, using the available M substates which remain after applying Pauli and removing indistinguishable states, you can only construct $J^\pi=4, 2, 0^+$. The parity is $(-1)^2$ i.e. positive

Three neutrons: $vf_{5/2}^3$

Go through the same procedure as with two neutrons and write out the allowed combinations of $M=m_1+m_2+m_3$, discarding those that violate Pauli such as (1/2,1/2,1/2), and remembering that the three neutrons are all indistinguishable, so that, for example all the following combinations are actually the same state and should only be counted once: (1/2, −1/2,5/2), (1/2,5/2, −1/2), (−1/2,5/2,1/2), (−1/2,1/2,5/2), (5/2,1/2, −1/2) and (5/2, −1/2,1/2).
The results are J=9/2, 5/2 and 3/2 (but you should check me out) and the parity is $(-1)^3$ i.e. negative.

Four neutrons: $\nu f_{5/2}^{4}$

If you run through the *M*-scheme process you will deduce that the allowed spin-parities are J^{π}=4, 2, 0^{+}. Therefore you could consider this configuration as two neutron holes i.e. $\nu f_{5/2}^{-2}$. Then couple the two identical neutron holes in the same way as we did above for the identical neutron particles.

Five neutrons: $\nu f_{5/2}^{5}$, or $\nu f_{5/2}^{-1}$

Only a single-neutron hole and so $J^{\pi}=\frac{5^{-}}{2}$

Six neutrons: $\nu f_{5/2}^{6}$

This j-shell is now full. The spin-parity is $J^{\pi}=0^{+}$. This is because the only allowed combination of *m*'s is:

$M = 5/2 + 3/2 + 1/2 - 1/2 - 3/2 - 5/2 = 0$.

All other combinations violate Pauli by having more than one neutron with a particular *m* value. This is a general result which is independent of the actual *j*-orbital involved.

Full j-orbitals can only couple to spin-parity 0^{+}.

Spins and Parities of Ground States and Low-Lying Levels

Ground states with full j-orbitals

The ground states of doubly-magic nuclei are composed of a series of full j-orbitals. So the ground states must be 0^{+}. Experimentally there are no exceptions. All ^{4}He, ^{16}O, ^{40}Ca, ^{56}Ni, ^{132}Sn…etc. have zero spin ground states.

Other cases of full j-orbitals have 0^{+}. For example, $^{90}_{40}\mathrm{Zr}_{50}$ has a zero spin ground state.

Some terminology:
- ***closed core*** = a series of full j-orbits
- ***magic core*** = a series of full j-orbits, then a sizeable gap to the next orbit
- ***doubly-closed core*** = closed core for both protons and neutrons
- ***doubly-magic core*** = magic core for both protons and neutrons

One particle outside a doubly-magic or doubly-closed core

The cores will contribute nothing; the spin of the nucleus is determined by the odd particle.

Eg. $^{41}_{20}\mathrm{Ca}_{21}$ the odd neutron sits in $1f_{7/2}$ so the spin-parity is 7/2-.

This works for all doubly-magic cores. It should also be okay for doubly-closed cores plus one, but it depends on the proximity of the next level up.

Eg. $^{91}_{40}\mathrm{Nb}_{41}$ the odd neutron sits in $1f_{7/2}$ so the spin-parity is 7/2-.

If you move the odd particle around to different orbitals you can make excited states.

Eg. $^{17}_{8}\mathrm{O}_{9}$ and $^{17}_{9}\mathrm{F}_{8}$ have an odd nucleon in $1d_{5/2}$, so the ground state has $J^{\pi}=5/2+$. Promoting the nucleon into the next excited state, $2s_{1/2}$, will create a low-lying $J^{\pi}=1/2+$ state.

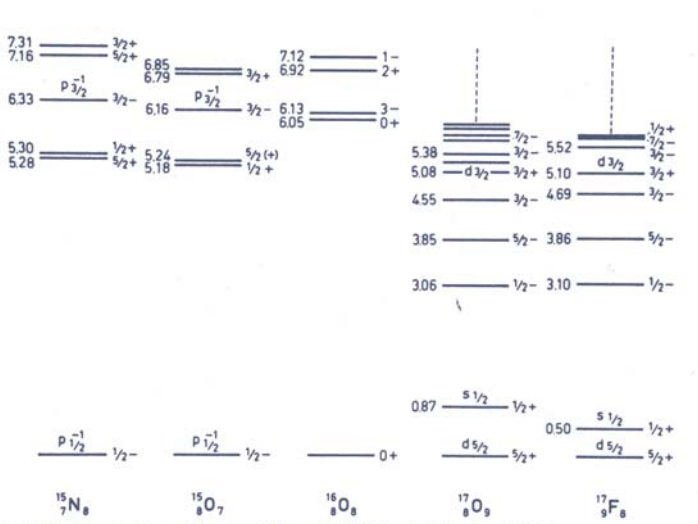


Fig. 17.11 Level schemes for some light nuclei (Bohr and Mottelson 1969).

The excitation energies are to a first approximation equal to the difference in the energies of the $1d_{5/2}$ and $2s_{1/2}$. But you'll find problems with this approach if you make detailed comparisons with data. This gets worse the more excitation energy you pump into the system, even with doubly-magic cores.
In order to properly describe excited states you need take into consideration the residual interactions.

Residual Interactions (Qualitative)

Residual interactions are an extra term in the Hamiltonian which goes beyond the mean-field approximation. They are invariably not small, so perturbation theory is hardly ever satisfactory. They are two-body in nature, depending on the coordinates and quantum states of two nucleons and are, in general, non central. This is a descriptive approach to give you a picture of what is going on. As with all such pictures, you need to take it with a pinch of salt; to deal with them properly you need an explicitly quantum mechanical description which we'll come to later.

Imagine a nucleon in a single-particle state, happily orbiting with quantum numbers n, ℓ and j. It is orbiting in the mean field generated by the average of the interactions with all the other nucleons, but its motion does not explicitly depend on coordinates or quantum numbers of other nucleons i.e. the potential generates a one-body force.
Let it interact via a residual interaction with another nucleon. This is a two-body interaction; the strength of the interaction depends on the coordinates of both nucleons. Like colliding snooker balls (short-range interactions), the nucleons can scatter into different orbits, as long as the orbitals into which they scatter are empty; Pauli must be obeyed. If the residual interactions play an important role, the nucleon will scatter between a subset of single-particle orbitals, occupying each one for certain fractions of the time.
In this new state of motion, there is a probability of finding the nucleon in a particular single-particle orbit specified by n ℓ j.

Neglecting the residual interaction, you have the mean-field eigenfunctions: $\Psi_{nucleon}=\Phi_{n\,\ell\,j}$.
Including the residual interaction requires a new set of eigenfunctions which we can express as a sum of the mean-field eigenfunctions: $\Psi_{nucleon}=\Sigma a_{n\,\ell\,j}\,\Phi_{n\,\ell\,j}$. This is the "mixing" discussed earlier on.
Here $a^{*}_{n\ell j}\ a_{n\ell j}$ is the probability of finding the nucleon in the particular mean-field eigenfunction, n ℓ j, during its continual scattering between orbitals.

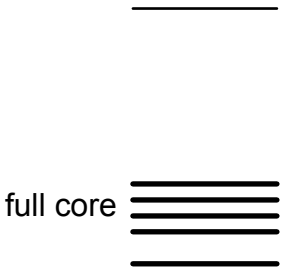
In this sense the residual interaction will *mix* different unperturbed single-particle wavefunctions, but the energy of the nucleon is also altered $E=\Sigma\, a^{*}_{n\ell j}\ a_{n\ell j}\ E_{n\ell j}$.

Remember that any wavefunction can be expanded into a particular basis set of eigenfunctions. Here we are expanding a complex state into the basis represented by single-particle wavefunctions. There are other

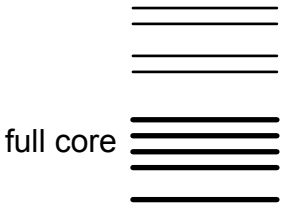
representations that we could use to describe a nuclear state. For example, vibrational or rotational wavefunctions will also provide basis sets that we could use. If we have a state that has a wavefunction that it dominated in the expansion in a particular basis by one single eigenfunction, then that basis will give a simple picture of the characteristics of the state. The basis is a good model.

For example, if $\Psi_{nucleus}=\Sigma a\ \Phi_{single\text{-}particle}$ where the sum goes over many different single-particle orbitals, then the state is not well described by the motion of single particles. But the same state might be described in a rotational basis set as $\Psi_{nucleus}\approx\varphi_{rotational}$, then in this basis the wavefunction is quite simple and the state is well described as a rotation. This is the quantum mechanical interpretation of the process of nuclear modelling.

We'll deal with this properly later, but we can already start to see cases where the independent-particle model will work and were it won't:



In a closed shell plus one nucleus, if the level gap between the core and the next levels up is larger than the average energy involved in a residual interaction, it is difficult to scatter particles into empty orbitals. Scattering doesn't happen often and the single valence nucleon is unaffected. It can be treated as an independent particle to a good approximation. With magic cores the gaps are always large. In closed cores the gap may be large but, as in the case at Z=40, it sometimes isn't.



If the energy gap is small, residual interactions will scatter nucleons into the empty orbitals quite often and the independent-particle model is a worse approximation.

In open-shell nuclei, residual interactions can play an significant role scattering nucleons between many different single-particle states for both protons and neutrons. Large mixing can occur and highly complex wavefunctions can arise if a single-particle basis is used. Other bases, like collective models, have better success in describing states simply between magic nuclei.

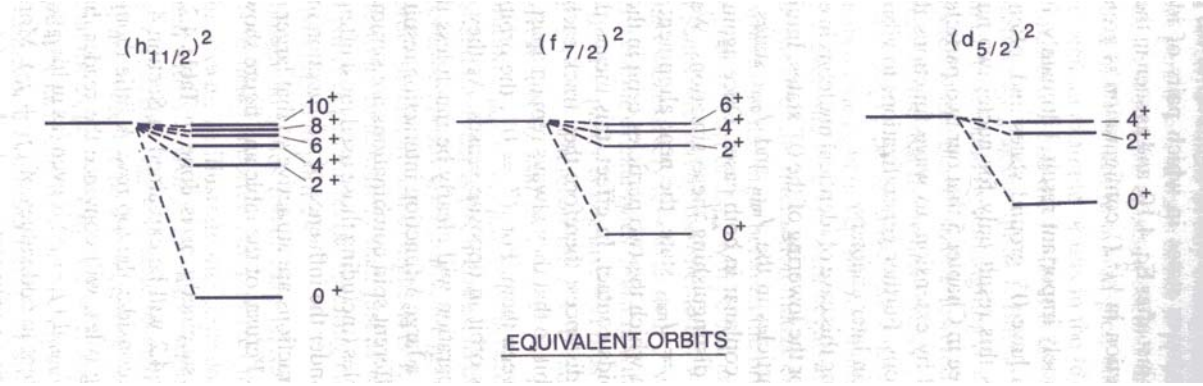
Residual Interactions and Two-Particle Configurations

For closed shells and full *j* orbitals, we have the result that *J*=0. What happens in an incompletely filled *j* orbit?

Take as an example, two particles in a particular orbital, j^2, which we know will couple to give J= 2j, 2j-2, …., 0 taking into account indistinguishability and Pauli principle. So far our model would say that the excitation energy of this state is just the sum of the energy of the two particles i.e. $2E_{n\ell j}$. All of these different spin couplings would be degenerate in this model. Experimentally it is found that these states are not degenerate.

Residual interactions between the two nucleons cause scattering between orbitals.The amount of scattering depends on the relative motion of the two nucleons. The relative motion of two nucleons depends on the *J* value of the pair. As a result, the residual interaction will lift the *J*-degeneracy discussed above and split these states.

For example, a simple residual force might be the delta interaction, which is explicitly short-ranged in fact only operates if the two particles are at the same position: $H_{delta}=V_0\delta(r_1,r_2)$. Calculations with this force lead to a fall in the 0^+ energy.



Most possible forms for the residual interaction will split states in a similar fashion, pushing the 0^+ state down to become the lowest lying state. This is the basis for an explanation for why all even-even nuclei have a 0^+ ground state.

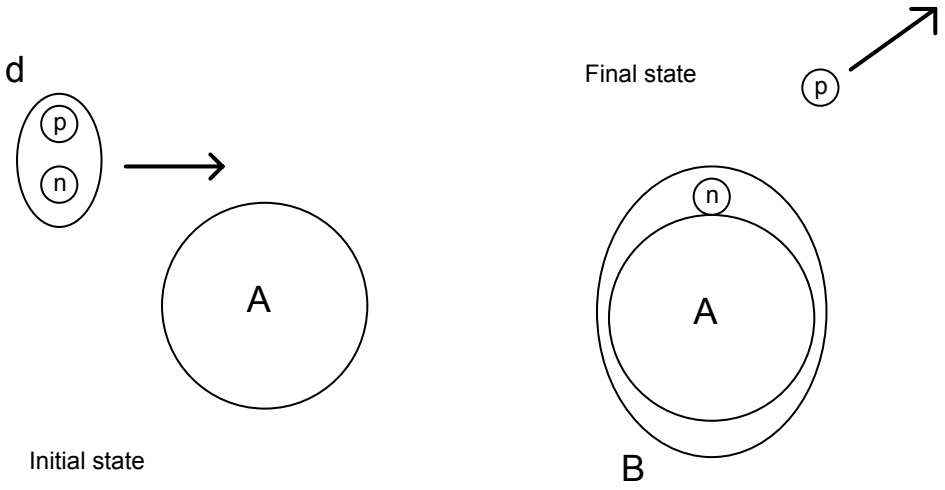
PC 4421 Lecture 7: Transfer Reactions

Introduction

We've talked a lot about how to cope with the problem of nuclear structure from the fundamental *ab initio* approaches using nuclear forces, through to mean-field theories and the problems of residual interactions. You should start asking some questions about how we know any of this is right. What experiments can you do to investigate whether single-particle descriptions are accurate? How do you know what energy the single-particle states have? How can you know whether a state in a nucleus with, say $J^{\pi}=9/2^{+}$, is one that is purely single particle in nature, with a wavefunction corresponding to a core plus a $g_{9/2}$ nucleon? How do you identify states which are mixed in nature with contributions from many different nucleon orbitals? There are many experimental observables we can use as probes; some of the best are nuclear reactions and electromagnetic moments.

Direct Single-Nucleon Transfer Reactions

The classic example of a single-nucleon transfer reaction is the A(d,p)B process. A neutron from the incident deuteron projectile is transferred to the target nucleus, A. The neutron occupies an unfilled single-particle state in the residual nucleus, B, and the rest of the projectile, now just a proton, flies onwards.

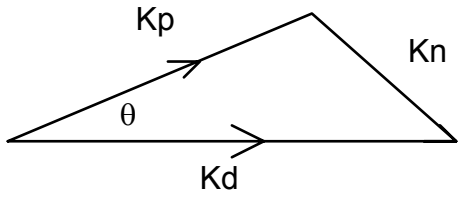


This is called a single-neutron stripping reaction. You can also pickup neutrons out of occupied single-particle states in a target in reactions such as (p,d). And there are proton-transfer reactions such as (d,^{3}he) and (^{4}he,^{3}h). Historically, the (d,p) reaction was the first to be studied and the forward or backward peaking in the angular distribution of the emitted proton suggested that the reaction was dominated by a direct, single-step process as opposed to a compound nucleus reaction where the whole deuteron is swallowed, there's lots of internal rearrangements then sometime last a proton pops out. The forward peaking suggested the simple picture of the neutron being transferred and the proton carrying on its way. To a first approximation, the emitted proton momentum, $\boldsymbol{k_p}$, is the sum of the translational momentum of incident deuteron plus the proton momentum with respect to the CM of the deuteron. Angular spread of the outgoing protons is then indicative of the momentum distribution of the proton inside the deuteron before the neutron was removed.

Such reactions identify single-particle states in a nucleus or the single-particle components in the wavefunction of the state, if it is mixed. A measurement of the energy of the ejectile ion, the proton in the case of (d,p), gives the excitation energy of the state populated by applying energy conservation. As

discussed below, the detailed shape of the angular distribution of the ejectile ions allows assignments to be made of the angular momentum transferred in the reaction, giving information about the spin and parity of the states populated in the residual nucleus, B. Measurements of the reaction rate or cross section gives a measure of the single-particle purity of the wavefunction of the residual state; if the state is empty you can easily put neutrons in it with (d,p). If it is partially occupied by scattering due to residual interactions there won't be room for as many neutrons and the cross section will be lower.

To make the analysis of the relative motion simple, assume that the deuteron and proton have sufficiently large kinetic energies that the Coulomb interaction on them can be ignored and think semi-classically to avoid dealing with the quantum mechanics of reaction theory. The incoming deuteron has a linear momentum of $\hbar\boldsymbol{k_d}$, the outgoing proton has $\hbar\boldsymbol{k_p}$ and the neutron carries a momentum, $\hbar\boldsymbol{k_n}$, into the target nucleus, A. These have to observe conservation of linear momentum such that: $\boldsymbol{k_n=k_p-k_d}$



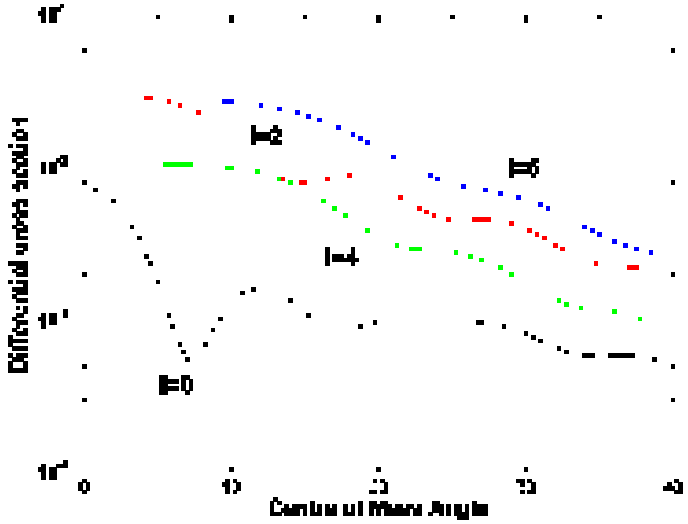
If the transfer of the neutron occurs at a certain distance *b* from the centre of the target nucleus, then the maximum angular momentum that can be transferred by the neutron is $\hbar k_n b$. This distance can be anything from zero up to the radius of the target, *R* (plus a little bit more to account for the range of the strong interaction if you wanted to be absolutely precise). This transferred angular momentum has to come from the relative orbital angular momentum between the projectile and the target, so the angular momentum taken from the entrance channel is restricted to:

$$k_n R \geq L$$

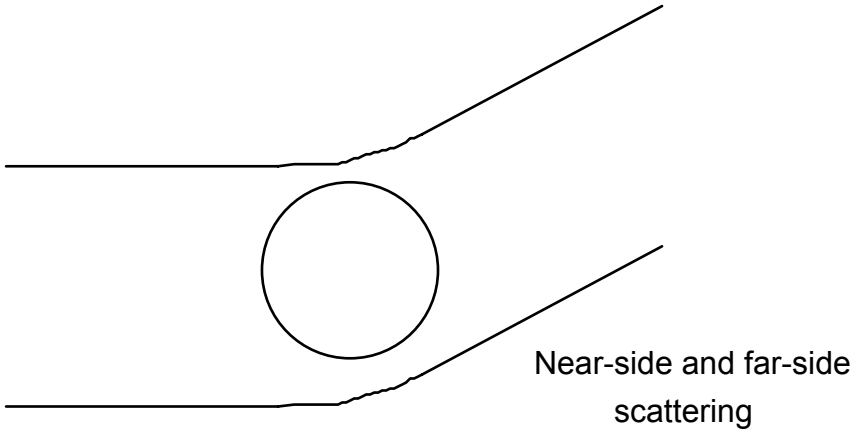
Given the vector diagram above and this inequality we can now understand why different *L* transfers have different angular distributions.
When *L=0*, the inequality is always satisfied, but it is always found to be peaked at an angle, θ=0. This is because the internal momentum of the proton is very small with respect to the translational momentum of the deuteron, and the proton therefore pretty much keeps going in the direction that the deuteron was travelling. When *L* is greater than zero, k_n has to be larger in magnitude than *L/R*. So looking at the vector diagram there is a minimum angle at which the transfer can take place. At this angle there will be a pronounced peak in the angular distribution, essentially for the same reason that the *L=0* is peaked at θ=0. This peak moves to greater and greater angles the larger the angular momentum transfer.

Once you know what L is you can then use angular momentum coupling to work out what the possible spin of residual nucleus. If you start off with an even-even target with J_A, then you are adding orbital angular momentum *L* and the intrinsic spin of the transferred nucleon, s=½, so J_B is the coupling of *L*, J_A and ½. On a spin zero target, for example, you end up with two possibilities: $J_B = L+½$ or $L-½$. Furthermore, remembering that the parity carried by a spherical harmonic wavefunction is $(-1)^L$, it should not be surprising that the parity change in the reaction is $(-1)^L$.

This analysis is semi-classical and so reality is likely to be fairly different. Here are some examples of angular distributions for various L transfers in the Sn(^{4}He,^{3}H) reaction.



The peak of the cross section does move out in angle with increasing L, but the maximum are wide and there are undulations in the angular distribution, which are also characteristic of L. There occur from quantum mechanical interference of ejectile proton wavefunctions generated by transfer of the neutron on one side of the target and the other which correspond to the same scattering angle.



With some reaction theory you can calculate the cross section for transfer to an ideal pure single-particle orbital. In reality the cross section is less than this:

$$\frac{d\sigma}{d\Omega} = S^2 \frac{d\sigma}{d\Omega}_{dwba}$$

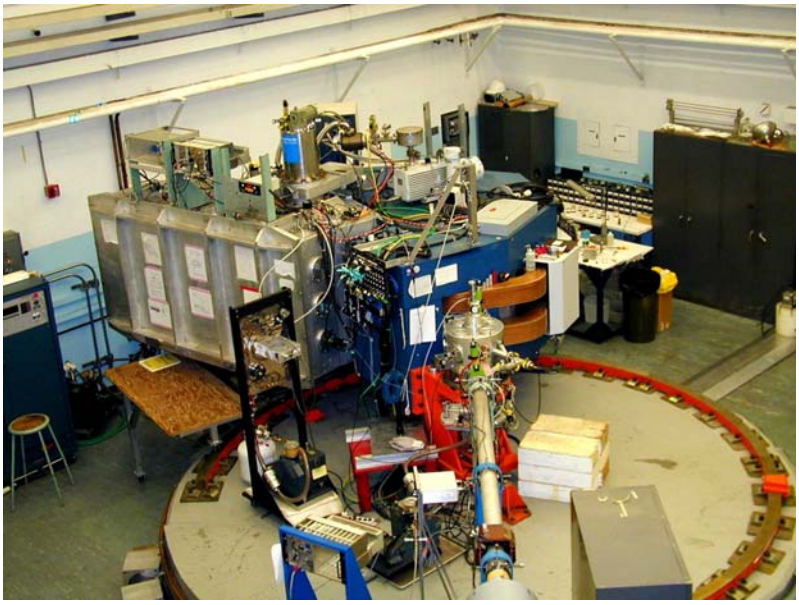
S^2 is the spectroscopic factor and is between 0 and 1. It measures the overlap of a pure njℓ single-particle state with the actual wavefunction the nucleon ends up in.

i.e if $|\psi\rangle \approx |\phi_{nj\ell}\rangle$ then $S = \langle\psi|\phi_{nj\ell}\rangle = \langle\phi_{nj\ell}|\phi_{nj\ell}\rangle = 1$

if $|\psi\rangle \approx \sum_{n'j'\ell'} a_{n'j'l'} |\phi_{n'j'\ell'}\rangle$ then $S = \langle\psi|\phi_{nj\ell}\rangle = \sum a_{n'j'\ell'} \langle\phi_{n'j'\ell'}|\phi_{nj\ell}\rangle = a_{nj\ell}$

So these reactions can probe the mixing of single-particle states produced by residual interactions.

Here's an example of a real experiment. The problem here was associated with measuring the purity of proton single-particle states in odd-A Sb (Z=51) isotopes. Such nuclei should be a closed magic proton core of Sn with Z=50 and an odd neutron. Excited states Sb should be formed by just moving the odd proton around the single-particle levels. But are the actual observed states based on this picture or are they mixed wavefunctions? The idea is to populate the states in Sn(^{4}He,^{3}H)Sb proton stripping reactions, measure the cross sections and thus figure out the spectroscopic factors.

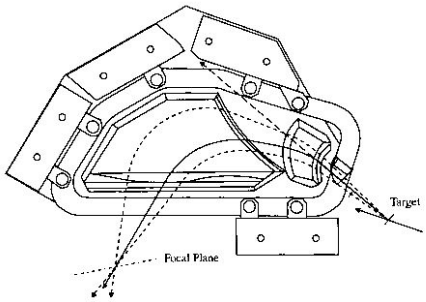


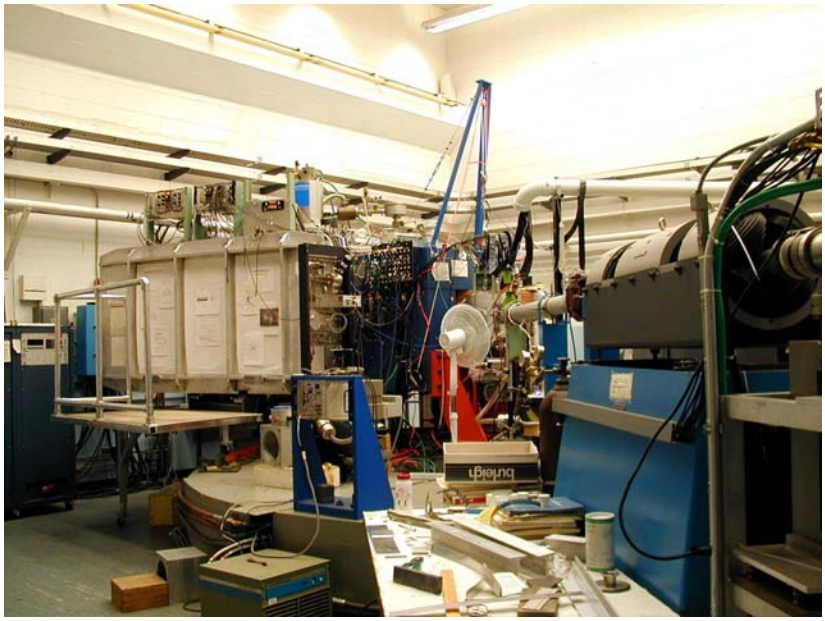
Fire a beam of high energy alpha particles from an accelerator onto a thin target.

Use a magnetic spectrometer to analyse the momenta of the reaction products, and thus the proton energies, from which you can get the excitation energies of the states populated.

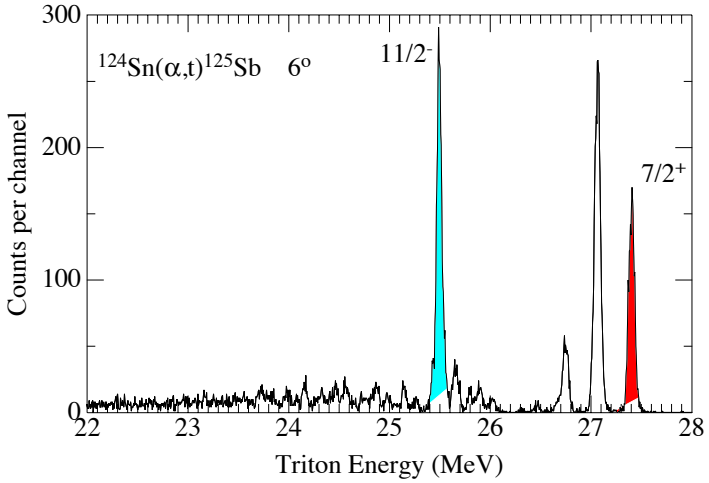
The beam needs transporting in a vacuum to avoid collisions with air molecules.

You need to detect the ejectile ions at the focal plane and measure their position along it which is related to their momentum.

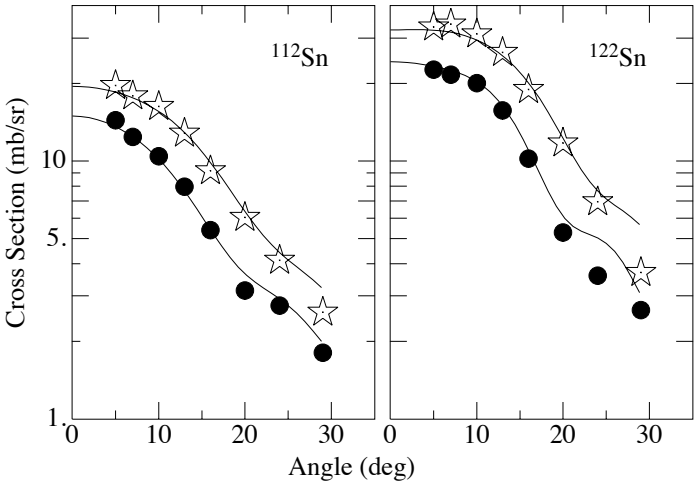




On the right is a spectrum from a reaction on a ^{124}Sn target. The physics interest here is in the $11/2^-$ and $7/2^+$ states and the question is, how much are these based on $h_{11/2}$ and $g_{7/2}$? They are clearly populated in the spectrum.



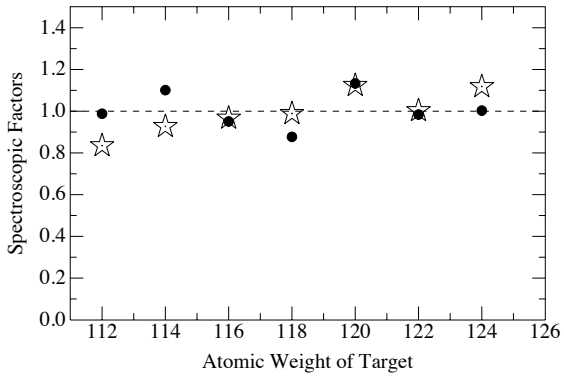
Below that are the angular distributions for these states, which are well reproduced by reaction theory for L=4 and L=5 transfers. Work out for yourselves which of the circles and stars corresponds to which L transfer. You could check this out in the original paper which is published in Physical Review Letters 92, 162501 (2004). Both this and the Nature paper, mentioned below, can be accessed from a University computer via the journal web pages associated with the John Rylands.



If I told you the stronger peak between the $11/2^-$ and $7/2^+$ states was characterised by L=2, could you identify what single-particle state it is?

The final result for the spectroscopic factors is at the bottom. All of these states appear to have S~1, and therefore are reasonably good single-particle states.

If you're interested in why this is so important to measure, there is a very accessible review of the experiment in the journal NATURE Vol 430, 29th July 2004, page 517. You have more than sufficient physics knowledge to understand all the details of this review so you're encouraged to read it.



PC 4421 Lecture 8: Magnetic Dipole Moments

Electromagnetic Multipole Moments

The electric or magnetic fields associated with any arbitrary charge or current distribution can be described as the sum of a series of multipoles each with a characteristic spatial dependence:

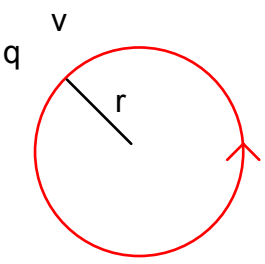
E= charge (L=0) *term in $1/r^2$ + dipole (L=1) * term in $1/r^3$ + quadrupole (L=2) * term in $1/r^4$+…..
M= dipole moment * term in $1/r^3$ + quadrupole moment * term in $1/r^4$+…..

For magnetic fields the magnetic monopole either does not exist or it is extremely rare, so the first term in the expansion does not exist.
For simple distributions the series terminate abruptly. For example, a sphere of charge just had a electric monopole term, a circular current loop purely a magnetic dipole term. Small distortions from sphericity introduce higher order multipoles. The first evidence for non-spherical nuclear shapes came from the observation of anomalously large electric quadrupole moments.
Each multipole has an operator, $\hat{O}$, associated with it that has a definite parity, i.e. a characteristic behaviour under the transformation **r**→-**r**. Electric moments have parity $(-1)^L$; magnetic moments have parity $(-1)^{L+1}$.
In quantum mechanics they are calculated by: $\int \psi^* \hat{O} \psi \, dV$. As ψ appears twice, its parity is not important, but if $\hat{O}$ has odd parity the integrand is an odd function and integrates to zero over all space. As a result all odd-parity moments must vanish. Other restrictions are placed on the existence of different multipole moments depending on the spin of the state of interest. In general, for a particular multipole to exist, the spin of the state has to be equal or greater than L.

Electric monopole moment:

This is just the charge on the nucleus.

Magnetic dipole moment:

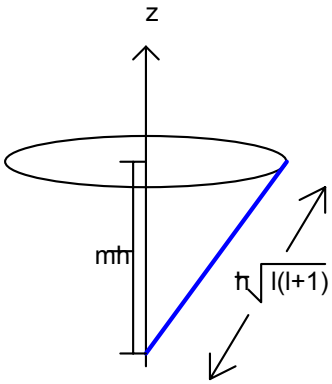


Classically, for a particle with charge, q, moving in a circular loop of radius, r, at speed, v, the magnetic dipole moment is given by:

$$\left|\underline{\mu}\right| = IA = \frac{q}{2\pi r / v}\pi r^2 = \frac{qvr}{2} = \frac{e}{2m}\left|\underline{\ell}\right|$$

Quantum mechanically you can replace classical quantities with their operators such that $\hat{\underline{\mu}} = \frac{e}{2m}\hat{\underline{\ell}}$

We need to know what the expectation value of the vector $\hat{\underline{\ell}}$ for a state which is an eigenfunction of $\hat{\ell}^2$ and $\hat{\ell}_z$. This requires a bit of thought, since the angular momentum vector itself is not constant of motion. Remember that the good quantum numbers are the length of the angular momentum vector and its projection on the z axis. One way of visualising this is to think of a vector of length $\hbar\sqrt{\ell(\ell+1)}$ which precesses around the z axis in such a way as to keep the projection on that axis constant, as in the next figure.



Writing out in component form $\left\langle \hat{\underline{\ell}} \right\rangle = \left\langle \hat{\ell}_x \right\rangle \underline{i} + \left\langle \hat{\ell}_y \right\rangle \underline{j} + \left\langle \hat{\ell}_z \right\rangle \underline{k}$

Appealing to the vector model illustrated on the left, the time averages are found to be $\left\langle \hat{\ell}_x \right\rangle = \left\langle \hat{\ell}_y \right\rangle = 0$ and $\left\langle \hat{\underline{\ell}} \right\rangle = \langle \ell_z \rangle \underline{k} = m\hbar \underline{k}$, where $\underline{k}$ is a unit vector in the z direction.

The magnetic moment is defined as the largest expectation value for the operator, which requires the highest value that the expectation of $\underline{\ell}$ can take, substituted into the above formula. This highest value is therefore $\ell\hbar$.

A fully quantum mechanical method gives an overall answer $\mu = \frac{e\hbar}{2m}\ell$.

If the particle is an electron, the multiplicative factor is known as the Bohr magneton, in units of eV/T:

$$\mu_B = \frac{e\hbar}{2m_e} = 5.7884 \times 10^{-5}$$

If the particle is a proton, it is known as the nuclear magneton, again in eV/T:

$$\mu_N = \frac{e\hbar}{2m_p} = 3.1525 \times 10^{-8}$$

So we can rewrite the magnetic moment as $\mu = \mu_N g_\ell \ell$ where g_ℓ is known as a g-factor and is 1 for protons and 0 for neutrons. The quantum mechanical operator can be rewritten as

$$\hat{\mu} = \frac{g_\ell \mu_N \hat{\ell}_z}{\hbar}$$

.

So much for orbital contributions, what about spin?

Define a similar contribution for intrinsic spin contributions to the magnetic moment:

$$\mu_s = \mu_N g_s s$$

where s is ½ for a fermion.

For *point-like* fermions the Dirac equation shows that the intrinsic spin g-factor is 2.0. In fact, a more accurate value for electrons is 2.0023…, due to QED corrections.

Measuring the magnetic moment of a free nucleon gives the following answers for the spin g-factors:

$$g_s^{\pi} = 5.5856912(22)$$

$$g_s^{\nu} = -3.8260837(18)$$

This has two important implications. Firstly, nucleons are not point fermions. And secondly, whilst the neutron has an overall charge of zero, it can only generate a magnetic moment if it has a charge distribution within it.

As you might imagine, nucleon configurations whose overall angular momentum couples to zero contribute nothing to the overall magnetic moment. Another interesting thing to keep in mind is that all nuclear magnetic moments are small <6μ_N.

Let's try again with the simplest nucleus, the deuteron:

Deuteron magnetic moment: the nucleon configuration can be written as $\pi s_{1/2} \nu s_{1/2}$. There is no orbital contribution and gs spin-parity is 1^+, so nucleon spins are "parallel" and the separate moments should add:

$$\mu_d = \frac{1}{2}\mu_N (g_s^{\nu} + g_s^{\pi}) = 0.879804\mu_N$$

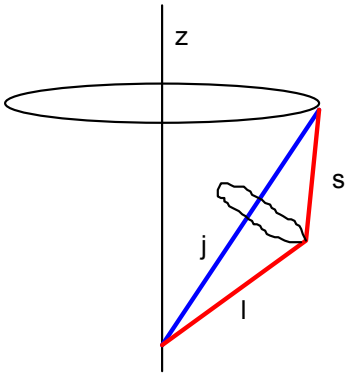
Experimentally the result is 0.8574376(4)μ_N. So on the right lines but what might be at issue?

(a) Firstly we know the ground state is not a pure S state, there is a small D contribution:

$$\psi_d = a_0\psi_{\ell=0} + a_2\psi_{\ell=2}$$
$$\langle\mu\rangle = a_0^2\mu_0 + a_2^2\mu_2$$

(b) There is reason to believe that free nucleon spin g-factors are not necessarily the best things to use. The nucleon-nucleon force can be thought of as exchange of pions, and these virtual particles can contribute to the magnetic moments 'in-medium'.

Single Nucleon in a j-orbital



Here's a case where ℓ is not zero. First consider the vector model in the diagram. In this case the orbital and spin angular momenta precess in such a way as to keep the total angular momentum vector of constant length. This total angular momentum itself precesses about the z-axis in such a way as to keep its projection on the z-axis a constant.

$$\langle\hat{\underline{\mu}}\rangle = \mu_N\left[g_\ell\langle\hat{\underline{\ell}}\rangle + g_s\langle\hat{\underline{s}}\rangle\right]/\hbar$$
$$= \mu_N\left[g_\ell\langle\hat{\underline{j}}\rangle + (g_s - g_l)\langle\hat{\underline{s}}\rangle\right]/\hbar$$

The last step uses $\hat{\underline{j}} = \hat{\underline{\ell}} + \hat{\underline{s}}$.

Now following the philosophy and definitions above it is relatively easy to work through to some simple formulae.

There are then two different results corresponding to the two different couplings, $j_>=\ell+s$ and $j_<=\ell-s$, which are known as the Schmidt limits:

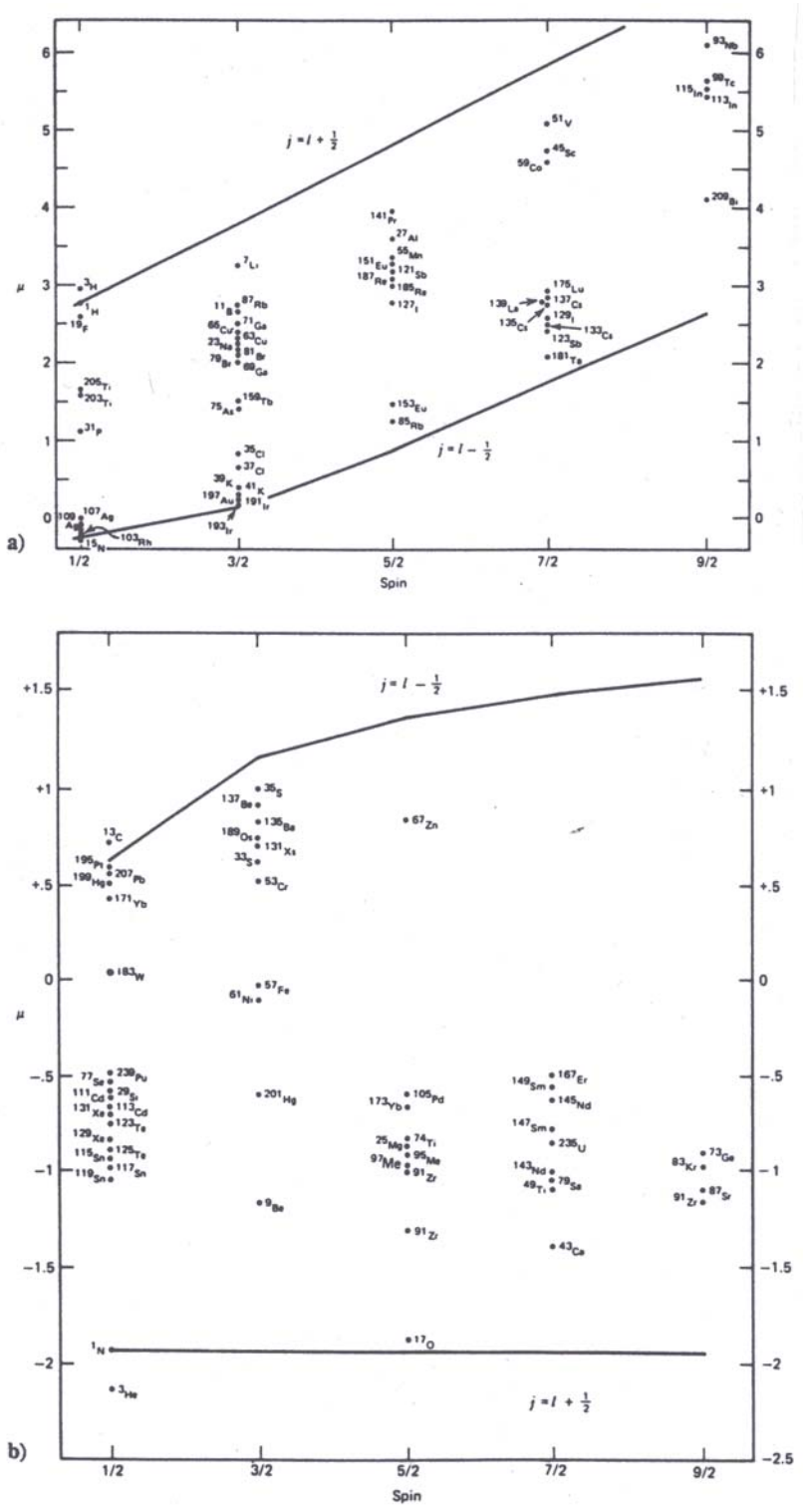
For $j_>$: $j=\ell+s$; $$\langle\mu\rangle = \left[g_\ell(j-1/2) + g_s/2\right]\mu_N$$

For $j_<$: $j=\ell-s$; $$\langle\mu\rangle = \left[g_\ell\frac{j(j+3/2)}{(j+1)} - g_s\frac{j}{2(j+1)}\right]\mu_N$$

In nuclei with a closed core with no spin and an odd nucleon, the magnetic moment comes from the valence particle, so the Schmidt limits should work. It turns out that the experimental values fall between these two limits with considerable scatter. If you arbitrarily reduce the spin g-factors to 60% of the free value you will get a better description. This is sometimes done with the excuse that it reflects the in-medium mesonic effects.

The considerable scatter in the data points indicates an oversimplification; many wavefunctions are actually more complicated than just a single-particle orbit outside an inert core and magnetic moments appear quite sensitive to small admixtures into the wavefunction.

More refined theories which properly account for the mixing of single-particle wavefunctions are needed to account for the details of magnetic moments.



PC 4421 Lecture 9: Electric Quadrupole Moments

Electromagnetic Multipole Moments

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For magnetic fields the magnetic monopole either does not exist or it is extremely rare, so the first term in the expansion does not exist.
For simple distributions the series terminate abruptly. For example, a sphere of charge just had a electric monopole term, a circular current loop purely a magnetic dipole term. Small distortions from sphericity introduce higher order multipoles. The first evidence for non-spherical nuclear shapes came from the observation of anomalously large electric quadrupole moments.
Each multipole has an operator, $\hat{O}$, associated with it that has a definite parity, i.e. a characteristic behaviour under the transformation **r**→-**r**. Electric moments have parity $(-1)^L$; magnetic moments have parity $(-1)^{L+1}$.
In quantum mechanics they are calculated by: $\int \psi^* \hat{O} \psi \, dV$. As ψ appears twice, its parity is not important, but if $\hat{O}$ has odd parity the integrand is an odd function and integrates to zero over all space. As a result all odd-parity moments must vanish. Other restrictions are placed on the existence of different multipole moments depending on the spin of the state of interest. In general, for a particular multipole to exist, the spin of the state has to be equal or greater than L.

Electric quadrupole moment:

Classically, the electric quadrupole moment of a charge distribution, $\rho_q(\mathbf{r})$, is given by:

$$eQ = \int \rho_q(\mathbf{r})(3z^2 - r^2)dV$$

For an orbiting point particle with charge, *e*, the charge distribution is related to the density distribution by $\rho_q(\mathbf{r}) = e\,\rho(\mathbf{r})$. The quadrupole moment is then written as:

$$Q = \int \rho(\mathbf{r})(3z^2 - r^2)dV = 3 < z^2 > - < r^2 >$$

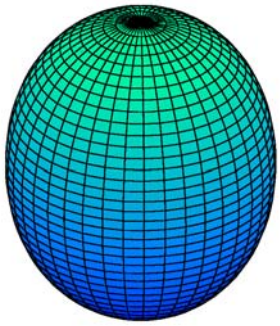
So what does this quantity actually tell us about? If the charge distribution is spherically symmetric then

$$< x^2 > + < y^2 > + < z^2 > = < r^2 >$$

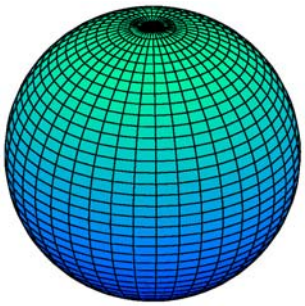
via the equation for a spherical surface. Also each of the three coordinate directions is equivalent, so this reduces to $3\langle z^2\rangle = \langle r^2\rangle$. As a result the quadrupole moment is zero for spherically symmetric distributions. A quadrupole moment therefore indicates the extent to which the nuclear shape, more precisely the nuclear charge distribution, is distorted away from a sphere.

One type of distortion away from sphericity is a cigar or *prolate* shape; imagine grabbing two sides of the sphere and pulling then away from each other. If we chose the *z* axis to be along this pulling direction, which is better described as an axis of symmetry, then the extent of the charge distribution in the *z* direction is greater than in the *x* and *y* directions. In fact the extent in the *z* direction is greater than the average extent over all directions. Thus $\langle z^2\rangle > \langle r^2\rangle$, and therefore the quadrupole moment is positive.

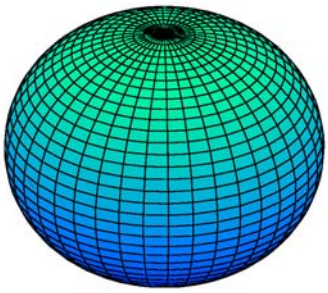
You can form another sort of shape by pushing two points on opposite sides of the sphere, squashing the charge distribution towards a plate-like shape. Such deformation is called *oblate*. Here the extent of the charge distribution is smallest in the *z* direction, giving $<z^2> < <r^2>$ and therefore a negative quadrupole moment.



Prolate



Spherical



Oblate

For a closed core of nucleons, we know that the overall angular momentum will couple to $J=0$. The spin and the orbital angular momentum have to be zero and so the wavefunction must have an angular part which is proportional to Y_{00}. This is actually independent of angles and therefore is a spherically symmetric wavefunction charge distribution. Closed-core nuclei should therefore have no quadrupole moment.
A closed-core plus one nucleus would therefore have a quadrupole moment due to the contribution of the odd valence nucleon. If we first think about a nucleon which is in an extreme orbit, where it just moves in the *xy* plane at $z=0$, then the quadrupole moment will be $Q=-<r^2>=-r^2$. A quadrupole moment of such a particle is therefore related to the averaged mean-square radius.

In a quantum mechanical approach, the classical quantities are replaced by their quantum mechanical operators and the quadrupole moments are calculated as follows:

$$Q = \int \varphi^* (3\hat{z}^2 - \hat{r}^2)\varphi \, dV \quad \text{for protons}$$

$$= 0 \quad \text{for neutrons}$$

There is no quadrupole moment for neutrons since they have no charge. If you take the wavefunctions from an independent-particle shell model and calculate the integral you can get a general formula which depends on the particles overall angular momentum, *j*:

$$Q_{\mathrm{sin}\,gle-particle} = -\frac{(2j-1)}{2(j+1)} < r^2 >$$

The dependence on $<r^2>$ is comfortingly similar to our simple picture of a particle orbiting in a classical orbit. To go from quantum mechanics to classical physics you could take the limit of very large *j*, much bigger than unity. In that limit the quantum mechanical expression becomes the same as the classical one.

We could just use the classical result to get an order of magnitude estimate of the sizes of quadrupole moments in nuclei. If the valence particle orbits near the surface of a nucleus, then $r \sim r_0 A^{1/3}$:

$$|Q| \leq r_0^2 A^{2/3} \approx 0.06 - 0.5 \text{ barn}$$

A *barn* is a convenient unit to use. Note that Q has the units of area and one barn is equivalent to 10^{-24} cm^2.

So does all this work? You'll be expected to have some idea about how nuclear moments are measured so you'd better read up on it now (Krane Chapter 16), but in essence they can be measured by their interaction with electromagnetic fields external to the nucleus. Here are some results that we can try to interpret with single-particle models.

		EXPERIMENTAL QUADRUPOLE MOMENTS			
		Single particle		Single hole	
Single-particle state	**Calculated Q for proton**	**Proton orbit**	**Neutron Orbit**	**Proton Orbit**	**Neutron Orbit**
$1p_{3/2}$	−0.013	−0.0366 ^{6}Li		+0.0407 ^{11}B	+0.053 ^{9}Be
$1d_{5/2}$	−0.036	−0.12 ^{19}F	−0.026 ^{17}O	+0.140 ^{27}Al	+0.201 ^{25}Mg
$1d_{3/2}$	−0.037	−0.08249 ^{35}Cl	−0.064 ^{33}S	+0.056 ^{39}K	+0.45 ^{35}S
$1f_{7/2}$	−0.071	−0.26 ^{43}Sc	−0.080 ^{41}Ca	+0.40 ^{59}Co	+0.24 ^{49}Ti
$2p_{3/2}$	−0.055	−0.209 ^{63}Cu	−0.0285 ^{53}Cr	+0.195 ^{67}Ga	+0.20 ^{57}Fe
$1f_{5/2}$	−0.086		−0.20 ^{61}Ni	+0.274 ^{85}Rb	+0.15 ^{67}Zn
$1g_{9/2}$	−0.13	−0.32 ^{93}Nb	−0.17 ^{73}Ge	+0.86 ^{115}In	+0.45 ^{85}Kr
$1g_{7/2}$	−0.14	−0.49 ^{123}Sb		+0.20 ^{139}La	
$2d_{5/2}$	−0.12	−0.36 ^{121}Sb	−0.236 ^{91}Zr		+0.44 ^{111}Cd

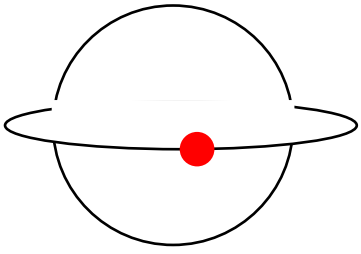
Things to note:

(i) The measured quadrupole moments for proton-particle states have the right sign, but generally the magnitude is larger than $Q_{\text{single-particle}}$.

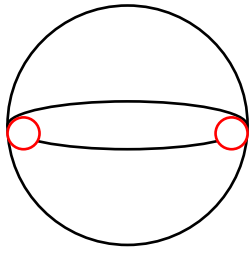
(ii) The measured quadrupole moments for proton-hole states have the opposite sign, and again have moments larger than $Q_{\text{single-particle}}$.

(iii) The measured quadrupole moments for neutron states are not zero, as expected for a neutral particle. They follow the same sign systematics as protons.

The signs can be understood by thinking about which overall shape that the charge distribution for the core-plus-valence-particle assumes. For a proton orbiting outside a closed core, charge is added to a spherical shape around the equatorial region. The overall time-averaged shape looks oblate. Compare this to a core plus a proton hole; material is removed from the equatorial region making it look prolate.



a time average of this would look oblate



a time average of this would look prolate

The reason why protons have higher quadrupole moments than expected from an independent-particle model is the same reason as that behind the neutron states having a non-zero moment. The core and the particle are not independent! There is an interaction between the core and the particle. For example, an odd neutron orbiting outside a spherical core will tend to interact with it, pulling it out towards the neutron. The resulting shape of the core will tend to be oblate as a result and so the system will have a negative quadrupole moment, despite the fact that the neutron has no charge. These effects are generally known as *core polarisation*. In the proton case, the independent particle model underestimates the quadrupole moment since the core polarisation distorts the spherical core away from sphericity increasing the quadrupole moment.

The effect of removing particles is less clear but can be understood by saying that a full spherical core has internal pushes and pulls due to the residual interactions which are balanced to give a spherical shape. Removing particles in the equatorial regions, removes interactions which would maintain the equatorial extent of the nucleus. As a result the core-plus-hole elongates into a prolate shape, thus giving a neutron hole state a non-zero moment and enhancing the prolate moment of a proton-hole state.
Often people will still try to force the independent-particle model on the results, even though there is core polarisation. You can do this by introducing an effective charge, e', for the particular single-particle orbital involved:

$$Q_{\mathrm{sin}\,gle-particle} = -\frac{(2j-1)}{2(j+1)}\frac{e'}{e} < r^2 >$$

The core polarisation effect is modelled into the appearance of an effective charge.

Quick note of caution:

As indicated above, quadrupole moments are measured by their interaction with an external electric field. This field points in a particular direction in space. The axis of symmetry will be at some angle with respect to the field direction. The results depend sensitively on that angle, but are independent of polar angle i.e. rotations of the system about the field direction. The bottom line is that the quadrupole moment coming directly from the experimental measurements, the *laboratory or spectroscopic* quadrupole moment, is actually the average of all possible rotations around the field direction. If you imagine spinning a cigar around an axis perpendicular to it, the time-averaged shape looks oblate! The laboratory quadrupole moment needs transforming into an *intrinsic* quadrupole moment before you can compare to theoretical estimates. This has already been done in the table above which lists intrinsic moments. If you look up data on quadrupole moments check what you are looking at. There is generally a sign change between intrinsic and spectroscopic quantities which can lead to confusion between oblate and prolate shapes!
Undergraduate students should be aware of this; postgraduates need to go and look up the details of the transformation and understand it in detail. See reference below.

Some other general electric moment results

An analysis of the actual operators for the electric moments will lead to a few general results about electric moments that are worth remembering.

(a) If a system has good parity, all odd electric moments, such as electric dipole, octupole moments etc., must disappear.

(b) For an electric 2^λ moment to exist, the spin of the state in question must be at least $\frac{1}{2}\lambda$. For example, in order to have a state with an electric quadrupole moment the spin of the state must be 1 or greater.

Undergraduates should just be aware of these results. Postgraduate students should go away and understand properly where they come from; work though Section 3.3 of Preston and Bhaduri Structure of the Nucleus, for example.

Electromagnetic Transitions

We have been dealing with moments involving calculation of the expectation of electromagnetic operators via integrals of the form $\int \psi^* \hat{O} \psi \, dV$. Similar electromagnetic operators can induce transitions between nuclear states which give rise to γ-ray emission. The series of electromagnetic multipole operators give rise to a series of different sorts of transitions: electric dipole, magnetic dipole, electric quadrupole etc. These differ in terms of the spin-parity changes that they induce.

Dipole photons carry away one unit of angular momentum. Since angular momentum is conserved, the difference between the spin of initial and final transitions is the photon angular momentum. You have to consider this as a vector sum and a better way of putting it is that the photon angular momentum and the spin of the final state must couple to result in the spin of the initial state. Thus emission of a dipole photon will change the nuclear spin by +1, 0 or −1 units of angular momentum. A quadrupole photon carries two units of angular momentum inducing changes +2,+1, 0, -1 or -2 units. An octupole photon carries three units and so on. *Stretched* transitions induce the maximum change in spin, for example stretched quadrupole transitions induce changes of +2 or -2; *folded* transitions induce less than this. This nomenclature comes from the pictures of the vector coupling. *Electric* and *magnetic* transitions differ in the parity changes they induce. Electric dipole, magnetic quadrupole, electric octupole etc. transitions change the parity of the nuclear state. Magnetic dipole, electric quadrupole, magnetic octupole etc. transitions do not change the parity of the nuclear state.

In general, the theory of electromagnetic transitions is complicated. There are some general statements that can be made. Usually there are many decay paths open to an excited state and the transition probability increases rapidly with transition energy, so the state will decay most strongly to the lowest state that it can get to according to angular momentum selection rules. However, the probability of a particular case rapidly decreases with increasing multipolarity to the extent that, unless there are special circumstances, only electric dipoles and quadrupole, and magnetic dipoles transitions are observed. Often in a particular transition more than one multipole is possible. For example, a nucleus decaying from spin 2^+ to spin 1^+ can go via a stretched magnetic dipole or a folded electric quadrupole; the resulting transition is said to be mixed and the *mixing ratio* tells you about the relative probability of the two options.

After these general energy and multipolarity dependences in γ-ray transition probabilities, there is also a dependence on the nuclear structure of the initial and final states i.e. their wavefunctions. From measurements of the lifetime of excited states, the transition probability may be extracted. The simple energy and multipolarity dependences can be stripped off, to leave a so-called *reduced transition probability* which should be dominated by nuclear structure effects. The reduced transition probabilities can be compared to the results of calculations within various models to give us information on what structures are involved. For example, simple estimates can be made using the wavefunctions from independent particle models. Here the assumption being made is that the transition can be attributed to changes in the motion of a single-nucleon alone. The transition probabilities which arise are called *Weisskopf units (WU) or single-particle estimates.* They are often used as convenient units in this kind of work. A transition rate of one WU would what you would expect for the contribution of one single particle. If a transition has a strength of about 1 WU then we'd expect it to involve transitions between single-particle states. If it is greatly enhanced above this estimate, then maybe more nucleons contribute. Given that we know residual interactions are an important part of nuclear structure, it is clear that in many cases such estimates are likely to be poor.

Undergraduate students should read up on the chapters in Krane on the background to gamma decay, multipolarity and transition rates. Postgraduate students are expected to know the detailed background to this including all the assumptions that go into the calculation of single-particle estimates.

PC 4421 Lecture 10: Pauli Principle, Antisymmetrisation and Isospin

The nucleons that make up the nucleus have two important properties. Firstly, you cannot distinguish one proton/neutron from another proton/neutron. All protons are indistinguishable and all neutrons are indistinguishable. We can extend this to also say that, as far as strong or nuclear interaction properties are concerned, no nucleon is distinguishable from any other nucleon. This charge independence symmetry is at the root of the concept of *isospin.* This is a seemingly obscure quantity but it allows simplicity and transparency when specifying wavefunctions and has some useful properties giving rise to useful selection rules.

Pauli Principle and Antisymmetrisation

Nucleons are fermions and therefore should obey the Pauli principle. We can guarantee this if we construct wavefunctions which are antisymmetric with respect to particle exchange.

Consider for now a simple two-particle system with no interactions between the two identical particles. Under these conditions the Hamiltonian is simply the sum of the Hamiltonians for the two particles alone:

$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

You can easily show by substitution that a simple product wavefunction, $\Psi=\varphi_a(r_1)\varphi_b(r_2)$, satisfies the Schrodinger equation, $\hat{H}\psi = E\psi$, if $E=E_1+E_2$. Here the a and b represent the quantum numbers of the two single-particle states, and r_1 and r_2 are the spatial coordinates of the two nucleons. *(Do it yourself to make sure!)* We're ignoring spin until later on.

There are problems with writing the wavefunction as $\Psi=\varphi_a(r_1)\varphi_b(r_2)$. It suggests that you can label the first nucleon and distinguish it from the second; if you exchange the first for the second nucleon you get a different state $\Psi=\varphi_a(r_2)\varphi_b(r_1)$. Also if the two single-particle states are the same, $a=b$, the wavefunction becomes $\Psi=\varphi_a(r_2)\varphi_a(r_1)$, rather than zero as expected by the Pauli principle.

We can construct something which obeys Pauli by forming the wavefunction:

$$\psi = \frac{1}{\sqrt{2}}\left[\varphi_a(r_1)\varphi_b(r_2) - \varphi_a(r_2)\varphi_b(r_1)\right]$$

By substitution, show that this wavefunction satisfies the Schrodinger equation for the two-particle system and that it is properly normalised.

It is clear that in this particular case if $a=b$, the wavefunction is zero and therefore the Pauli principle is obeyed. If you perform a particle exchange operation on this wavefunction, where you swap the first for the second ($1\rightarrow2$) nucleon and the second for the first ($2\rightarrow1$) nucleon, you end up with the final answer $-\Psi$. This wavefunction is therefore antisymmetric under particle exchange. Generally, wavefunctions must be antisymmetric to be consistent with the Pauli principle. But here we've been only considering simple spatial wavefunctions!

In general, the Hamiltonian depends on both spatial and spin components. Consider a simple separation of spin and spatial coordinates can be performed such that the wavefunction is written as a product of a spatial and a spin part, ΨX. In order to be consistent with the Pauli principle, it is the overall wavefunction that must be antisymmetric. This means that either the spatial part is antisymmetric combined with a symmetric spin part, or the spatial part is symmetric and the spin part is antisymmetric.

Consider the possible spin wavefunctions of two identical independent nucleons. They both have spin-1/2 and so the system can couple to give and overall spin of S=0 or 1.

Let's take the S=1 possibilities first. To have S=1, we must have wavefunctions with m_S=+1, 0 and −1. And remember that $M_S=m_{s1}+m_{s2}$. To make M_s=1 we require m_{s1} and m_{s2}=+½. For M_s=−1 we require m_{s1} and m_{s2}=−½. If we swapped 1 for 2 and visa versa for these wavefunctions we would see that they are symmetric under particle exchange since each nucleon has the same quantum numbers. (We would therefore have to have an antisymmetric spatial component). The M_S=0 wavefunction could be made from either $m_{s1=}$+½ and m_{s2}=−½, or $m_{s2=}$+½ and m_{s1}=−½. In order to make the symmetry consistent within the triplet of states we would therefore construct the spin component of the wavefunction for the S=1 states as follows:

S=1 TRIPLET	Symmetric spin component of wavefunction	Antisymmetric spatial component of wavefunction
M_S=+1	$X = X_{+1/2}(1)\, X_{+1/2}(2)$	
M_S=0	$X = \sqrt{2^{-1}}[X_{+1/2}(1)\, X_{-1/2}(2) + X_{-1/2}(1)\, X_{+1/2}(2)]$	$\Psi = \sqrt{2^{-1}}[\varphi_a(r_1)\varphi_b(r_2) - \varphi_b(r_1)\varphi_a(r_2)]$
M_S=−1	$X = X_{-1/2}(1)\, X_{-1/2}(2)$	

You can also show that the form chosen for the S=1, M_S=0 wavefunction is correct by applying a lowering operator to the S=1, m_S=+1 wavefunction, a raising operator to the S=1, m_S=−1 wavefunction, or using Clebsch-Gordan coefficients. *Postgraduate students should do all of these for themselves!*

The S=0, M_S=0 wavefunction has either $m_{s1=}$+½ and m_{s2}=−½, or $m_{s2=}$+½ and m_{s1}=−½. We need to construct a wavefunction out of these possibilities with definite particle-exchange symmetry and we've already used a symmetric combination above. It also must be orthogonal to the S=1 wavefunctions. *You should convince yourselves that the following is suitable.* Since it is an antisymmetric spin wavefunction, we need to combine it with a symmetric spatial component.

S=0 SINGLET	Antisymmetric spin component of wavefunction	Symmetric spatial component of wavefunction
M_S=0	$X = \sqrt{2^{-1}}[X_{+1/2}(1)\, X_{-1/2}(2) - X_{-1/2}(1)\, X_{+1/2}(2)]$	$\Psi = \sqrt{2^{-1}}[\varphi_a(r_1)\varphi_b(r_2) + \varphi_b(r_1)\varphi_a(r_2)]$

Things are getting complicated! If we had two protons or two neutrons, we would need to construct antisymmetric wavefunctions. If we had a proton and a neutron we would not.

Remember though…..

This is a simplified approach. The simple separation of spin and spatial components discussed here is not so simple in the case where there is coupling between spin and spatial variables such as a spin-orbit term in the Hamiltonian. But one still needs to make sure that the overall wavefunction is antisymmetric with respect to particle exchange. Here the spin-orbit coupling would be done first, and then antisymmetrisation as a second step. For example, a $\pi d_{5/2} f_{7/2}$ configuration coupled to overall spin, J, would have an antisymmetrised wavefunction $\Psi = \sqrt{2^{-1}}[\{\varphi_{d5/2}(r_1)\varphi_{f7/2}(r_2)\}_J - \{\varphi_{f7/2}(r_1)\varphi_{d5/2}(r_2)\}_J]$.

Remember back to the M-scheme, where we explicitly imposed the effects of indistinguishablility and Pauli principle on coupling possibilities when combining single-particle states where spin-orbit terms had been included. This restricted the possible spins of a proton-proton or neutron-neutron system, but not a proton-neutron system. For example, $\pi d_{5/2}^2$ or $\nu d_{5/2}^2$ will only couple of J=0,2, or 4, whereas $\pi d_{5/2}\, \nu d_{5/2}$ can couple to J=0, 1, 2, 3, 4 or 5.

Isospin

You can invent a scheme to simplify things a little which then takes on more significance than you would expect. Protons and neutrons are identical as far as the operation of the strong nuclear force is concerned. Here are a few observations that indicate that we could start to treat them as two different types of the same particle:

(a) The proton-neutron mass difference is tiny, $\Delta m/m=0.14\%$.

(b) In low-energy (<5 MeV) np and pp scattering, the cross section for the ^{1}S channel is equal to within a few % if Coulomb effects are corrected.

(c) Change all the protons in a nucleus to neutrons, and all the neutrons to protons, and generate its mirror system. Apart from small Coulomb effects and the n-p mass difference, the energy levels are remarkably similar. The nuclear interactions are therefore unchanged if n-n forces are exchanged for p-p forces and the nuclear force must be CHARGE SYMMETRIC.

(d) Gradually exchange protons, one by one for neutrons and generate a sequence of nuclei of the same mass but different numbers of protons and neutrons. States in nuclei in this isobaric sequence have analogues in the other members of the sequence. The nuclear interactions between n-p and p-p and n-n are therefore the same and the nuclear force must be CHARGE INDEPENDENT.

An example was discussed before in ^{30}Si, ^{30}P and ^{30}S where analogue states were seen in all three. Some states though were unique to ^{30}P and we will see that these are states which are allowed in an np system but forbidden in the pp or nn cases by Pauli.

This is the origin of the name *nucleon.* Heisenberg was the first to treat protons and neutrons as two substates of the same particle, the nucleon back in 1932. This is a two substate system, rather like intrinsic spin-½ which can have substates $m_s=+½$ or $-½$, hence the name of this new characteristic, *isospin.*

A nucleon has isospin $t=½$; a proton has $t_z=-½$ and a neutron has $t_z=+½$. This z doesn't refer to real space anymore; isospin operates in a fictitious new space called isospin space. Don't think too much about this, in a sense it is not real. We're inventing something which is useful to us, more in a book keeping sense for the moment. All the quantum mechanical mathematics of spin operators, Pauli spin matrices, angular momentum coupling and raising/lowering operators can be applied to isospin in a completely analogous way, but we're not going to complicate things any further with needless mathematics. *Unless you're a postgraduate student; if you are you need to go and read in detail about these things.* You need to think about a wavefunction now with three components: spatial, spin and isospin. We're going to see an example of isospin used in anger to classify some states.

Example: the two-nucleon system

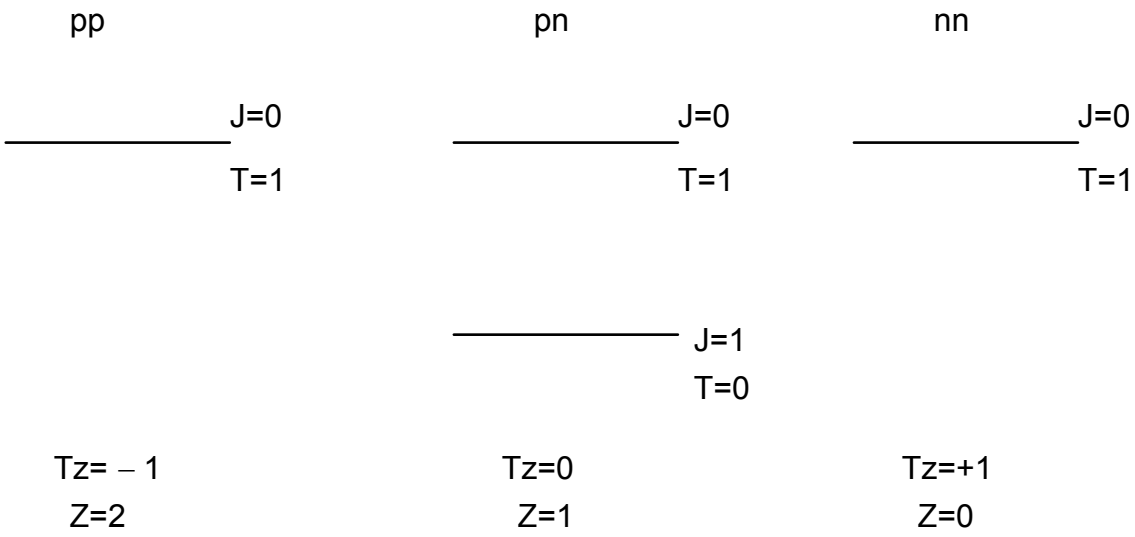
Take two nucleons and couple their isospin together. Each nucleon carries $t=½$, so we can couple them together to make $T=0$ or 1. The third components couple according to $T_z=t_{z1}+t_{z2}$. A system of states is then generated completely analogous to the spin components discussed above. The $T=0$ state is a singlet with $T_z=0$, and it is antisymmetric under particle exchange. The $T=1$ coupling is a triplet of states with $T_z=+1$, 0, and −1 and is symmetric under particle exchange. What does all this mean?

We have two nucleons so we have generated nuclei with $A=2$. The third component tells us something important. Protons individually have $t_z=-½$ and neutrons $t_z=+½$, so the third component is all wrapped up in what electrical charge the system has. The quantity, $-(t_z-½)$, tells us the charge on a nucleon. In a multinucleon system, the overall charge can be found by summing $-(t_z-½)$ over all the nucleons. Doing this gives you, $Z=-(T_z-A/2)$. For the $A=2$ nuclei, $T_z=+1$, 0, and −1 must therefore correspond to $Z=$ 0, 1 and 2, or equivalently two neutrons (a dineutron), the deuteron and two protons (a diproton).

Notice that in the dineutron and diproton, there is no T=0 state since it is prevented by the Pauli principle. But in the deuteron, both T=0 and T=1 states are available.

In addition, for the A=2 case we would expect that the spatial wavefunction is going to be $s_{1/2}$ for both nucleons. The spatial wavefunction in this case cannot be antisymmetric, and only a symmetric version is non-zero. *Prove this by looking at the spatial two-particle wavefunctions above and substitute in the same single-particle states.* To get an overall antisymmetric wavefunction, if the spin part is symmetric, the isospin part must be antisymmetric, or visa versa. So the T=1 (symmetric) state must have J=0 (antisymmetric). The T=0 state must have J=1 for the same reason.

Combining this with the knowledge of the deuteron we have from before, namely the ground state is J=1 and all other states are unbound and at higher energies, we can draw a diagram summarising all of this.



We've used charge independence to tell us that, apart from Coulomb effects and pn mass differences, the T=1 states should be at the same energy.
We already can use this to tell us something new. We would expect that the diproton and the dineutron are not bound nuclei. Two identical nucleons cannot stick together under nuclear forces. You can do experiments that confirm this prediction.

Notice that for the deuteron two isospin couplings are possible, T=0 and T=1. We see experimentally that the T=0 coupling is lowest. It turns out that for most nuclei, many isospin couplings are available, but usually the one that is lowest in energy is $T=T_z$.

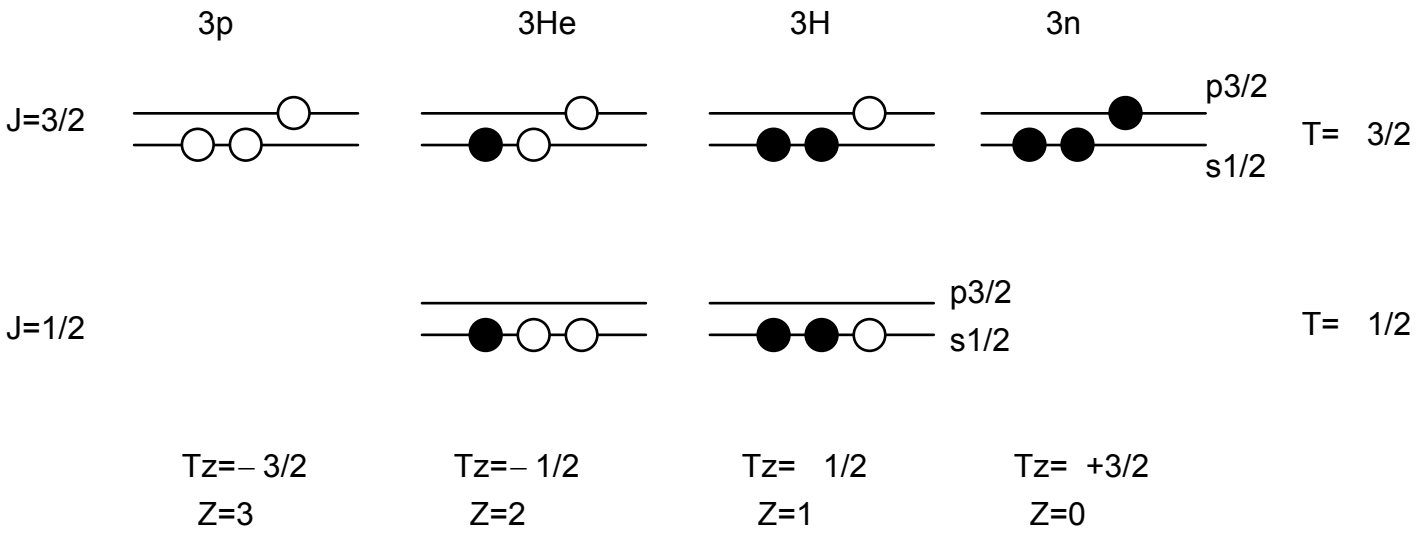
Take a nucleus composed of A nucleons, with Z protons and N neutrons. The T_z of the nucleus is $(N-Z)/2$. Many values of the isospin are available by coupling together the isospin of each nucleon i.e. couple ½, A times. The maximum value of the isospin is then $A/2$. T cannot be lower than T_z. If you can't immediately see this, consider that if you had a state with m_j=+2, you know that J couldn't be 0 or 1 as they only have substates m_j=0 or m_j=+1, 0 and −1.

For example, ^{30}S has A=30, Z=14 and N=16:

$Tz=½(N-Z)$=+1
Maximum T=15
Minimum T=1
Ground-state T=1

Example: the Three-Nucleon System

Here is a pictorial representation of the A=3 system. Isospin coupling suggests that the various possibilities are T=3/2 with T_z=+3/2, +1/2, −1/2 and −3/2, or T=1/2 with T_z= +1/2 and −1/2. *Convince yourself that these couplings work and that these states are associated with the particular A=3 nuclei shown below.* There is a difference here compared to the A=2 system in that we have to take into account two single-particle orbitals, $p_{3/2}$ and $s_{1/2}$, rather than just the latter. On the diagram each state in the final system is shown as a pair of lines with dots to represent the details of the configurations involved in the states. The very lowest states have all three nucleons in the $s_{1/2}$ orbital, which can only happen with the 2pn and p2n systems by Pauli and therefore must be the T=1/2 states in ^{3}He and ^{3}H. The pair of nucleons of the same type has to be coupled to spin-zero giving an overall J=1/2 for the spin of these states.



An example of a T=3/2 state, is the T_z=3/2 case of three neutrons. The lowest corresponding configuration has to be $\nu s_{1/2}^2 p_{3/2}$, filling the single-particle levels according to Pauli, with an overall spin J=3/2. You can then move from the T_z=3/2 system to the T_z=1/2 system by changing one neutron into a proton; an alternative language would be to apply an isospin lowering operator to the wavefunction. Sticking to the lowest energy configuration would suggest that the $p_{3/2}$ neutron is the one to change, to produce the lowest T=3/2 state in ^{3}H with a configuration, $\nu s_{1/2}^2 \pi p_{3/2}$. This also has spin J=3/2 and is clearly at a higher energy compared with the $\nu s_{1/2}^2 \pi s_{1/2}$ T=1/2 ground state in ^{3}H. Applying isospin lowering operators will progressively move you through the T=3/2 states in the A=3 multiplet; the lowest configuration will have J=3/2 and these form a set of isobaric analogue states, more accurately resonances as these states and actually all unbound.

You don't necessarily have to covert the $p_{3/2}$ neutron in the T=3/2 state in the three neutron system to move to T=3/2 states in ^{3}H. You could have chosen an $s_{1/2}$ neutron, but this would make the configuration $\nu s_{1/2} p_{3/2} \pi s_{1/2}$. This configuration is more excited than the $\nu s_{1/2}^2 \pi p_{3/2}$ T=0 J=3/2 state, since a neutron pair is broken. It also can couple to a variety of spins. These constitute other, more highly excited, T=3/2 states in ^{3}H.

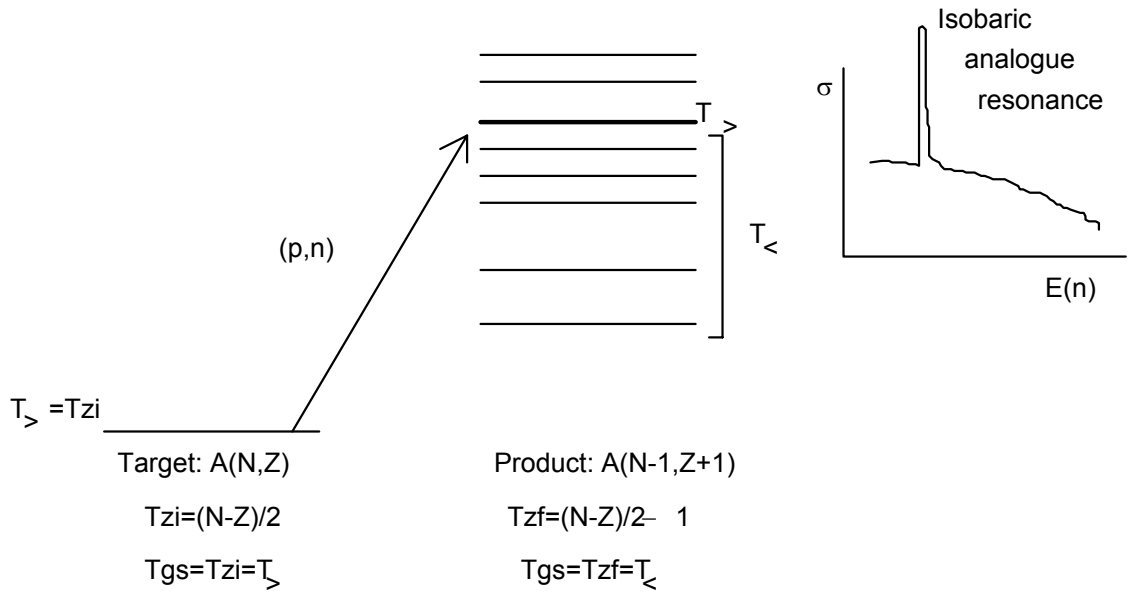
In this example you can see that isospin is telling you about particular configurations of nucleons. The T=3/2 states have two nucleons in $s_{1/2}$ and one in $p_{3/2}$. The T=1/2 states have three nucleons in $s_{1/2}$. The third component, T_z, tells you which nucleus you are in, or how many protons and neutrons there are. Obviously because of Pauli some particular T states are not present for particular T_z; there are no T=1/2 states in the 3n system because of this, but then that is obvious because T_z=3/2 which cannot support T=1/2. Isospin gives us a convenient mathematical (and computational) language with which to describe the similarity of protons and neutrons, indistinguishablility and the need to obey Pauli.

Isospin Transitions and Selection Rules

Isospin now takes off on its own and becomes even more useful. We now have another quantum number and quantum numbers often have selection rules which can be useful when we discuss changes.
For example, you are probably used to selection rules in atomic transitions where photons are usually emitted which carry off 1 unit of angular momentum. Due to angular momentum conservation, states can only decay to other states where the change in angular momentum is −1, 0 or +1. This selection rule can be determined by considering the angular momentum coupling between initial and final states and the photon. Here are a couple of isospin selection rules to wet your appetite, there are many more. *Postgraduates should look up the isospin selection rules for electromagnetic transitions.*

(a) Beta decay
In β decay, either a proton changes to a neutron in β+ decay, or a neutron turns into a proton in β− decay. In other words, this is a process where T_z changes by −1 or +1. You could write an operator driving such decays in terms of isospin raising and lowering operators if you wanted.
In particular, remember that isobaric analogue states have nucleons in exactly the same configurations. If you β decay between isobaric analogue states, all that happens is that a proton switches into a neutron. Its configuration doesn't alter, so this change occurs without altering its state of motion, it doesn't need to leap up to another energy level or change its spin coupling. Such transitions therefore happen with must greater probability than transitions between other states. In a β decay process, if it is energetically possibly, the majority of the decay strength will populate the isobaric analogue state. These very fast decays are called *superallowed* transitions and there are many examples of such decays between the ground states of mirror nuclei such as $^{3}H \rightarrow {}^{3}He$ and $^{48}Ca \rightarrow {}^{48}Ti$. *Postgraduates should read up on the details of the theory of beta decay and understand log(ft) values.*

(b) (p,n) reactions:
The (p,n) reaction is similar to β decay in that the target nucleus loses a neutron and gains a proton. The reaction can also be modelled using an isospin lowering operator. If the initial and final states share the same *T* value, again the configurations will be identical other than some minor effects due to Coulomb differences. Reactions between such isobaric analogue states will therefore be much easier than to other states. In a (p,n) reaction, these isobaric analogue reactions stand out as marked resonances in the neutron energy spectrum above the mass of reactions to other states. The transition is illustrated in the diagram below. *Figure through for yourself what the isospin of the ground state of the target and the product is. Where are states in the product with the same isospin as the ground state of the target?*



PC 4421 Lecture 11: Coping with Residual Interactions, Two Particle Systems and Configuration Mixing

This section is essential for postgraduate students, but might enlighten an interested undergraduate!

Two particles outside a closed core nucleus is a good system to use to illustrate how to cope with residual interactions. We saw that configurations such as $h_{11/2}^2$ can couple to J=0, 2, 4$^+$ and from an independent-particle model all these spin states would have the same energy. In reality, such degeneracy is lifted and in general energy of the states depends on the spin with the J=0 generally coming lowest. This effect is due to mixing with configurations other than $h_{11/2}^2$. The nucleons interact with each other, scattering between different configurations such that for any particular state the nucleons will be found for certain amounts of time in each contributing configuration. We need to translate these qualitative ideas into some quantum mechanics. If the residual interaction is small, perturbation theory can be used; you should be familiar with such methods from third-year quantum mechanics *(if not, make sure you are before proceeding)*. Otherwise you have to resort to the methods of matrix diagonalisation discussed here.

Here is an outline of the basic problem:

Model: An inert core plus two valence nucleons.
Assumptions: The core is not excited or perturbed by the valence nucleons (no core polarisation).
The only residual interaction is between the two valence nucleons.
Hamiltonian: $\hat{H} = \hat{h}_0(1) + \hat{h}_0(2) + V_{12}$
h_0 are the mean-field potentials for the valence nucleons
V_{12} is the residual interaction between the valence nucleons

The independent-particle model is taken as the starting point. We're used to this now so here just a summary of the main ideas:

Independent-particle Hamiltonian: $\hat{H}_0 = \hat{h}_0(1) + \hat{h}_0(2)$

Single-particle Schrodinger equations:

$$\hat{h}_0(1)\varphi_{j_a m_a}(1) = e_1\varphi_{j_a m_a}(1) \quad \text{and} \quad \hat{h}_0(2)\varphi_{j_b m_b}(2) = e_1\varphi_{j_b m_b}(2)$$

Full Schrodinger equation: $H_0\psi = E\psi$

Solutions: $\psi = \varphi_{j_a m_a}(1)\varphi_{j_b m_b}(2)$ with $E = e_1 + e_2$

These solutions should not be surprising. We have two particles outside an inert core; the energy is the sum of the energy of the two valence nucleons.

Technical Issues: Simple product wavefunctions are not normally enough:

(a) You have two particles contributing to the wavefunction so you should couple these together to produce a good overall nuclear spin. To do this properly requires Clebsch-Gordan coefficients:

$$\psi(j_a(1), j_b(2); JM) = \sum_{m_a m_b} \left\langle j_a m_a j_b m_b \middle| JM \right\rangle \varphi_{j_a m_a}(1)\varphi_{j_b m_b}(2)$$

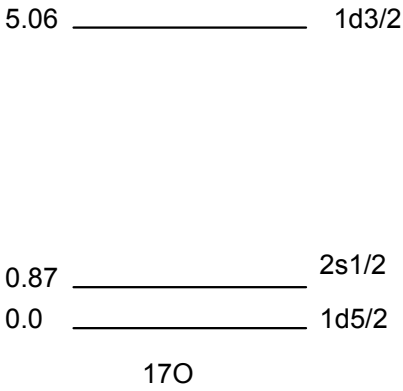
(b) Also the wavefunction needs to be made antisymmetric to obey the Pauli principle:

$$\psi(j_a(1), j_b(2); JM) = \frac{1}{\sqrt{2}} \sum_{m_a m_b} \langle j_a m_a j_b m_b | JM \rangle \left[\varphi_{j_a m_a}(1) \varphi_{j_b m_b}(2) - \varphi_{j_a m_a}(2) \varphi_{j_b m_b}(1) \right]$$

Now if $j_a=j_b$ and $m_a=m_b$, Ψ is zero as required.

To show you how to proceed further we need to take a specific example. We're going to calculate states in ^{18}O. At low excitation energies, this should be viewed as ^{16}O, a nice stable doubly-closed magic core, plus two valence neutrons in the sd shell.

We first need to know what energies the valence neutrons might have. We could calculate this as suggested above, but we could also take empirical energies from experiment. The low-lying levels of ^{17}O should look like an inert core plus one neutron, with excitations being made by promoting the neutron between different single-particle states.



Only the $2s_{1/2}$ and $1d_{5/2}$ orbitals appear at low excitation energies in ^{17}O. We'd therefore expect that low-lying states in ^{18}O would correspond to configurations of two neutrons arranged in these two orbitals. Technically we would say that the *model space* includes $2s_{1/2}$ and $1d_{5/2}$ orbitals only. We'll neglect $1d_{3/2}$ for now and comment on the restrictions of the model space later.

We can use these single-particle energies to make the first guess in the independent-particle model at the structure of ^{18}O, by coupling the single-particle spins and adding the energies.

Configuration	Possible Spins	Excitation Energy $E=e_1+e_2$
$d_{5/2}^2$	$0,2,4^+$	0
$s_{1/2}^2$	0^+	1.74
$d_{5/2}s_{1/2}$	$2,3^+$	0.87

Notice that there are two 0^+ states in the simple model space at low excitation energy. A residual interaction could scatter the two neutrons between these two configurations making a real 0^+ state which was a mixture of both $d_{5/2}^2$ and $s_{1/2}^2$ configurations. There are also two 2^+ state which can mix. The 3 and 4^+ states, within this particular model space, do not have any other states of the same spin to mix with and therefore remain pure independent-particle model states with configurations as in the table. As we will see, despite the lack of mixing, their energies do shift a little.

So how do we deal the residual interaction when it mixes the 0^+ states, for example? The independent-particle model suggests that the unmixed eigenfunctions are:

$$\phi_1 = \left| d^2_{5/2};0 \right\rangle \quad \text{and} \quad \phi_2 = \left| s^2_{1/2};0 \right\rangle$$

In reality, the residual interaction mixes them to give the real eigenfunctions. We can express these mixed eigenfunctions as a sum of the unmixed, eigenfunctions:

$$\Psi_1 = a_{11}\phi_1 + a_{12}\phi_2 \quad \text{and} \quad \Psi_2 = a_{21}\phi_1 + a_{22}\phi_2$$

The unmixed eigenfunctions are solutions to the independent-particle Hamiltonian, H_0. But we want solutions to the "real" Hamiltonian with residual interactions included i.e. H_0+V_{12}. These solutions are $\Psi_{1,2}$ and actually if we determine the constants, a_{11}, a_{12}, a_{21} and a_{22}, we have the problem solved.

Now we're going to do some maths to manipulate the equations we already have above into a form which makes them easier to solve. We're going to briefly write things in a more general fashion so we can cope in situations where there are, for example, more than two states that might mix. We will take the mixed eigenfunctions above and substitute them into the full Schrödinger equation. *If at any point you are confused by notation, just take the simple two-state case above and follow the steps using those equations.*

In general, the mixed eigenfunctions can be written as:

$$\Psi_p = \sum_k a_{kp}\phi_k$$

Substituting into the full Schrodinger equation:

$$(H_0 + V_{12})\Psi_p = (H_0 + V_{12})\sum_k a_{kp}\phi_k = E_p\Psi_p = E_p\sum_k a_{kp}\phi_k$$

Our problem, as stated above, is to find the a coefficients which give us the mixed wavefunctions and E_p, the energy of the states of the full Hamiltonian.

Multiply through the equation using one particular unmixed eigenfunction, ϕ_l :

$$\begin{aligned}
\phi_l^*(H_0 + V_{12})\sum_k a_{kp}\phi_k &= E_p\sum_k a_{kp}\phi_l^*\phi_k \\
\sum_k a_{kp}\phi_l^*(H_0 + V_{12})\phi_k &= E_p\sum_k a_{kp}\phi_l^*\phi_k \\
\sum_k a_{kp}(\phi_l^* H_0\phi_k + \phi_l^* V_{12}\phi_k) &= E_p\sum_k a_{kp}\phi_l^*\phi_k \\
\sum_k a_{kp}(\varepsilon_k\phi_l^*\phi_k + \phi_l^* V_{12}\phi_k) &= E_p\sum_k a_{kp}\phi_l^*\phi_k
\end{aligned}$$

In the last few steps you have to be careful about the operators on the left-hand side. We know that the unmixed wavefunctions are eigenfunctions of the independent-particle Hamiltonian and therefore $H_0\phi_k = \varepsilon_k\phi_k$, where ε_k are the unmixed energies in the final step.

Now integrate over all space and use the results of orthonormality i.e. $\int \phi_l^* \phi_k d\tau = \delta_{lk}$

$$\sum_k a_{kp}(\varepsilon_k \int \phi_l^* \phi_k d\tau + \int \phi_l^* V_{12} \phi_k d\tau) = E_p \sum_k a_{kp} \int \phi_l^* \phi_k d\tau$$

$$\sum_k a_{kp}(\varepsilon_k \delta_{kl} + \int \phi_l^* V_{12} \phi_k d\tau) = E_p \sum_k a_{kp} \delta_{kl}$$

$$\sum_k a_{kp} H_{lk} = E_p a_{lp}$$

We've just introduced a new quantity, $H_{lk} = \varepsilon_k \delta_{kl} + \int \phi_l^* V_{12} \phi_k d\tau$. This, if you know the operator for the residual interaction, is just a number. Remember that this is not really just one equation, it is a set of equations. With a bit more staring you should be able to see that these equations represent a matrix equation:

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & \cdots & H_{1n} \\ H_{21} & H_{22} & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ H_{n1} & \cdots & \cdots & \cdots & H_{nn} \end{pmatrix} \begin{pmatrix} a_{1p} \\ a_{2p} \\ \vdots \\ \vdots \\ a_{np} \end{pmatrix} = E_p \begin{pmatrix} a_{1p} \\ a_{2p} \\ \vdots \\ \vdots \\ a_{np} \end{pmatrix} \quad \text{or} \quad \mathbf{H a_p} = E_p \mathbf{a_p}$$

$$\begin{pmatrix} H_{11} - E_p & H_{12} & \cdots & \cdots & H_{1n} \\ H_{21} & H_{22} - E_p & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ H_{n1} & \cdots & \cdots & \cdots & H_{nn} - E_p \end{pmatrix} \begin{pmatrix} a_{1p} \\ a_{2p} \\ \vdots \\ \vdots \\ a_{np} \end{pmatrix} = 0$$

Either the vectors, $\mathbf{a}_p$, are all zero and there is a null solution, or the determinant of the matrix is zero:

$$\begin{vmatrix} H_{11} - E_p & H_{12} & \cdots & \cdots & H_{1n} \\ H_{21} & H_{22} - E_p & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ H_{n1} & \cdots & \cdots & \cdots & H_{nn} - E_p \end{vmatrix} = 0$$

Let's go back to the specific case of the two 0^+ states to get a better impression of where this manipulation has got us. Explicitly we have a two by two determinant:

$$\begin{vmatrix} 2\varepsilon_{d5/2} + \left\langle d_{5/2}^2 \middle| V_{12} \middle| d_{5/2}^2 \right\rangle - E_p & \left\langle d_{5/2}^2 \middle| V_{12} \middle| s_{1/2}^2 \right\rangle \\ \left\langle s_{1/2}^2 \middle| V_{12} \middle| d_{5/2}^2 \right\rangle & 2\varepsilon_{s1/2} + \left\langle s_{1/2}^2 \middle| V_{12} \middle| s_{1/2}^2 \right\rangle - E_p \end{vmatrix} = 0$$

Or using the notation that we introduced above:

$$\begin{vmatrix} H_{11}-E_p & H_{12} \\ H_{21} & H_{22}-E_p \end{vmatrix} = 0$$

All operators that represent real things are Hermitian and satisfy the condition, $H_{12}=H_{21}$, so evaluating the determinant gives a simple quadratic equation with two solutions, which correspond to E_1 and E_2:

$$E^2 - E(H_{11}+H_{22}) - H_{12}^2 + H_{11}H_{22} = 0$$

Using the quadratic formula and tidying up:

$$E = \frac{(H_{11}+H_{22})}{2} \pm \frac{1}{2}\left[(H_{11}-H_{22})^2 + 4H_{12}^2\right]^{1/2}$$

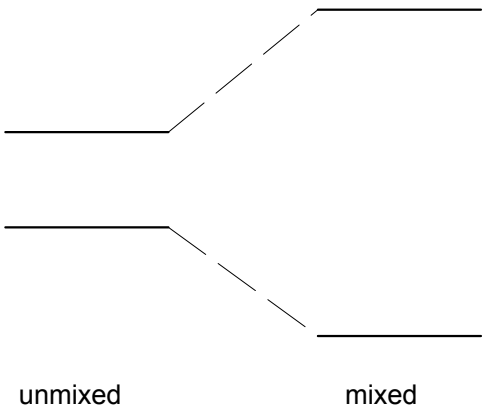
These are the energies after taking into account the residual interaction. The difference between the new energies is:

$$\Delta E = \left[(H_{11}-H_{22})^2 + 4H_{12}^2\right]^{1/2}$$

Remember the definition, $H_{11} = \varepsilon_1 + \int \phi_1^* V_{12} \phi_1 d\tau$, where the first term is the unperturbed energies.

The second term in this definition is actually the result you would get from first-order perturbation theory. The separation of the two perturbed states is minimised if $H_{11}=H_{22}$. In other words, if the first-order perturbation theory results in degenerate states, the full mixing calculation still pushes the states apart by at least $2H_{12}$. In the mixing process it is as if the two states repel each other.

In the limit of weak mixing, $|H_{11}-H_{22}|>>|H_{12}|$, the final energy separation tends towards $\Delta E= H_{11}-H_{22}$. This suggests that the effect of mixing depends on how close together in energy the states are with respect to the strength of the residual interaction; states close together mix a lot and those widely spaced hardly at all. This fits with our previous qualitative statements about the residual interaction scattering nucleons between configurations; if the configurations are closely lying, it is easy to scatter whereas if they are widely spaced there may not be sufficient interaction to raise them from one to another.



Just to comfort those people who feel happy with perturbation theory and maybe thinking there should be a connection, if you take the result for the new eigenvalues and, assuming that $|H_{11}-H_{22}|>>|H_{12}|$, expand the square root, you end up with:

$$E_1 = H_{11} + \frac{H_{12}^2}{H_{11}-H_{22}} + \ldots \quad \text{and} \quad E_2 = H_{22} + \frac{H_{12}^2}{H_{22}-H_{11}} + \ldots$$

These results are therefore the series of various perturbative orders, first-order perturbation theory result, followed by the second-order term and so on. This exact method is therefore consistent with the results of perturbation theory in the limit where such an approach is acceptable. Remember though that in nuclei, the residual interaction is usually too strong to allow perturbative approaches.

To summarise, if we know the so-called *matrix elements* of the residual interaction: $\langle \phi_i | V_{12} | \phi_j \rangle$ (more on this later) we can solve the determinant problem and find the perturbed energies. In the above situation there are only two states, and the two-by-two determinant is equivalent to two simultaneous equations which are solvable as a quadratic. If there are larger numbers of states mixing this algebraic method is not possible. It is, in fact, mathematically equivalent to *diagonalising the matrix* and there are a variety of numerical methods that can be employed to do this and therefore solve the determinant problem.

To obtain the mixed wavefunctions we need to deduce the coefficients, a_{lp}, which can be done by substituting back the newly found perturbed energies, E_p, back into the matrix equations. In the simple 2x2 case, the results are:

$$\Psi_1 = \frac{(E_2 - H_{22})\phi_1 + H_{12}\phi_2}{\left\{(E_2 - H_{22})^2 + H_{12}^2\right\}^{1/2}} \quad \text{and} \quad \Psi_2 = \frac{H_{12}\phi_1 + (E_1 - H_{11})\phi_2}{\left\{(E_1 - H_{11})^2 + H_{12}^2\right\}^{1/2}}$$

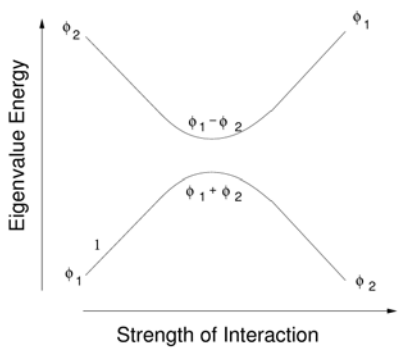
Run through explicitly the algebraic steps performed up to this stage for the two-state mixing problem.
The notation used is such that Ψ_1 is the mixed state with the lowest energy.

If you think about what happens as the residual interaction reduces to zero, $V_{12} \rightarrow 0$ then $H_{12} \rightarrow 0$, and in the above expressions wavefunctions tend towards the unperturbed eigenfunctions:

$$\Psi_1 \rightarrow \phi_1 \quad \text{and} \quad \Psi_2 \rightarrow \phi_2 .$$

If the residual interaction becomes very strong, then all terms in the above expressions are small other, other than H_{12}, and as a result, $\Psi_1 \rightarrow \phi_2$ and $\Psi_2 \rightarrow \phi_1$.

There is an intermediate region where they are very mixed, but remember that the states are always separated by at least $2H_{12}$, so they never actually cross each other. At this position of maximal mixing the wavefunctions are equal mixtures of both. The lower state having a coherent mix: $\Psi_1 = (\phi_1 + \phi_2)/\sqrt{2}$ and $\Psi_2 = (\phi_1 - \phi_2)/\sqrt{2}$. The situation looks something like the figure below.



Residual Interactions

We are now in a position to cope with residual interactions, except that we need one final piece of information, V_{12}, in order to be able to calculate the matrix elements for the diagonalisation process. There are many different approaches that can be taken:

(a) From the best bare nucleon-nucleon force and try to derive the residual interaction to the mean-field potential. This is very complicated.

(b) Use the basic feature of the nucleon-nucleon force such as short-range nature and so on, to write down a simple form for the residual interaction that can be dealt with in a mathematically simple way. These so-called *schematic* interactions include the surface delta interaction. This incorporates the short range nature of the nucleon force and the lack of net forces in the nuclear interior to give a force with the form:

$$V_{12} = -4\pi V_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

Integrals resulting from the use of the SDI come out as a function of the strength of the force and the nuclear radius parameter, V_oR_o. Comparison of results with data allows this parameter to be fixed.

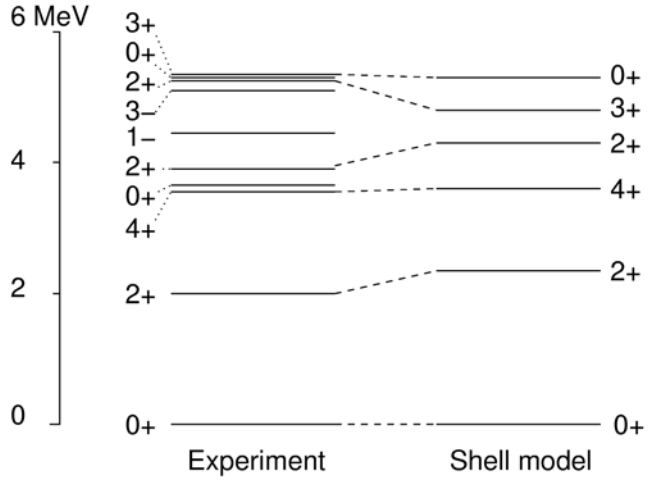
(c) It turns out that the two-body matrix elements of the residual interaction between two nucleons in specific orbits actually depend on the model space you are using. Larger model spaces tend to give better results when compared to experiment. But the larger the model space, the more complex the situation becomes. We had two 2^+ states in ^{18}O in the $s_{1/2}d_{5/2}$ space. For ^{154}Sm, which has 12 protons and 10 neutrons in the shells above Z=50 and N=82, there are 3×10^{14} different 2^+ states. This space is restricted to the shells in which the valence nucleons are filling and we're excluding already cross-shell excitations. But this is already too many to deal with even with the very best modern computing, so you *always* have a restricted model space. Therefore many people have taken an empirical approach where they use results from very simple nuclei, such as the magic core plus two nucleons, to deduce the matrix elements by fitting experimental data to calculations. The single-particle energies can also be fitted to magic core plus one nucleon systems. Then these *empirical* matrix elements are used to try to understand the structures of states in more complex nuclei.

In passing, we have just dealt with two nucleons outside of a closed core and dealt with two-body matrix elements like $\left\langle j^2; JM \left| V_{12} \right| j'^2; J'M' \right\rangle$.

With more nucleons outside the core, in principle you need to deal with matrix elements like $\left\langle j^n; JM \left| V_{12} \right| j'^n; J'M' \right\rangle$. It turns out that such matrix elements can be reduced to sums over two-body matrix elements using things call *coefficients of fraction parentage*.

Results from SDI Calculations of ^{18}O

So we now know about all of the ingredients to a shell-model calculation. Here are some results of an SDI-based calculated of the low-lying states in ^{18}O.



This calculation was done in the model space, $d_{5/2}s_{1/2}$, with an SDI interaction with V_oR_o=1.057 MeV. There is a one-to-one correspondence between the calculated states and some of the low-lying levels in ^{18}O known form experiment, with excitation energies reasonably well reproduced for those states. Some improvement can be made if an interaction with a finite range is used.

The wavefunction of the ground state is $0.929(d_{5/2}^2)_{J=0}+0.371(s_{1/2}^2)_{J=0}$. In other words, a nucleon can be found with 86% probability in the $d_{5/2}^2$ configuration and 14% in the $s_{1/2}^2$.

The wavefunction of the first 2^+ state is more mixed $0.764(d_{5/2}^2)_{J=2}+0.645(s_{1/2}\ d_{5/2})_{J=2}$. This reflects the fact that the two 2^+ states in the unperturbed picture are closer together in energy than the two 0^+ states. The off-diagonal matrix elements, responsible for the mixing, are actually smaller in the 2^+ states than the 0^+ case.

Notice that the 3+ and 4+ states, despite not mixing, do move in energy when the residual interaction is taken into account. They are the sole state of this spin and the Hamiltonian matrix will be 1x1 with an element, $H_{11} = \varepsilon_1 + \langle \phi_1 | V_{12} | \phi_1 \rangle$. The shift is due to the second term, the diagonal matrix element of V_{12}.

There are negative-parity states which are not accounted for in this model space; the $d_{5/2}$ and $s_{1/2}$ orbitals can only generate positive parity. The negative-parity states necessarily involve cross-shell excitations, such as exciting neutrons from the p shell up into the sd shell. A $d_{5/2}p_{1/2}^{-1}$ excitation can couple to J^π=3 or 2^- and a $d_{5/2}p_{3/2}^{-1}$ configuration can generate states with J^π=4,3,2, or 1^-.

There is also a low-lying 0^+ state without a theoretical parallel. This turns out to be based on promoting a pair of neutrons from the p shell up into the sd shell. To a first approximation, an independent-particle picture would put this at high excitation. However, such an excitation takes advantage of the attractive residual interaction to pull the state down. When the pair was in the p shell, there is a reasonably large energy gap before it can scatter up into the sd shell and so not much cross-shell scattering happens. Now the pair is in the sd shell, it can easily scatter between the orbitals in the sd shell, which are closely lying in energy. The residual interaction helps to bring the configuration to low energies and we'd expect the wavefunction of this low-lying state to be very mixed. Such excitations are known as core excitations.

The Road to Collective States

With strong residual interactions and large model spaces, some states can be large admixtures of many single-particle states. These sums of states can be so large that the description within the single-particle basis set is cumbersome and doesn't give a nice simple interpretation of the structure. Other basis sets might give a simpler wavefunction and therefore a nicer interpretation. Often a very mixed state falls low in excitation energy, due to the repulsion from the states above with which it mixes. Notice in the discussion above that the state pushed lowest in excitation energy by strong mixing tends to be a coherent mixture of single-particle orbitals i.e. each admixture has the same phase. The low-lying 0^+ state in ^{18}O is a 4-particle 2-hole core excitation which has a complex structure in a single-particle basis. However, there is a sequence of states above it that look like a rotational band! This core excited state apparently is deformed. If the residual interaction is repulsive, the coherent state is pushed up; this is the origin of the extremely collective giant resonance states you'll hear about in the Nuclear Reactions course.

Such extreme mixing can lead to many interesting properties such as increased transitions strengths, above and beyond single-particle rates as many nucleons contribute coherently to a transition. Excitations are no longer just the changes in the motion of one or two nucleons; they involve contributions from many nucleons, maybe in fact all the valence particles. Such excitations become better described in terms of collective wavefunctions representing the motion of the bulk material of the nucleus. For example, thinking about ripples on the surface of a nuclear liquid drop, or rotations of a deformed speck of nuclear matter might be a more useful approach. Here's where the second half of the course begins which will discuss in detail the models of nuclei involving rotations and vibrations.