On single nucleon wave functions

Igal Talmi

The Weizman Institute of Science

Rehovot, Israel

The main success of the nuclear shell model

- Nuclei with “magic numbers” of protons and neutrons exhibit extra stability.
- In the shell model these are interpreted as the numbers of protons and neutrons in closed shells, where nucleons are moving independently in closely lying orbits in a common central potential well.
- In 1949, Maria G.Mayer and independently Haxel, Jensen and Suess introduced a strong spin-orbit interaction. This gave rise to the observed magic numbers 28, 50, 82 and 126 as well as to 8 and 20 which were well understood.

The need of an effective interaction in the shell model

- In the Mayer-Jensen shell model, wave functions of magic nuclei are well determined. So are states with one valence nucleon or hole.
- States with several valence nucleons are degenerate in the single nucleon Hamiltonian. Mutual interactions remove degeneracies and determine wave functions and energies of states.
- In the early days, the rather mild potentials used for the interaction between free nucleons, were used in shell model calculations. The results were only qualitative at best.

Theoretical derivation of the effective interaction

A litle later, the bare interaction turned out to be too singular for use with shell model wave functions. It should be renormalized to obtain the effective interaction. More than 50 years ago, Brueckner introduced the G-matrix and was followed by many authors who refined the nuclear many-body theory for application to finite nuclei.

- Starting from the shell model the aim is to calculate from the bare interaction the effective interaction between valence nucleons. Also other operators like electromagnetic moments should be renormalized (*e.g.* to obtain the neutron effective charge!)
- Only recently this effort seems to yield some reliable results like those obtained by Aldo Covello et al. This does not solve the major problem - how independent nucleon motion can be reconciled with the strong and short ranged bare interaction.

The simple shell model

- In the absence of reliable theoretical calculations, matrix elements of the effective interaction were determined from experimental data in a consistent way.
- Restriction to two-body interactions leads to matrix elements between *n*-nucleon states which are linear combinations of two-nucleon matrix elements.
- Nuclear energies may be calculated by using a smaller set of two-nucleon matrix elements determined consistently from experimental data.

The first successful calculation – low lying levels of ^{40}K and ^{38}Cl

- In the simplest shell model configurations of these nuclei, the 12 neutrons outside the ^{16}O core, completely fill the $1d_{5/2}$, $2s_{1/2}$, $1d_{3/2}$ orbits while the proton $1d_{5/2}$ and $2s_{1/2}$ orbits are also closed.

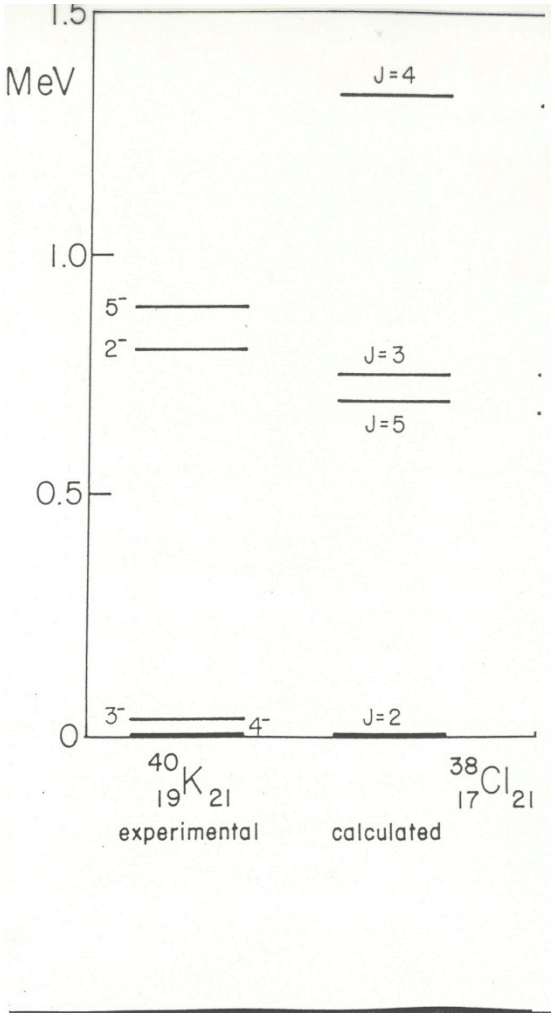
- The valence nucleons are
  in ^{38}Cl: one $1d_{3/2}$ proton and a $1f_{7/2}$ neutron
  in ^{40}K: $(1d_{3/2})^3 J_p=3/2$ proton configuration and
  a $1f_{7/2}$ neutron.

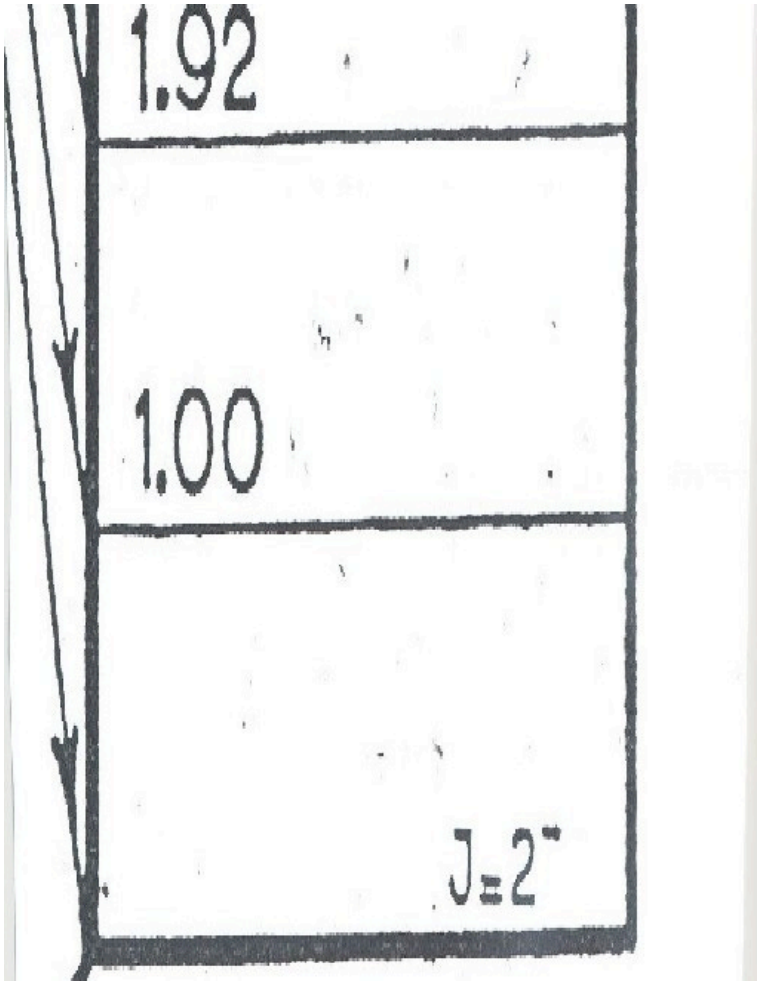
- In each nucleus there are states with J=2, 3, 4, 5

- Using levels of ^{38}Cl, the ^{40}K levels may be calculated and *vice versa.*

Comparison with 1954 data

only the spin 2^- agreed with our prediction





We were disappointed but not surprized. Why?

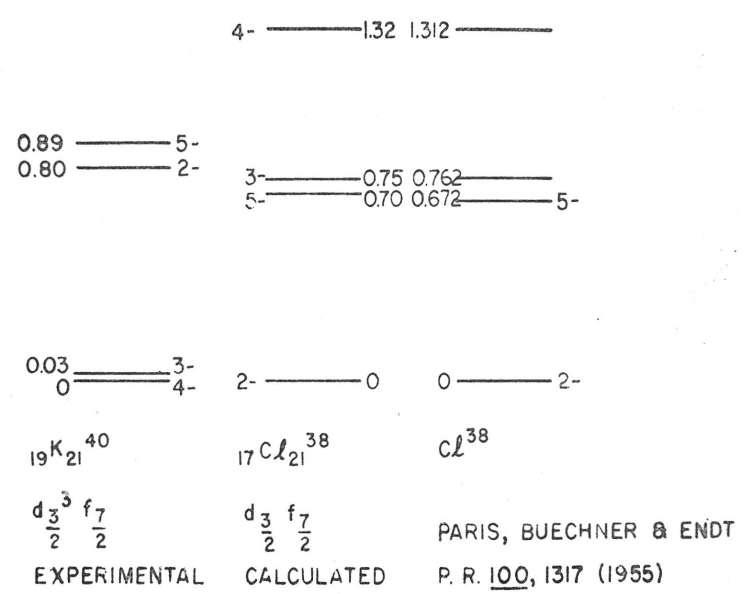
- The assumption that the states belong to rather pure *jj*-coupling configurations may have been far fetched. Also the restriction to two-body interactions could not be justified *a priori*.

- There was no evidence that values of matrix elements do not appreciably change when going from one nucleus to the next.

- Naturally, we did not publish our results

  but then…

Comparison of our predictions with experiment in 1955



Conclusions from the relation between the ^{38}Cl and ^{40}K levels

- The restriction to two-body effective interaction is in good agreement with some experimental data.

- Matrix elements (or differences) do not change appreciably when going from one nucleus to its neighbors (Nature has been kind to us).

- Some shell model configurations in nuclei are very simple. It may be stated that Z=16 is a proton magic number (as long as the neutron number is N=21).

Effective interactions, no longer restricted by the bare interactions, have been adopted

- This was the first successful calculation and it was followed by more complicated ones carried out in the same way.
- The complete *p*-shell, $p_{3/2}$ and $p_{1/2}$ orbits (Cohen and Kurath), Zr isotopes (mostly the Argonne group), the complete $d_{5/2}$,$d_{3/2}$,$s_{1/2}$ shell (Wildenthal, Alex Brown et al) and others.
- This series culminated in more detailed calculations including millions of shell model states, with only two-body forces (Strasbourg and Tokyo). Not all matrix elements determined.

General features of the effective interaction extracted even from simple cases

- The T=1 interaction is strong and attractive in J=0 states.
- The T=1 interactions in other states are weak and their *average* is repulsive.
- It leads to a seniority type spectrum.

- The *average* T=0 interaction, between protons and neutrons, is strong and attractive.
- It breaks seniority in a major way.

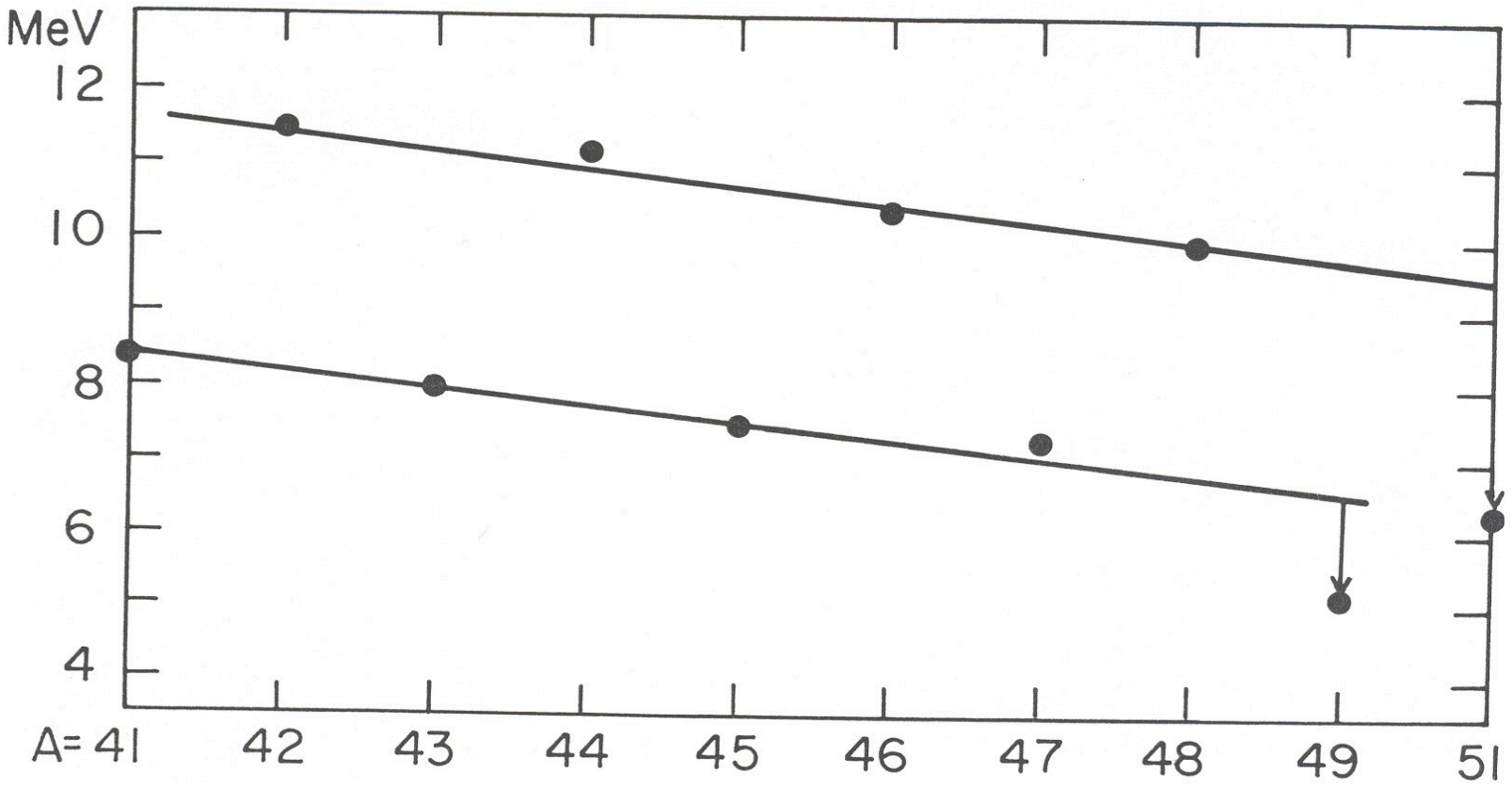
Consequences of these features

- The potential well of the shell model is created by the attractive proton-neutron interaction which determines its depth and its shape.

- Hence, energies of proton orbits are determined by the occupation numbers of neutrons and *vice versa*.

- These conclusions were published in 1960 addressing ^{11}Be, and in more detail in a review article in 1962.

Neutron separation energies from calcium isotopes

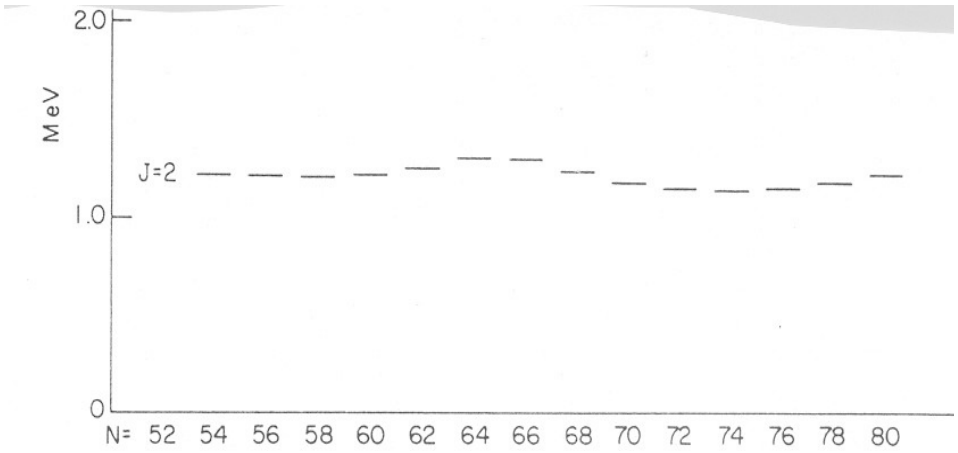


A direct result of this behavior is that magic nuclei are not more tightly bound than their preceding even-even neighbors.

Their magic properties (stability etc.) are due to the fact that nuclei beyond them are less tightly bound.

In semi-magic nuclei, with only valence protons or neutrons experiment shows features of generalized seniority

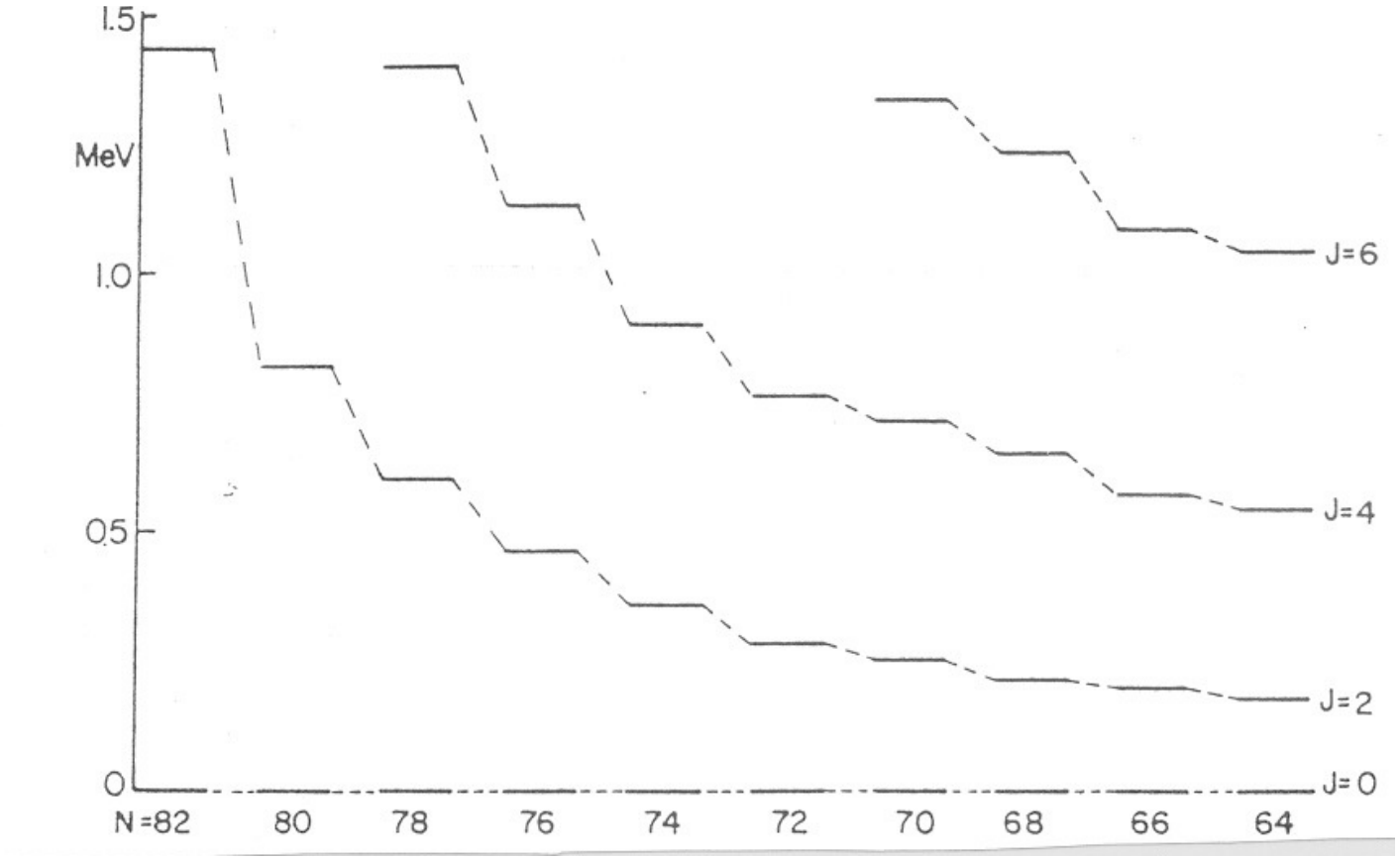
Constant 0-2 spacings in Sn isotopes



- The monopole part of the T=0 interaction affects positions of single nucleon energies.
- The quadrupole-quadrupole part in the T=0 interaction breaks seniority in a major way.
- In nuclei with valence protons and valence neutrons it leads to strong reduction of the 0-2 spacings – a clear signature of the transition to rotational spectra and nuclear deformation.

Levels of Sm (Z=56) isotopes

Drastic reduction of 0-2 spacings



In this picture, the real wave functions may be very different from shell model ones. They must have strong admixture of the latter. Still, there are experimental data indicating the reality of shell model wave functions. They are still used in the calculation of various observables. It seems as if the "wounds" inflicted on shell model wave functions by the strong two-body correlations occupy only a rather small volume.

Some exaples of using single nucleon wave functions

- In the theory of direct reactions they are assumed to take place near the boundary of the nucleus. The value of the wave function of the single nucleon which is removed or added in that region, is important.
- Electromagnetic moments and transitions are calculated by using single nucleon wave functions. In some of them, the actual shape of the radial part plays an important role.
- How real are single nucleon wave functions?

Is the Shell-Model Concept Relevant for the Nuclear Interior?

J. M. Cavedon, B. Frois, D. Goutte, M. Huet, Ph. Leconte, C. N. Papanicolas,[a]
X.-H. Phan, S. K. Platchkov, and S. Williamson

Département de Physique Nucléaire à Haute Energie, Centre d'Etudes Nucléaires de Saclay, F-91191 Gif-sur-Yvette Cédex, France

and

W. Boeglin and I. Sick

Department of Physics, University of Basel, Basel, Switzerland

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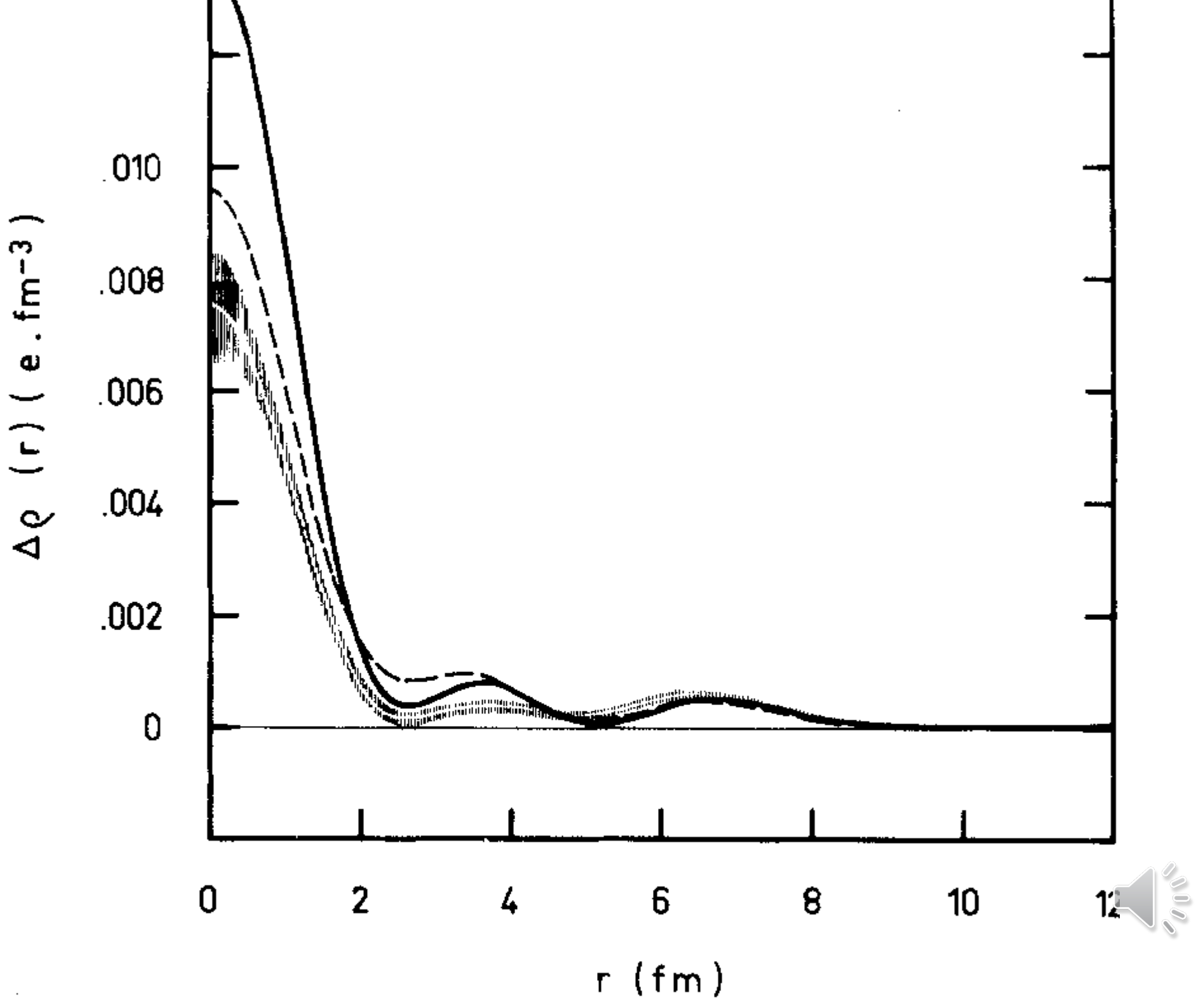
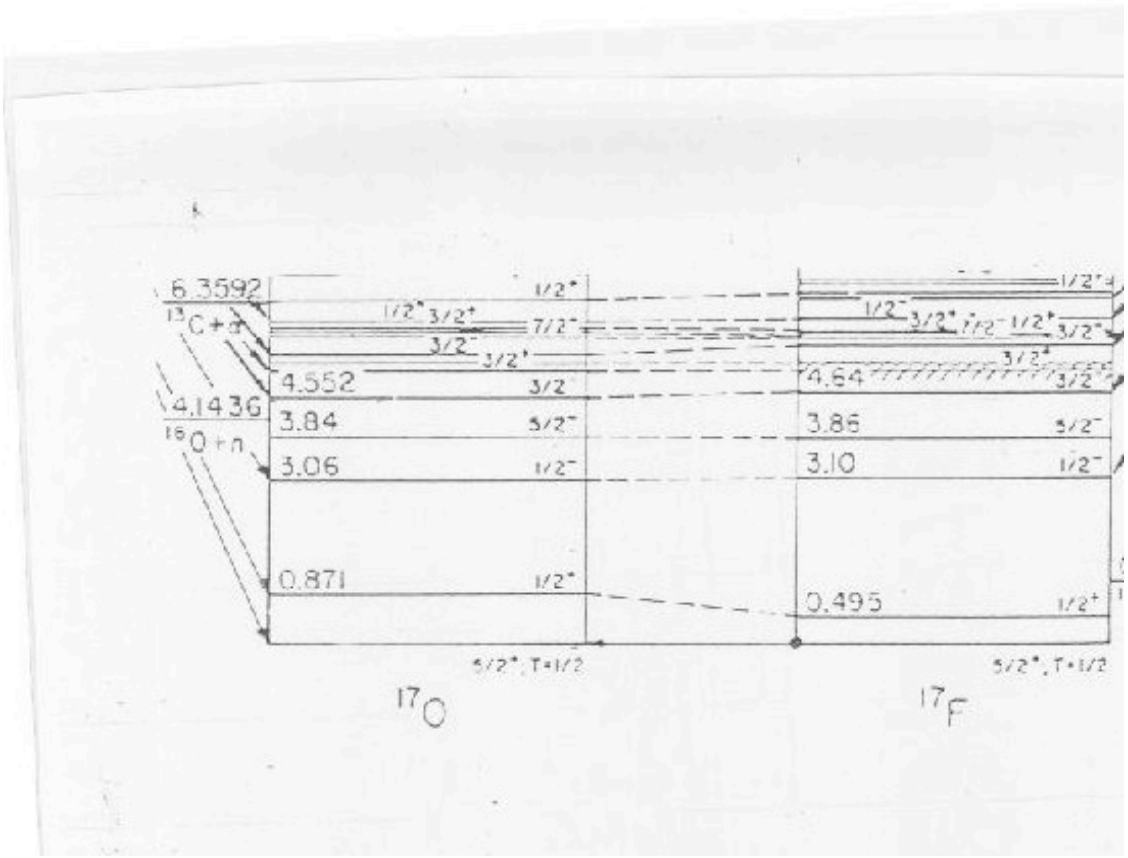
The 3*s* radial wave function $R(r)$ has been determined by electron scattering from ^{206}Pb and ^{205}Tl. The shape of $R(r)$ in the central region of the nucleus is used to test the validity of the independent-particle shell model at large nuclear density.


.010
.008
.006
.004
.002
0
Δρ (r) (e . fm⁻³)
0
2
4
6
8
10
12
r (fm)

- Coulomb energy differences between mirror nuclei are usually calculated by using single nucleon wave functions.

- Their values depend on the nature of the single nucleon wave function.

Coulomb energy differences of $1d_{5/2}$ and $2s_{1/2}$ orbits



Origin of the difference

- Consider various single particle wave functions in a given potential well. If the bottom of the well is raised, single particle energies are moved upwards.
- Due to the centrifugal potential, the following rule applies. The loss of binding energy is higher for states with higher orbital angular momenta.
- In the case of the Coulomb potential, this effect can be directly calculated.
- There are other ways to raise the bottom of the potential well.

- The average effective interaction between protons and neutrons is attractive.
- It creates the potential well of the shell model.
- Removing proton pairs coupled to J=0 makes the potential energy of valence neutrons less attractive.

ı the B^{12} data as well as on the data for the first
=1 levels in C^{12}.[2] The center of mass of the
'o $p_{1/2}$ levels lies at 0.59 Mev while that of the two
$_2$ levels lies at 2.03 Mev above the ground state.

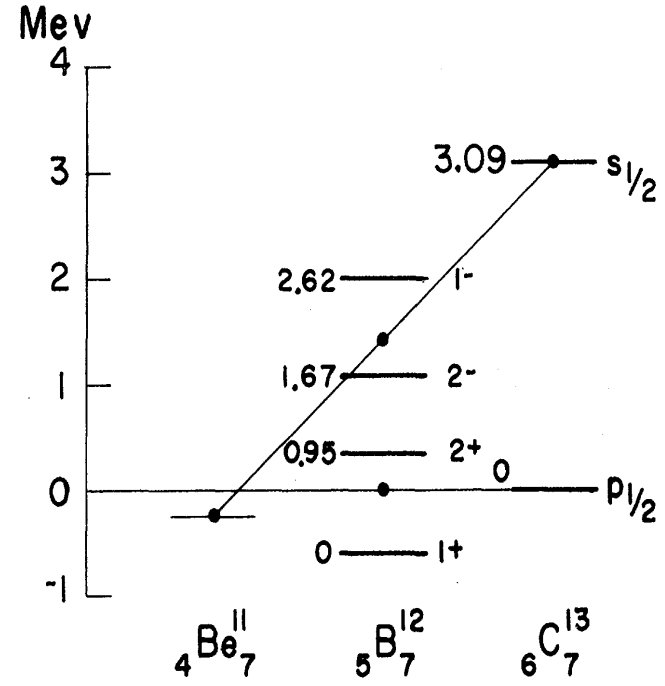


FIG. 1. Competition between $s_{1/2}$ and $p_{1/2}$ levels.

Our result about the C[13] spin was actually
not only on O^{17} and N^{16} but on many more dat
In the present case there are not enough data
the result obtained above on Be^{11} is not that
tain. The error involved in our estimate can
roughly obtained by considering the Be^{11} bind
energy. The separation energy of the $s_{1/2}$ neu

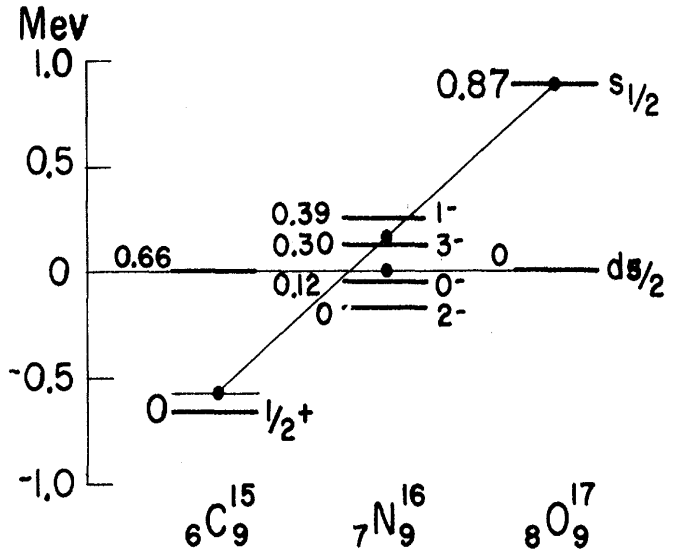


FIG. 2. Competition between $d_{5/2}$ and $s_{1/2}$ levels

- The graphs shown before are not merely extrapolations.
- They are graphic solutions of exact, even though simple, shell model problems.
- The matrix elements were taken from energies of nearby nuclei.
- The simple argument is qualitative and yet seems to agree with the more detailed calculation.

A common prescription to determine the wave function of a valence nucleon

- A potential well, like a Wood-Saxon one, is chosen. Its radius is determined by measurements of the charge distribution of the nucleus considered.
- The depth of the well is chosen so that the single nucleon energy is equal to its measured separation energy E_{A+1}-E_A .
- What is the reason for this choice?

When the valence nucleon is bound, the energy of the system is the binding energy of the nucleus with A+1 nucleons, E_{A+1} (binding energies in this paper are *negative*). When the valence nucleon is *adiabatically* removed, for very large distances, the *core* and the removed nucleon are independent of each other. The core, the nucleus with A nucleons, is in its ground state with energy E_A. The valence nucleon has in this situation, the energy $E=E_{A+1}- E_A$. Its wave function is

$$[\, R(r)/r]Y_{lm}(\vartheta, \varphi\,) \qquad (1)$$

and, for very large r, it is the solution of the radial part of the Schroedinger equation in which the interaction, as well as the centrifugal potential, no longer appear

$$-(h^2/2m)R'' = ER = (E_{A+1}- E_A)R \qquad (2)$$

From this equation follows that the asymptotic form of R is given by

$$R(r)=Cr^k exp(-[(2m/h^2)|E_{A+1}- E_A|]^{1/2}r) \quad \text{for} \quad r \to \infty \qquad (3)$$

The values of C and of k are determined by the solution of the equation for small values of r.

- This prescription will be examined by looking at Hartree-Fock theory in which the potential well is determined by the mutual (effective) interaction of the nucleons.
- The results will be applicable to the way single nucleon wave functions are constructed.

For simplicity, consider a spherical nucleus whose A nucleons occupy closed shells of protons and neutrons. The single nucleon energy of a valence orbit may be defined in three ways.

It may be defined by

$$E_{A+1} - E_A$$

Another possibility is the energy of a nucleon in an unoccupied orbit in the potential well created by the A nucleons in their ground state.

The third possibility is to use the single valence nucleon energy in the nucleus with A+1 nucleons. Even if the A nucleons in the core remain in closed shells, their state is not the original one. The core is polarized by the valence nucleon. Hence, it has less binding which is more than compensated by a stronger interaction with the valence nucleon.

The ground state energy of the nucleus with closed shells (core) is given by the lowest value of the variational integral

$$E_A=\int \Phi_A^*\left(\sum_i t_i+\sum_{ij} V(i,j)\right)\Phi_A d(1)d(2)\ldots d(A) \qquad (4)$$

In (4), t_i is the kinetic energy of the i-th nucleon and $V(i,j)$ is the effective interaction between nucleons i and j. The energy of the lowest *unoccupied* orbit in the (spherical) field of the core is given by

$$E^0_{A+1}=\int (\Phi_A^* u_0^*)_a\left(\sum_i t_i+\sum_{ij} V(i,j)\right)(\Phi_A u_0)_a d(1)d(2)\ldots d(A)d(A+1)=$$

$$E_A+\int (\Phi_A^* u_0^*)_a\left(t_{A+1}+\sum_i V(i,A+1)\right)(\Phi_A u_0)_a d(1)d(2)\ldots d(A)d(A+1)=$$

$$E_A + \varepsilon_0 \qquad (5)$$

The single nucleon wave function u_0 is the solution of the Schroedinger equation where the potential energy is equal to the expectation value

$$\int \Phi_A^*\left(\sum_i V(i,A+1)\right)\Phi_A d(1)d(2)\ldots d(A) \qquad (6)$$

and the energy eigenvalue is ε_0.

Since Φ_A is not varied, the integral (5) is higher than the energy of the nucleus with A+1 nucleons, $E^0_{A+1} \geq E_{A+1}$. From (5) then follows the inequality

$$\varepsilon_0 \geq E_{A+1} - E_A \qquad (7)$$

The relation

$$\varepsilon_0 \geq E_{A+1} - E_A$$

was derived for HF energies. Naturally, E_{A+1} may be replaced by the experimental binding energy.

Also E_A may be replaced by the experimental binding energy of the core. The relation holds since the core wave function is not varied. No matter how well it could reproduce the core experimental binding energy, the integral is always higher than, or equal to, the experimental E_{A+1}.

Next, the third choice of single nucleon energy will be considered

Thus, we write

$$E_{A+1}=\int (\Phi'_A{}^* u^*)_a(\Sigma_i t_i+\Sigma_{ij} V(i,j))(\Phi'_A u)_a d(1)d(2)\ldots d(A)d(A+1)=$$

$$\int \Phi'_A{}^*(\Sigma_i t_i+\Sigma_{ij} V(i,j))\,\Phi'_A d(1)d(2)\ldots d(A)+$$

$$\int (\Phi'_A{}^* u^*)_a(t_{A+1}+\Sigma_{iA+1} V(i,A+1))(\Phi'_A u)_a d(1)d(2)\ldots d(A)d(A+1)=$$

$$E_A' + \varepsilon \qquad (8)$$

The amount $E_A' - E_A$ is called the *rearrangement energy*. It will be denoted RE and is always non negative, $RE \geq 0$. Subtraction of E_A leads to another inequality

$$\varepsilon = E_{A+1} - E_A + (E_A - E_A') \qquad (9)$$

and hence,

$$\varepsilon \leq E_{A+1} - E_A \qquad (10)$$

The inequalities (7) and (10) may be combined into

$$\varepsilon \leq E_{A+1} - E_A \leq \varepsilon_0 \qquad (11)$$

Koopmans Theorem

It follows that if and only if, the core is not polarized by the valence nucleon, the following equality is obtained

$$\varepsilon = E_{A+1} - E_A = \varepsilon_0$$

Koopmans was well aware of this condition unlike some authors of recent papers and books.

It is clear that the choice of E_{A+1} - E_A as the single nucleon energy is the exact one for a potential well which is not changed by adding a valence nucleon. The question is whether this is a reasonable model for dynamic nuclei

.

A real nucleus is polarized by valence nucleons in which case the expectation value of its Hamiltonian in the state with A+1 nucleons is higher than its binding energy.

There is ample evidence for polarization of the core by valence nucleons. For example, the change of charge radii when neutrons are added to a nucleus as well as electromagnetic transitions due to the neutron effective charge.

The discussion started from the single nucleon wave functions which are determined by a fixed potential well. The depth of the potential is determined by choosing the value of the single nucleon energy. If it is made equal to the *separation energy*, the wave function will have the correct asymptotic tail. The main bulk of such a wave function may be a rather poor approximation of the exact wave function. This is due to the polarization of the *real core* by the valence nucleon and the resulting *rearrangement energy*.

From the discussion presented here, it follows that a better approximation is obtained by using a single nucleon energy which is lower than the separation energy.

ε

$$\varepsilon = E_{A+1} - E_A + (E_A - E_A')$$

Which wave functions gives a better description?

- The one with the correct asymptotic tail

or

- The one whose main bulk is determined by the interaction with the core nucleons

- I hope that I convinced you that it is the second choice.

After all, it stands to reason that it is the dog who should wag his tail rather than the tail wagging the whole body of the dog.