Pairing, seniority and the BCS model

May 2, 2013

$$\langle \boldsymbol{r}|p\rangle = R_{n_p l_p j_p}(r)\left[Y_{l_p}(\hat{r})\chi_{1/2}\right]_{j_p m_p}$$

Uncoupled scheme

$$\Psi_a(pq;\boldsymbol{r}_1\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}\Big[R_p(r_1)\left[Y_{l_p}(\hat{r}_1)\chi_{1/2}\right]_p R_q(r_2)\left[Y_{l_q}(\hat{r}_2)\chi_{1/2}\right]_q$$
$$- R_p(r_2)\left[Y_{l_p}(\hat{r}_2)\chi_{1/2}\right]_p R_q(r_1)\left[Y_{l_q}(\hat{r}_1)\chi_{1/2}\right]_q\Big]$$

jj coupling scheme

We have also seen that one can choose another coupling scheme, in which the two particles carry total angular momentum $\boldsymbol{J} = \boldsymbol{j}_p + \boldsymbol{j}_q$ with projection $M = m_p + m_q$, such that $|j_p - j_q| \leqslant J \leqslant j_p + j_q$ and $-J \leqslant M \leqslant J$. This is called *coupled*-scheme. In this scheme the two-particle wave function reads,

$$\Psi_a(pq,JM;\boldsymbol{r}_1\boldsymbol{r}_2) = \mathcal{N}\Big[R_p(r_1)R_q(r_2)\left[\left[Y_{l_p}(\hat{r}_1)\chi_{1/2}\right]_{j_p}\left[Y_{l_q}(\hat{r}_2)\chi_{1/2}\right]_{j_q}\right]_{JM}$$
$$- R_p(r_2)R_q(r_1)\left[\left[Y_{l_p}(\hat{r}_2)\chi_{1/2}\right]_{j_p}\left[Y_{l_q}(\hat{r}_1)\chi_{1/2}\right]_{j_q}\right]_{JM}\Big] \quad (3)$$

The quantum numbers associated to this wave function are $\{n_p n_q l_p l_q j_p j_q JM\}$.

$$\left\{|\alpha\rangle = |pq;JM\rangle\right\}$$

$$\langle 12|j_p j_q; JM\rangle_a = N\big(\langle 12|j_p j_q; JM\rangle - (-1)^{j_p+j_q-J}\langle 12|j_q j_p; JM\rangle\big) \tag{4.9}$$

If $j_p = j_q$, then $(-1)^{j_p+j_q} = -1$ and

$$\langle 12|j_p^2; JM\rangle_a = N\big(1 + (-1)^J\big)\langle 12|j_p^2; JM\rangle \tag{4.10}$$

J must be even and $N = 1/2$ (since $\langle j_p^2; JM|j_p^2; JM\rangle = 1$). Otherwise $N = 1/\sqrt{2}$.

As a consequence of the generalized Pauli principle a symmetric space-spin wave function must be combined with an antisymmetric isospin function or *vice versa*. In both cases the complete wave function is antisymmetric under the interchange of all coordinates of the two particles. This leads to the general statement that one obtains allowed two-particle states $|(lj)^2\rangle_{JT}$ only for

$$J + T = \text{odd}$$

$1-(-1)^{J+T}$

$$|a \otimes b\rangle_B = \frac{1}{\sqrt{2}}(|a_1 \otimes b_2\rangle + |a_2 \otimes b_1\rangle) \qquad \text{bosons; symmetric}$$

$$|a \otimes b\rangle_F = \frac{1}{\sqrt{2}}(|a_1 \otimes b_2\rangle - |a_2 \otimes b_1\rangle) \qquad \text{fermions; anti-symmetric}$$

✧Convenient to describe processes in which particles are created and annihilated;
✧Convenient to describe interactions.

First quantizalton: Slater determinant		Second quantizalton

$$\Psi_{jk}(q_1, q_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_j(q_1) & \psi_k(q_2) \\ \psi_j(q_2) & \psi_k(q_2) \end{vmatrix} \Rightarrow |jk\rangle = a_j^\dagger a_k^\dagger |0\rangle$$

States

$a_i^\dagger \|0\rangle$	one-particle state	
$a_i^\dagger a_j^\dagger \|0\rangle$	two-particle state	described by Slater determinants in first quantization
$a_i^\dagger a_j^\dagger \ldots a_n^\dagger \|0\rangle$	N-particle state	

Examples of one and two-particle operators

First quantizaiton

Second quantizaiton

(1) $H_0 = \sum_{i=1}^{N} h_i$

$h_i = -\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}$

$H_0 = \sum_{i=1}^{N} \varepsilon_i \, a_i^{\dagger} a_i$

eigenvalue of h_i

One-body operator in second quantization

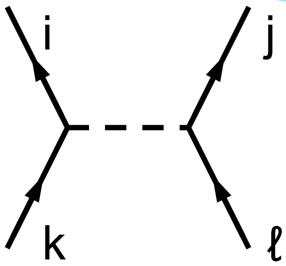
One-body operators depend upon one radial coordinate **r** only. In second quantization a one-body operator $\hat{M}$ can be written as,

$$\hat{M} = \sum_{pq} \langle p|\hat{M}|q\rangle c_p^{\dagger} c_q$$

where p and q run over all single-particle states (particle- as well as hole-states).

Occupation Number Formalism

$$V_{ijkl} a_i^+ a_j^+ a_k a_\ell$$



To proof that this is correct we will evaluate the matrix element of $\hat{M}$ between two single-particle states, i. e. (A+1)-states of the form $|i\rangle = c_i^\dagger|0\rangle$ for which $n_i = 0$. The final result of this calculation sould be that we get the matrix element itself again.

We then evaluate

$$
\begin{aligned}
\langle i|\hat{M}|j\rangle =& \langle 0|c_i\hat{M}c_j^\dagger|0\rangle = \sum_{pq}\langle p|\hat{M}|q\rangle\langle 0|c_i c_p^\dagger c_q c_j^\dagger|0\rangle \\
=& \sum_{pq}\langle p|\hat{M}|q\rangle\langle 0|\, c_i c_p^\dagger\, c_q c_j^\dagger + c_i c_j^\dagger\, c_p^\dagger c_q\,|0\rangle \\
=& \sum_{pq}\langle p|\hat{M}|q\rangle\Big[(1-n_i)\delta_{ip}(1-n_j)\delta_{qj} + (1-n_i)\delta_{ij}n_p\delta_{pq}\Big] \\
=& (1-n_i)(1-n_j)\langle i|\hat{M}|j\rangle + (1-n_i)\delta_{ij}\sum_p n_p\langle p|\hat{M}|p\rangle
\end{aligned}
\tag{1}
$$

and we see that with $n_i = n_j = 0$ we get the matrix element we needed, i. e. $\langle i|\hat{M}|j\rangle$, but that there is also another contribution which appears only when $i = j$. This corresponds to the sum of the mean values of $\hat{M}$ over all hole states. It is the interaction of the particles in the A-nucleon core among themselves, leaving the particle in the (A+1)-nucleus untouched. This term is called "core polarization".

The antisymmetrized two-particle states are,

$$|ij\rangle_a = c_i^\dagger c_j^\dagger |0\rangle \Longrightarrow {}_a\langle ij| = \langle 0|(c_i^\dagger c_j^\dagger)^\dagger = \langle 0|c_j c_i \tag{7.41}$$

and the matrix element is,

$$ {}_a\langle ij|\hat{M}|kl\rangle_a = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{M}|\gamma\delta\rangle \langle 0|c_j c_i : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : c_k^\dagger c_l^\dagger|0\rangle \tag{7.42}$$

Since the mean value of operators in normal form vanishes, the terms that survive contain only contractions. They are,

$$c_j c_i : c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma : c_k^\dagger c_l^\dagger = \left[\overline{c_i c_\alpha^\dagger}\,\overline{c_j c_\beta^\dagger} - \overline{c_i c_\beta^\dagger}\,\overline{c_j c_\alpha^\dagger}\right]\left[\overline{c_\gamma c_k^\dagger}\,\overline{c_\delta c_l^\dagger} - \overline{c_\gamma c_l^\dagger}\,\overline{c_\delta c_k^\dagger}\right] \tag{7.43}$$

which give,

$$\begin{aligned} {}_a\langle ij|\hat{M}|kl\rangle_a = &\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|\hat{M}|\gamma\delta\rangle \Big[(1-n_i)\delta_{i\alpha}(1-n_j)\delta_{j\beta} - (1-n_i)\delta_{i\beta}(1-n_j)\delta_{j\alpha}\Big] \\ &\times \Big[(1-n_k)\delta_{k\gamma}(1-n_l)\delta_{l\delta} - (1-n_k)\delta_{k\delta}(1-n_l)\delta_{l\gamma}\Big] \\ =&(1-n_i)(1-n_j)(1-n_k)(1-n_l)\Big[\langle ij|\hat{M}|kl\rangle_a - \langle ji|\hat{M}|kl\rangle_a\Big] \\ &- (1-n_i)(1-n_j)(1-n_k)(1-n_l)\Big[\langle ij|\hat{M}|lk\rangle_a - \langle ji|\hat{M}|lk\rangle_a\Big] \end{aligned} \tag{7.44}$$

The matrix element antisymmetrized to the right only becomes,

$$\langle ji|\hat{M}|kl\rangle_a = \langle ji|\hat{M}\left[|kl\rangle - |lk\rangle\right] = \langle ij|\hat{M}\left[|lk\rangle - |kl\rangle\right] = -\langle ij|\hat{M}|kl\rangle_a$$

and Eq. (3) becomes,

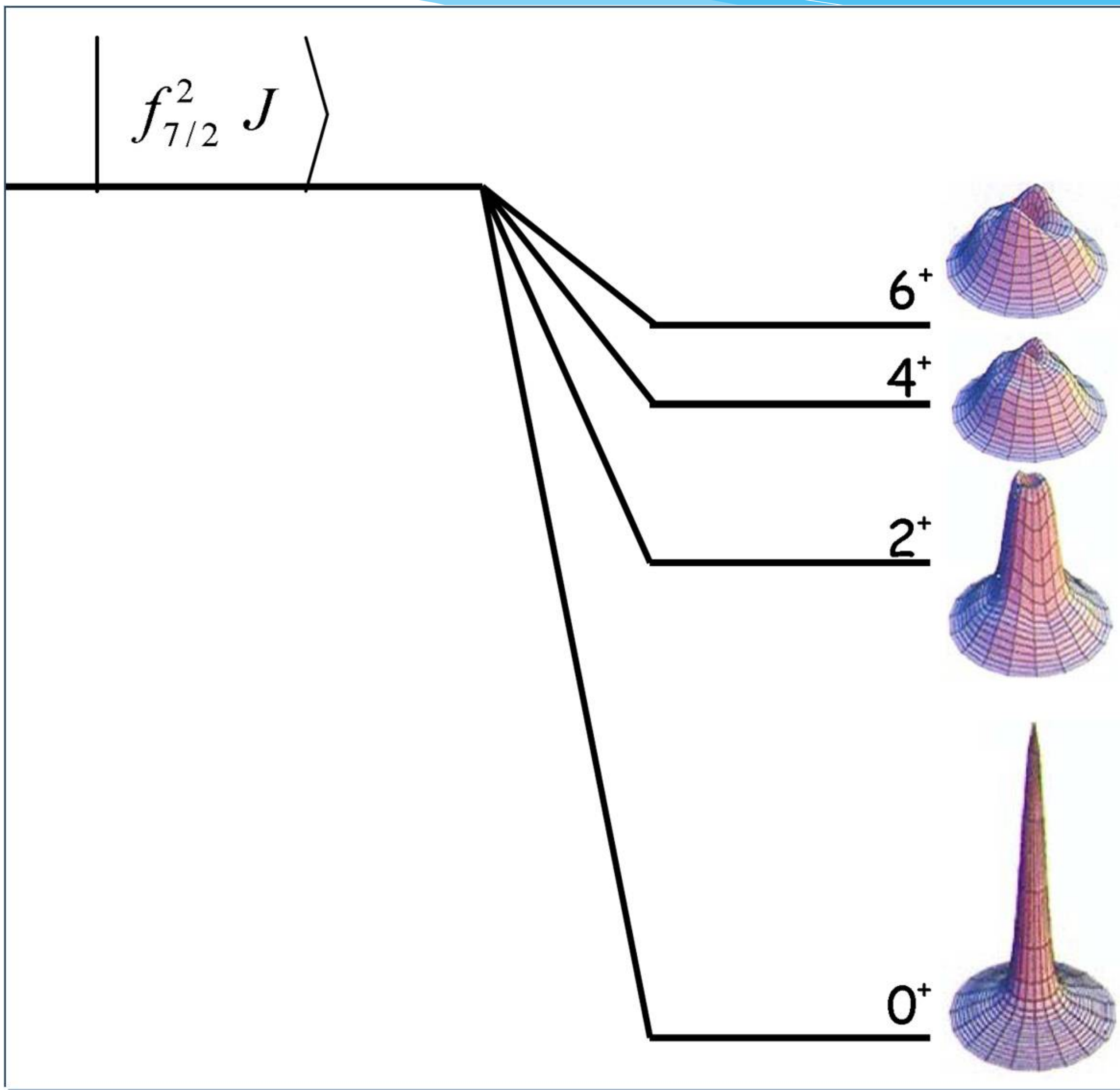
$$_a\langle ij|\hat{M}|kl\rangle_a = (1-n_i)(1-n_j)(1-n_k)(1-n_l)\,_a\langle ij|\hat{M}|kl\rangle_a$$

The Hamiltonian becomes,

$$H = \sum_{\alpha\beta}\langle\alpha|T|\beta\rangle c_\alpha^\dagger c_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\gamma\delta\rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma.$$

Two particles in a single j shell

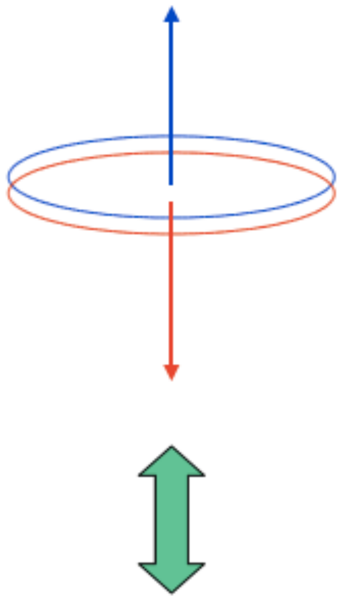
The *J=0 pairing interaction* is the dominant component of the nuclear interaction.



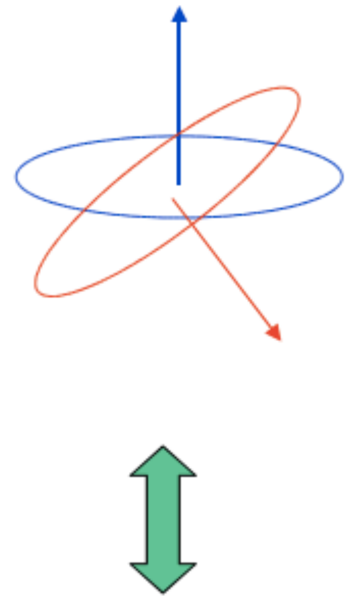
Even-even nuclei have $J = 0$ ground states. Göppert-Mayer (1950) showed that the $J = 0$ coupling of two nucleons in a single j-shell is energetically favored for a short-ranged, attractive nucleon-nucleon force. This is due to the large overlap of single-particle orbitals with $\pm m$ angular momentum projection.

$$|J = 0, M = 0\rangle = \frac{1}{\sqrt{2}} \sum_m \langle j, j, m, -m|00\rangle a_m^\dagger a_{-m}^\dagger |-\rangle.$$

Simple interpretation:



I=0 pair



$I \neq 0$ pair

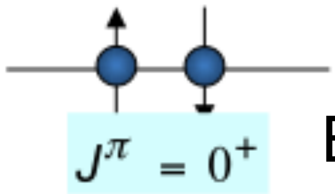
The spatial overlap is the largest for the I=0 pair.

"Pairing Correlation"

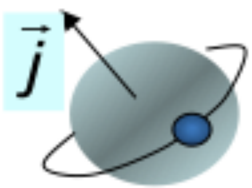
Reminder: Seniority symmetry

1943 Racah

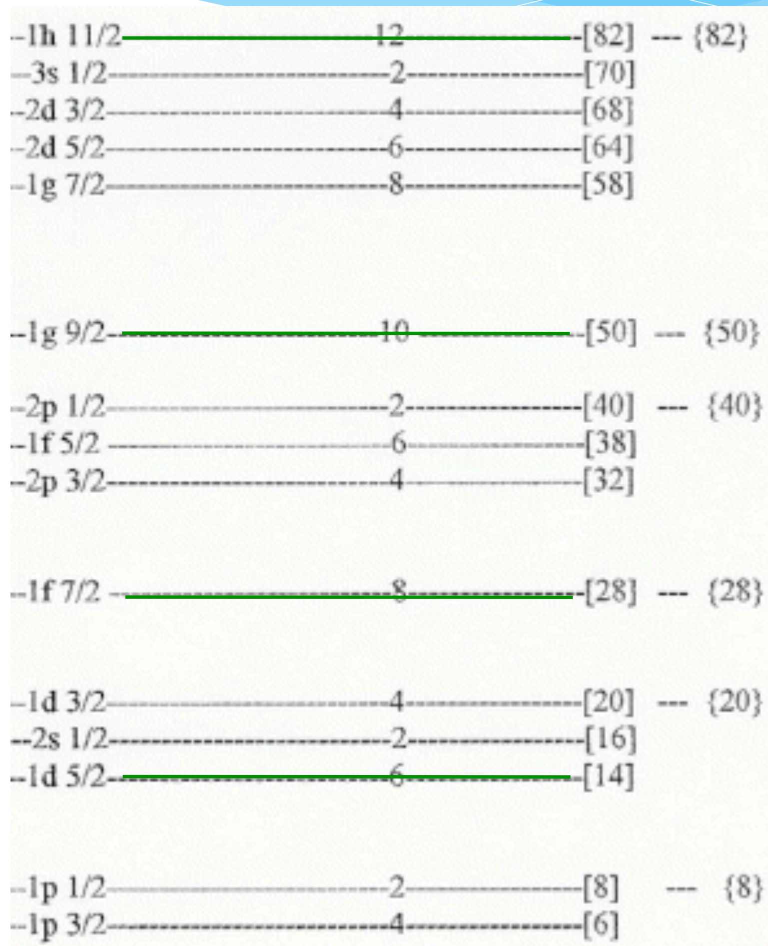
1949 Goeppert-Mayer



Even-even



Odd-A

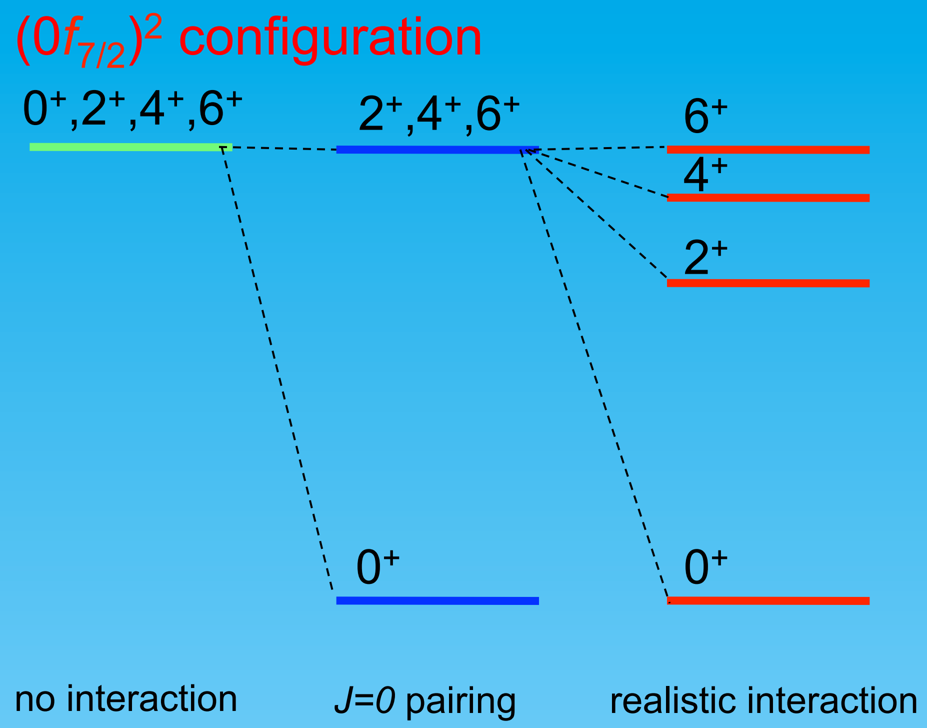


Mean field theories

- Single-particle model
  HO, WS…
- Hartree-Fock (density functional) approaches
  Skyrme force, boson exchange potentials
- Shell model
  Monopole

http://www.nobelprize.org/nobel_prizes/physics/laureates/1963/mayer-lecture.pdf

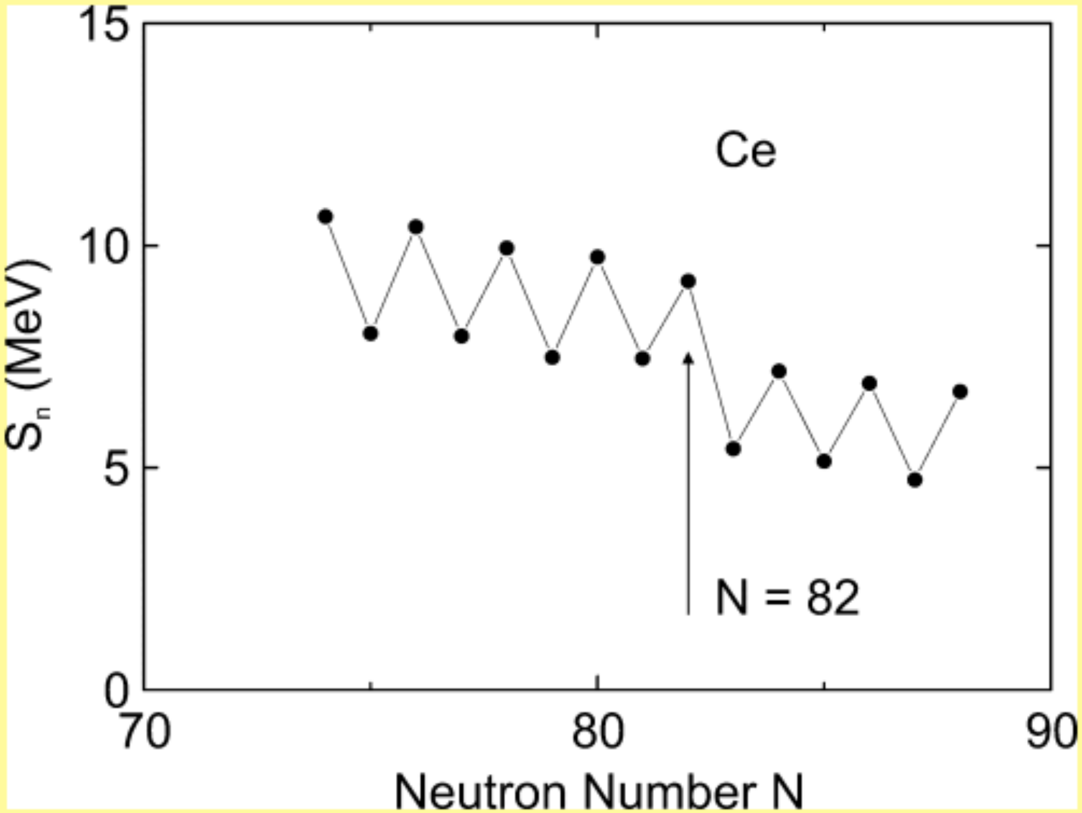
Realistic interaction and monopole pairing



- ❖J=0 interactions are strongly attractive.
- ❖Seniority is conserved when j<9/2
- ❖Pairing interaction conserves seniority

$$\left\langle j^2 JM_J \left| \hat{V}_{\text{pairing}} \right| j^2 JM_J \right\rangle = \begin{cases} -\frac{1}{2}(2j+1)g_0, & J=0 \\ 0, & J \neq 0 \end{cases}$$

(i) Odd-even effect: mass of an odd-even nucleus is larger than the mean of adjacent two even-even nuclear masses → shows up in S_n and S_p for all nuclei.



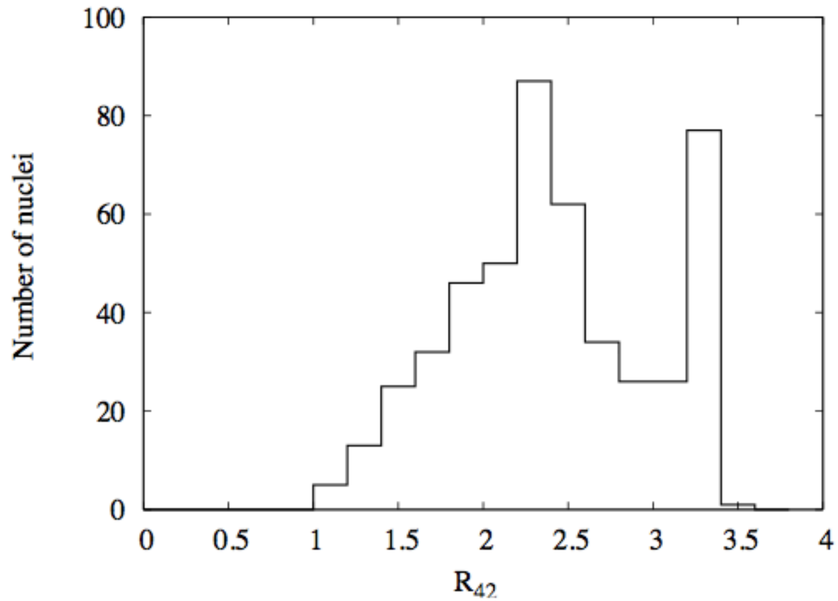
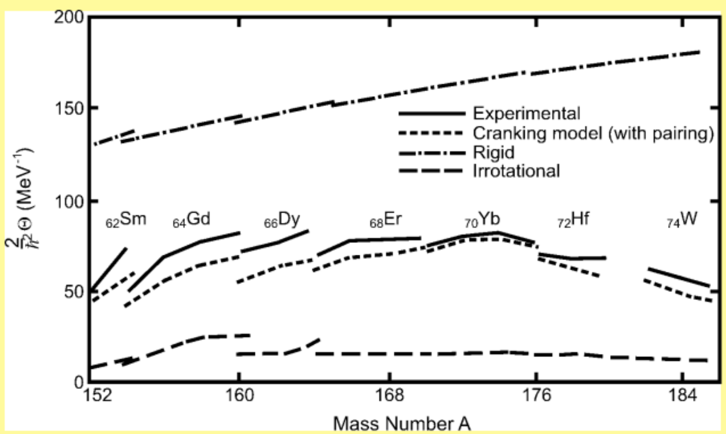


Figure 5.3: Distribution of nuclei with respect to deformation indicator R_{42}. Taken from GF Bertsch, arXiv:1203.5529.

(v) Moment of inertia: extracted from level spacing in rotational bands

$$E = \frac{\hbar^2}{2\Theta} J(J+1)$$

deviates about a factor of two from the rigid rotor values.



- $\Theta_{irrot} < \Theta_{exp} < \Theta_{rigid}$
- Pairing correlations have a dramatic influence on collective modes.

9.1 Pairing gaps: odd-even binding energy differences

The basic hallmarks of pair condensates are the odd-even staggering in binding energies, the gap in the excitation spectrum of even systems, and the compressed quasiparticle spectrum in odd systems. To examine odd-even staggering, it is convenient to define the even and odd neutron pairing gaps with the convention

$$\Delta^{(3)}_{o,Z}(N) = \frac{1}{2}(E_b(Z,N+1) - 2E_b(Z,N) + E_b(Z,N-1)), \text{ for } N \text{ odd}, \tag{9.1}$$

$$\Delta^{(3)}_{e,Z}(N) = -\frac{1}{2}(E_b(Z,N+1) - 2E_b(Z,N) + E_b(Z,N-1)), \text{ for } N \text{ even}. \tag{9.2}$$

where N and Z are the neutron and proton numbers and E_b is the binding energy of the nucleus. The proton pairing gaps are defined in a similar way. With the above definition, the gaps are positive for normal pairing.

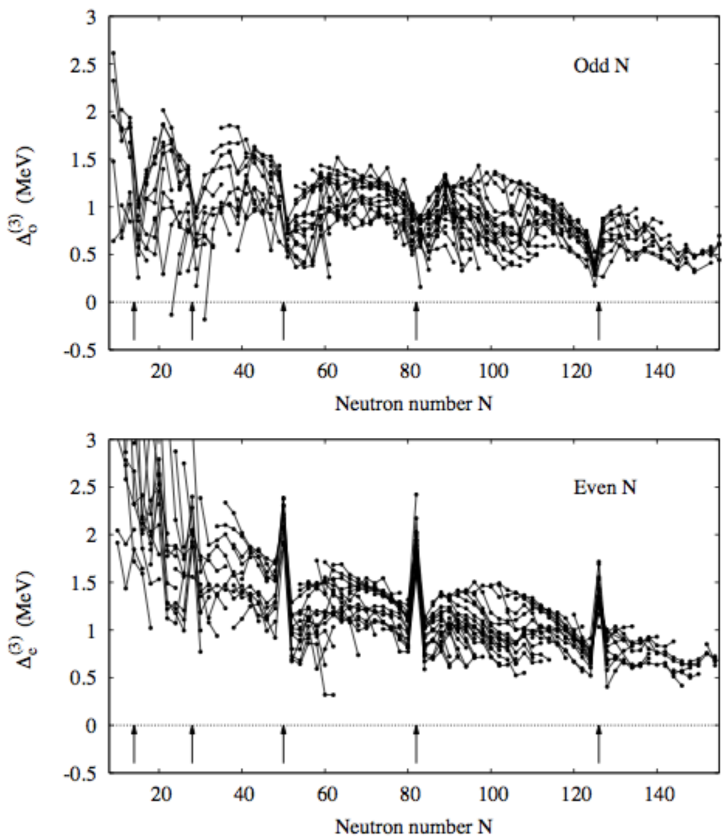


Figure 9.1: Upper panels: odd-N pairing gaps. Lower panels: even-N pairing gaps. Typically, the odd-N nuclei are less bound than the average of their even-N neighbors by about 1 MeV. However, one sees that there can be about a factor of two scatter around the average value at a given N.

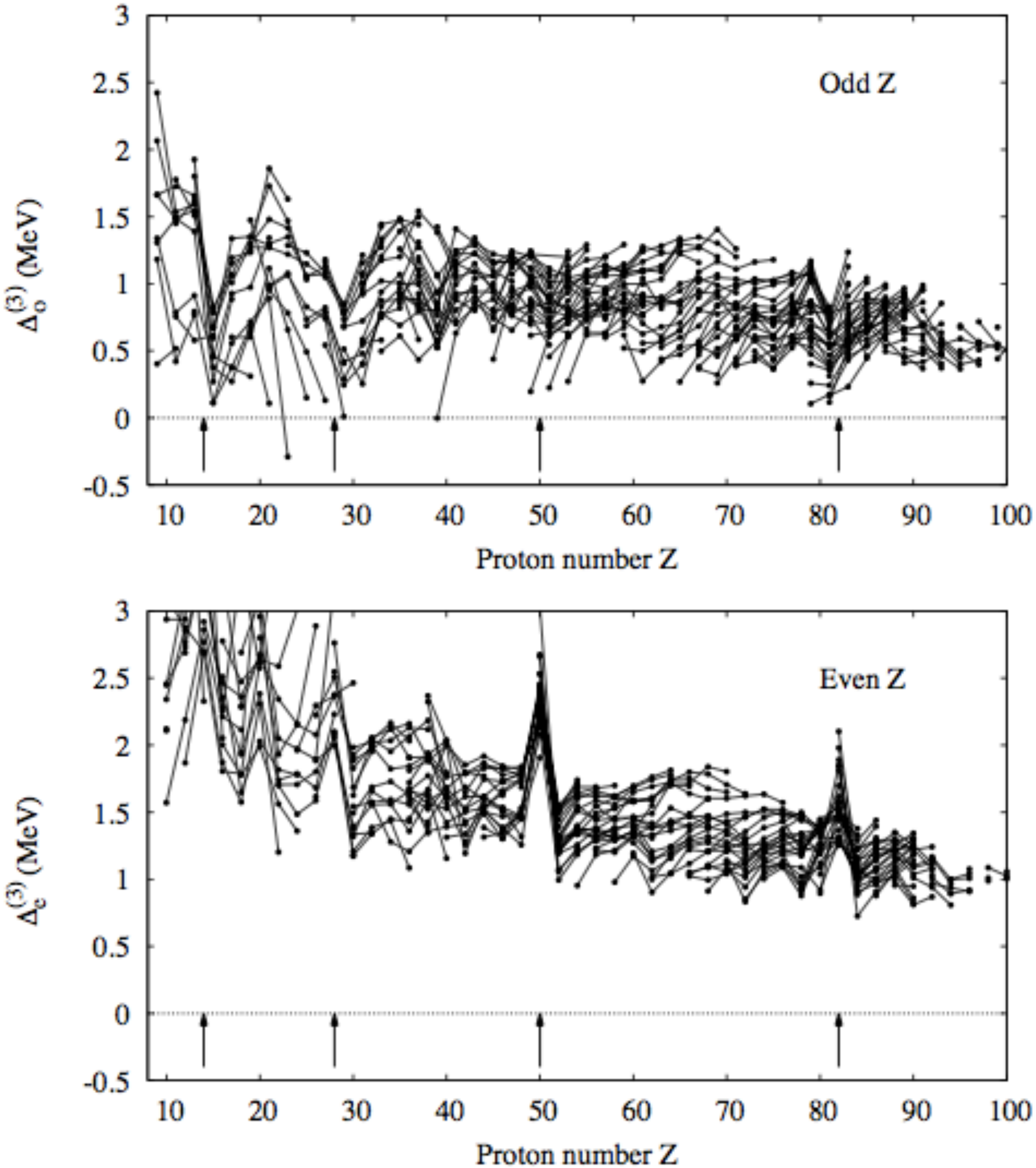


Figure 9.2: Upper panels: odd-Z pairing gaps. Lower panels: even-Z pairing gaps.

The seniority model

The seniority model provides a simple model for pairing phenomena.
System: N fermions in a single j-shell.
Hamiltonian:

$$\begin{aligned} H &= -G \sum_{m,m'>0} \hat{a}^\dagger_m \hat{a}^\dagger_{-m} \hat{a}_{-m'} \hat{a}_{m'} \\ &= -G \hat{S}_+ \hat{S}_- \end{aligned}$$

where

$$\hat{S}_+ = \sum_{m>0} \hat{a}^\dagger_m \hat{a}^\dagger_{-m} \quad \text{and} \quad \hat{S}_- = \left(\hat{S}_+\right)^\dagger .$$

Rewrite Hamiltonian as

$$H = -G\left(\vec{S}\cdot\vec{S} - \hat{S}_0^2 + \hat{S}_0\right)$$

in terms of total quasi-spin

$$\vec{S} = \sum_{m>0} \vec{s}^{(m)}.$$

and total z-component of quasi spin

$$\hat{S}_0 = \sum_{m>0} \hat{s}_0^{(m)} = \frac{1}{2}(\hat{N} - \Omega).$$

Here, $\Omega = j + 1/2$ is the maximal number of pairs for a single j-shell. The eigenvalues S of total quasi-spin are

$$S = \frac{1}{2}|N - \Omega|, \ldots, \frac{1}{2}\Omega - 1, \frac{1}{2}\Omega.$$

Thus, the energies of the seniority model are

$$E(S, N) = -G\left[S(S+1) - \frac{1}{4}(N-\Omega)^2 + \frac{1}{2}(N-\Omega)\right].$$

Alternatively, one uses the *seniority* quantum number $s = \Omega - 2S$

$$E(s, N) = -\frac{G}{4}\left[s^2 - 2s(\Omega + 1) + 2N(\Omega + 1) - N^2\right].$$

Note:

- s counts number of unpaired nucleons.
- ground state has minimal seniority $s = 0$ (or maximal quasi spin $S = \Omega/2$)
- for fixed N, excitations depend only on seniority quantum number
- $E(N, s = 2) - E(N, s = 0) = G\Omega$

Two-particle spectrum of pure pairing force: $J = 0$ ground state is separated from degenerate $J = 2, 4, 6, \ldots, 2j - 1$ levels.

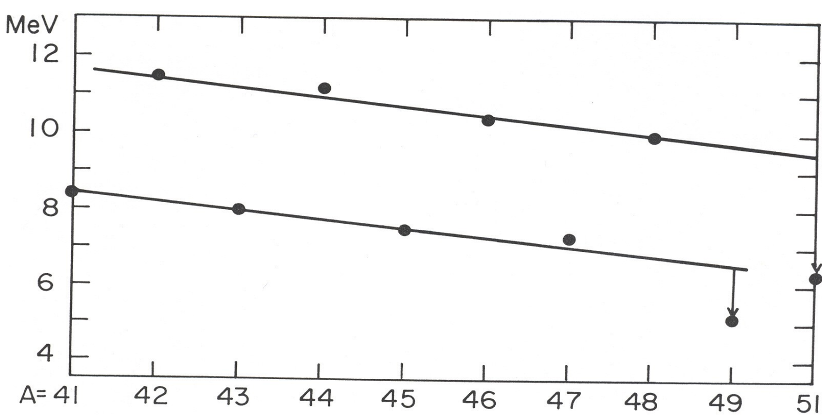
Seniority coupling and binding energy

Semi-magic nuclei

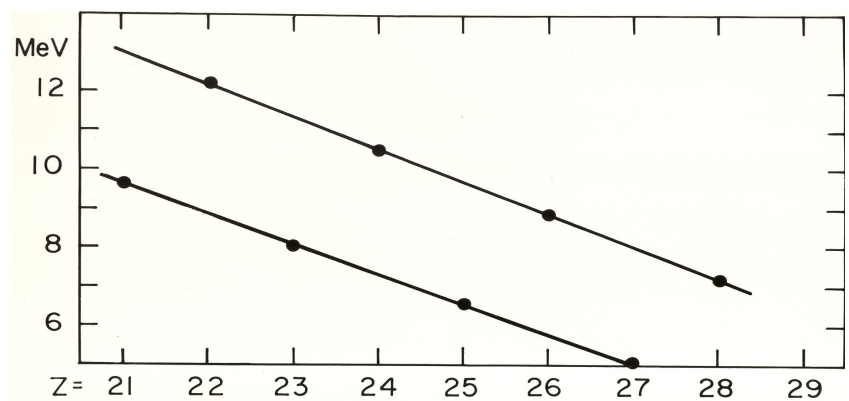
$$\hat{V} = a + b\mathbf{t}_1 \cdot \mathbf{t}_2 + GP_0,$$

Binding energies of ground states in j^n configuration

$$E\left(j^n\right) = Cn + \frac{1}{2}n(n-1)\alpha + \left[\frac{1}{2}n\right]\beta$$



Neutron separation energies from Ca isotopes

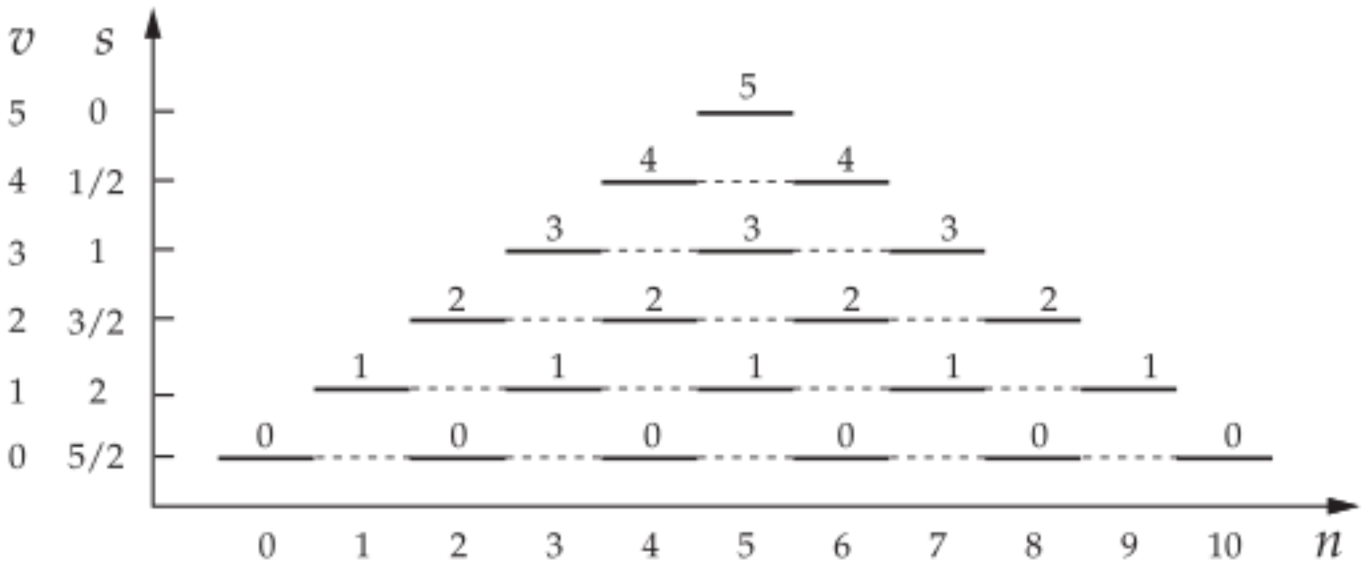


Proton separation energies from *N*=28 isotones

I. Talmi, Simple models of complex nuclei (Harwood, Chur, Switzerland, 1993)

The spectrum with a pairing interaction

USp(10) irreps in the j=9/2 shell



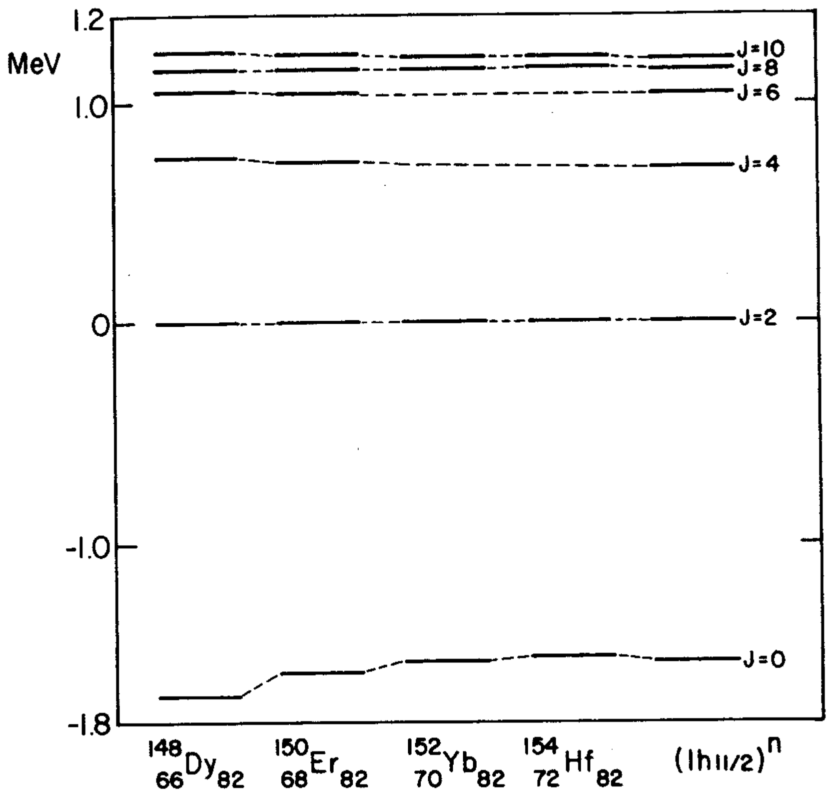
v: Seniority
s: Quasispin

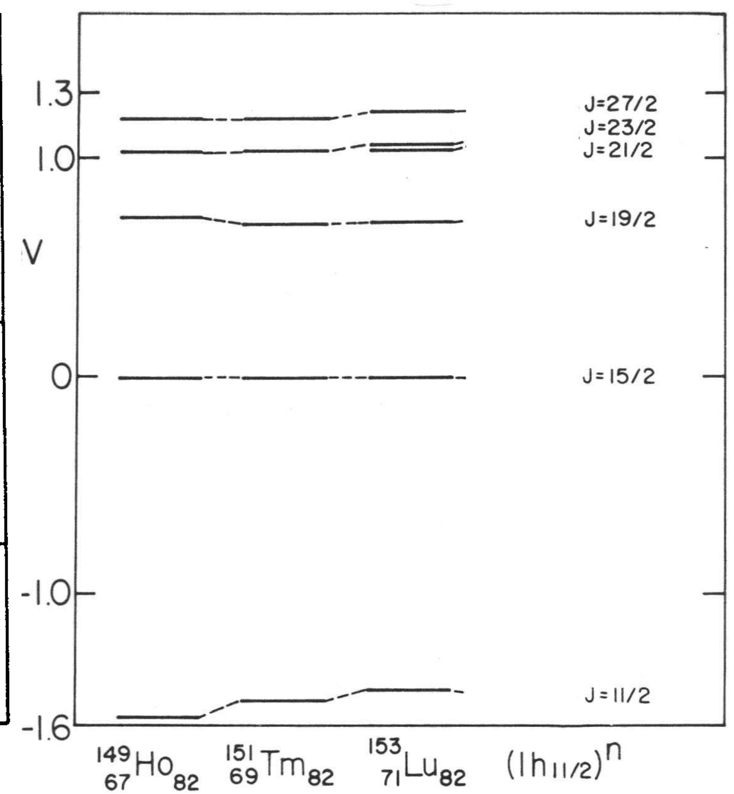
D. J. Rowe, M. J. Carvalho, and J. Repka, Rev. Mod. Phys. 84, 712 (2012).

Seniority coupling scheme with realistic interaction

$$|\text{g.s.}\rangle = |\nu = 0; J = 0\rangle = (P_j^+)^{n/2}|\Phi_0\rangle$$
$$|\nu = 2; JM\rangle = (P_j^+)^{(n-2)/2}A^+(j^2JM)|\Phi_0\rangle$$

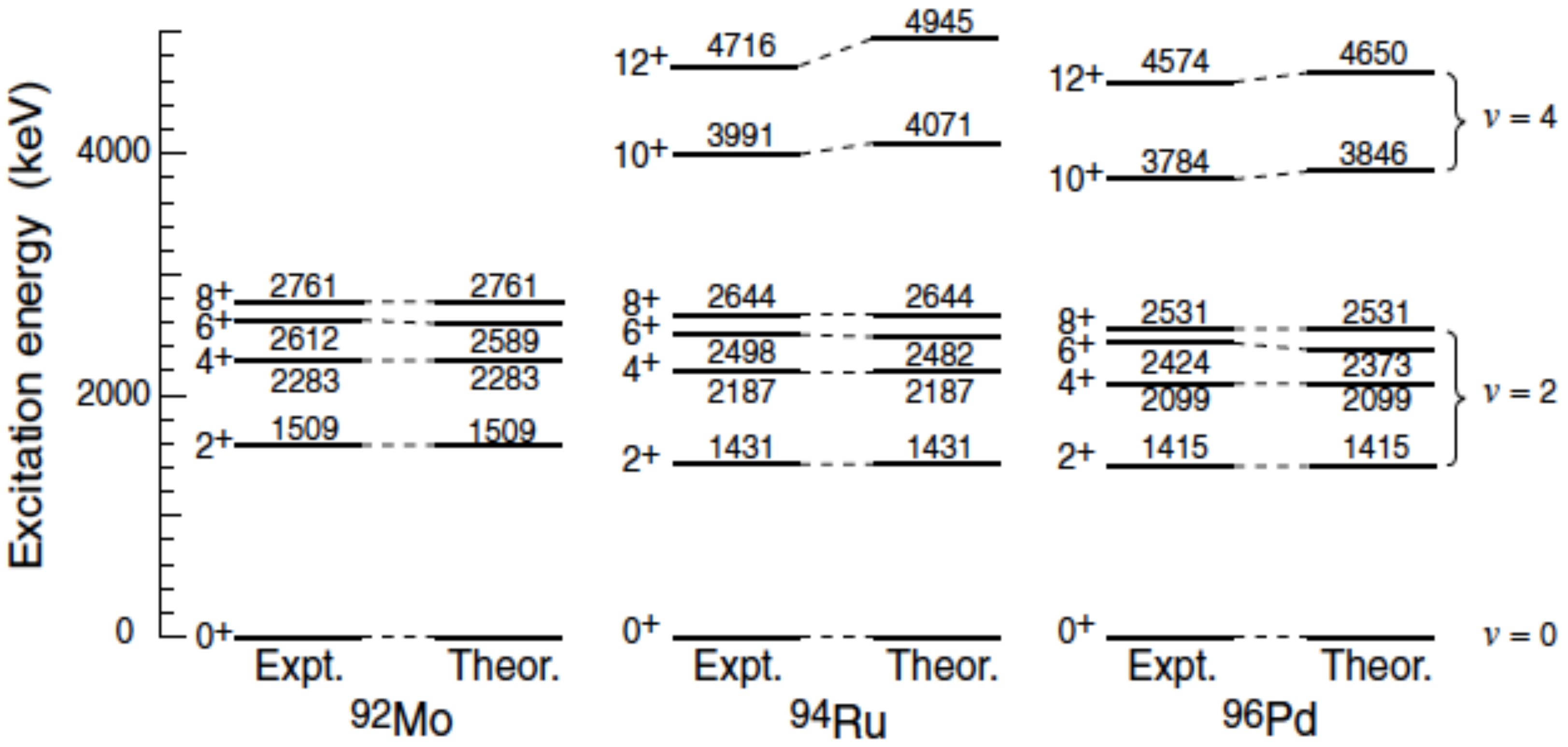
Energy levels of $0h_{11/2}$ protons in N=82 isotones





I. Talmi, Simple models of complex nuclei

Energy levels of $0g_{9/2}$ protons in N=50 isotones



D.J. Rowe and G. Rosensteel, Phys. Rev. Lett. ***87*** *(2001) 172502*

Conservation of seniority

the rotationally invariant interaction has to satisfy **[(2*j* − 3)/6]** linear constraints to conserve seniority.

$$j = 9/2: 65v_2 - 315v_4 + 403v_6 - 153v_8 = 0$$

$$j = 11/2: 1020v_2 - 3519v_4 - 637v_6 + 4403v_8 - 2541v_{10} = 0$$

$$j = 13/2: 1615v_2 - 4275v_4 - 1456v_6 + 3196v_8 - 5145v_{10} - 4225v_{12} = 0$$

$j = 15/2$

$$1330V_2 - 2835V_4 - 1807V_6 + 612V_8 + 3150V_{10} + 3175V_{12} - 3625V_{14} = 0,$$

and

$$77805V_2 - 169470V_4 - 85527V_6 - 4743V_8 + 222768V_{10} + 168025V_{12} - 208858V_{14} = 0.$$

I. Talmi, Simple Models of Complex Nuclei
D.J. Rowe and G. Rosensteel, Phys. Rev. Lett. 87, 172501 (2001).
P. Van Isacker and S. Heinze, Phys. Rev. Lett. 100, 052501 (2008).
CQ et al., PRC 82, 014304(2010)