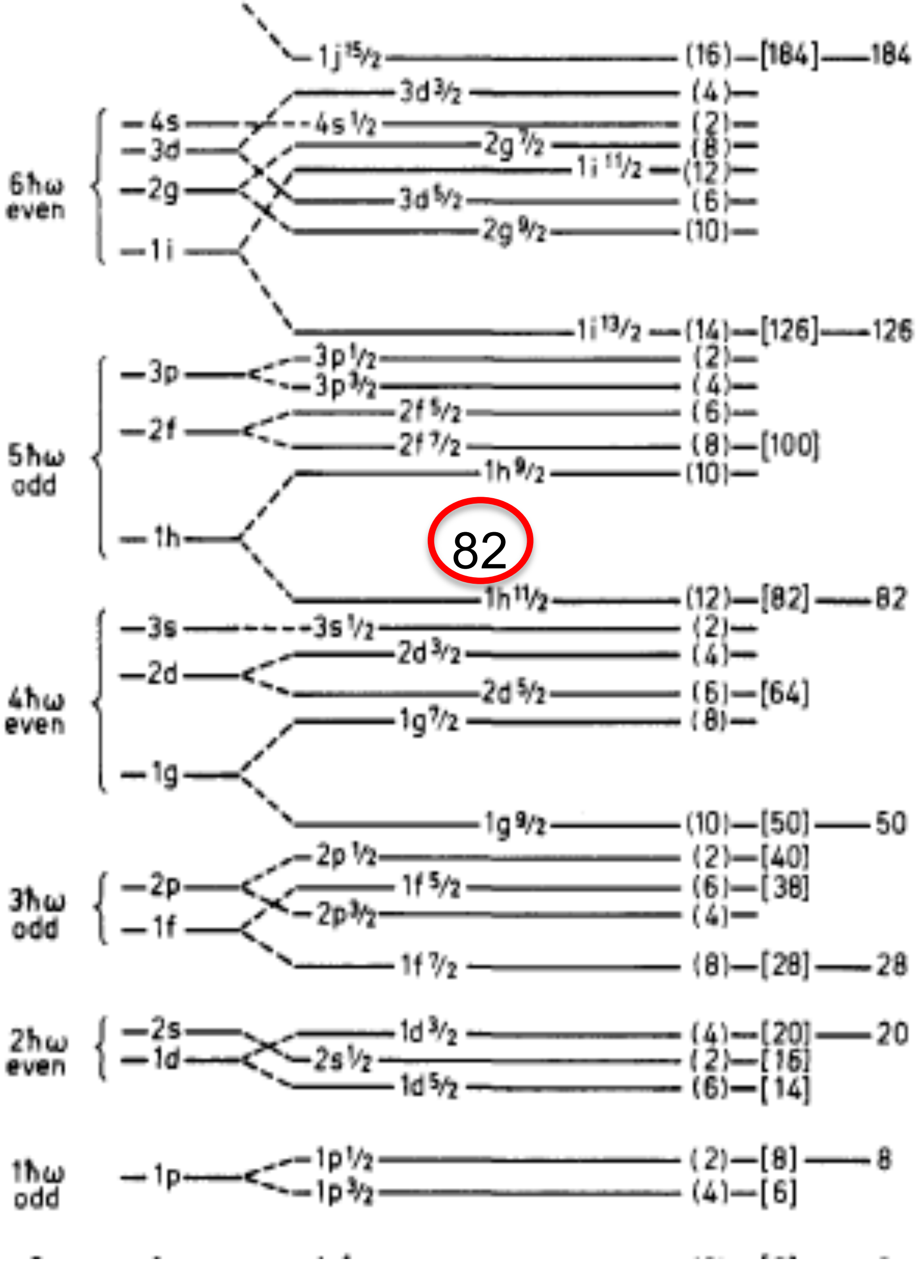
Enrico Vigezzi INFN Milano

PAIRING CORRELATIONS AND COLLECTIVE EXCITATIONS

Theory service for the low-energy nuclear physics community:
A hands-on workshop, ECT*, 7-9 July 2025

The quantum numbers of the energy levels observed in nuclei adjacent to the closed shell ^{132}Sn are as expected, according to the spherical shell model



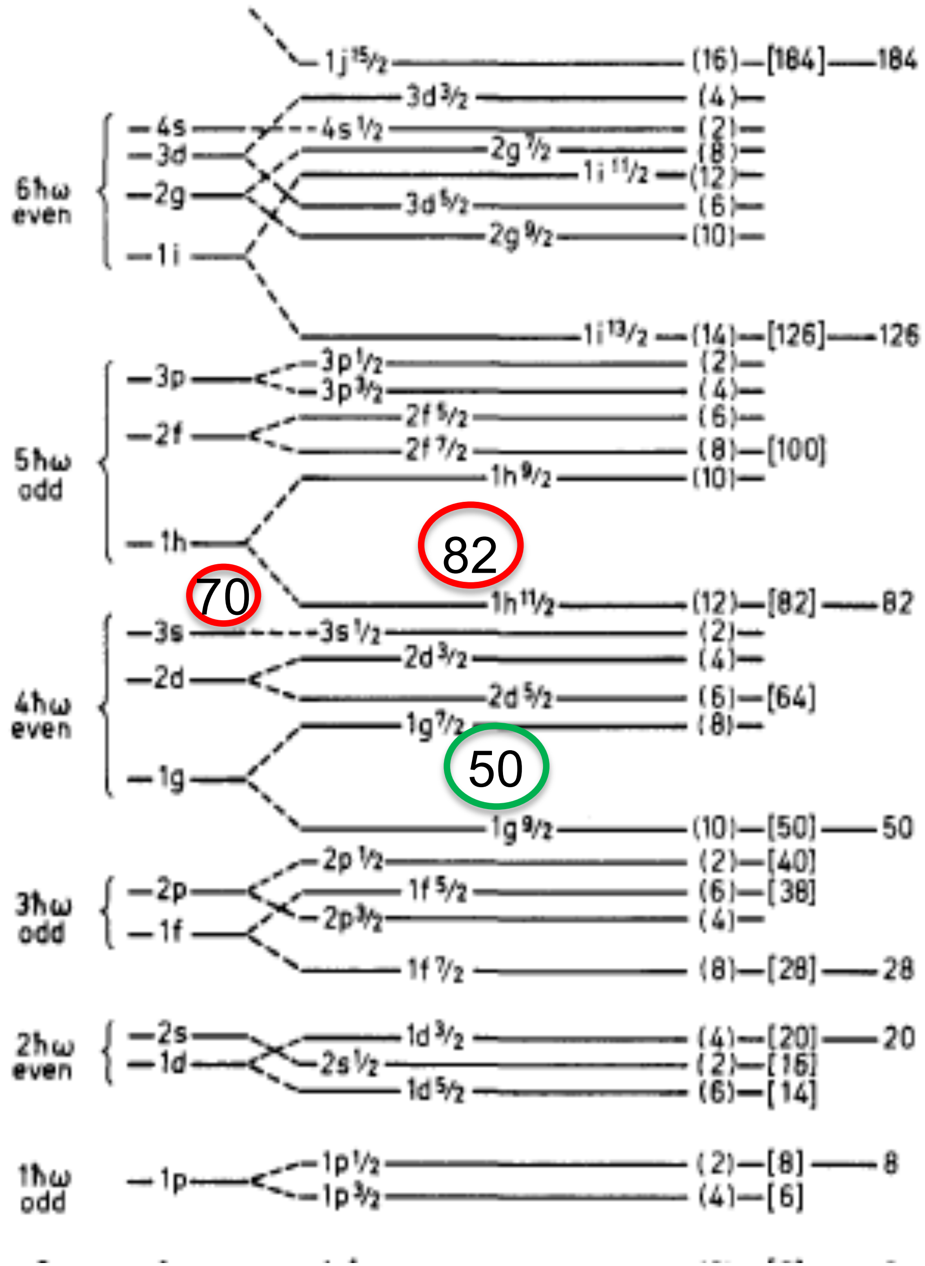
$^{133}_{50}Sn_{83}$

E(level) (keV)	J^{π}(level)
0.0	7/2-
853.7 3	3/2-
1363 31	(1/2-)
1560.9 5	(9/2-)

$^{131}_{50}Sn_{81}$

E(level) (keV)	J^{π}(level)
0.0	(3/2+)
0.0+X	(11/2-)
331.73 10	(1/2+)
1654.53 8	(5/2+)
2434.13 7	(7/2+)

The quantum numbers of the lowest energy levels observed in the odd nuclei adjacent to ^{120}Sn are the same, NOT as expected according to the spherical shell model



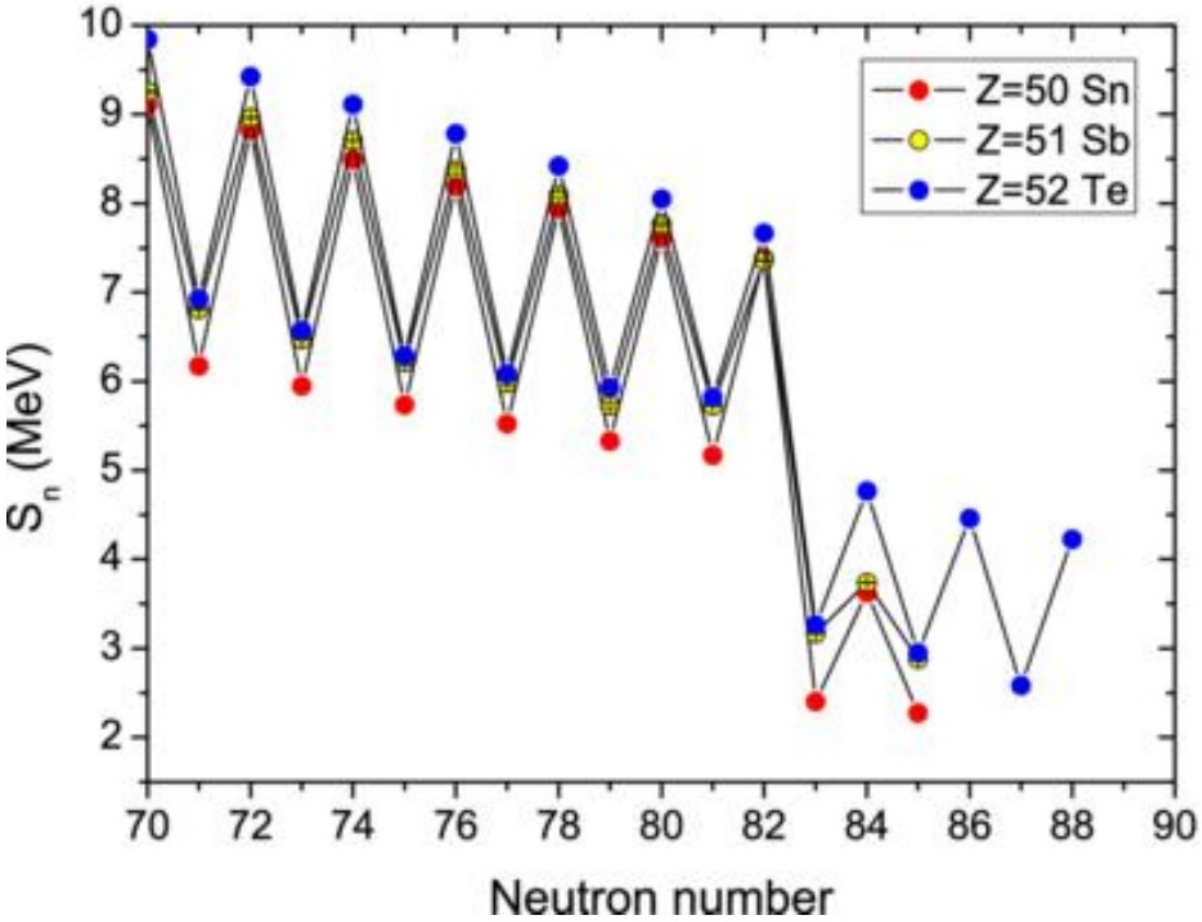
$^{121}_{50}Sn_{71}$

E(level) (keV)	J^{π}(level)
0.0	3/2+
6.31 6	11/2-
60.34 2	1/2+
663.63 6	7/2-,9/2-
869.25 5	5/2+
908.8 3	5/2+
925.59 5	7/2+
949.2 5	7/2-

$^{119}_{50}Sn_{69}$

E(level) (keV)	J^{π}(level)
0	1/2+
23.871 8	3/2+
89.531 13	11/2-
787.01 4	7/2+
920.51 14	3/2+
921.39 15	5/2+

The neutron separation energies along the Z=50 chain show a pronounced odd-even effect: it is more difficult to extract a neutron from a nucleus with N even, than from a nucleus with N odd



It looks as if particles and holes lose their identity, and neutron pairs have some extra binding.

It is possible to to account for these experimental facts, and still adopt a mean field picture, by extending the Hartree-Fock ansatz and introducing a new vacuum.

HF/KS ground-state:

Slater determinant of particles

$$a_p^\dagger|\Phi\rangle = |p\rangle \qquad E = \varepsilon_p$$

$$a_h|\Phi\rangle = |h^{-1}\rangle \qquad E = -\varepsilon_h$$

BCS (Bardeen-Cooper-Schrieffer):

Slater determinant of **quasiparticles**

$$\begin{aligned} \beta_k^\dagger &= u_k a_k^\dagger + v_k a_{\bar{k}}, \\ \beta_k &= u_k a_k + v_k a_{\bar{k}}^\dagger. \end{aligned}$$

$$\beta_k^\dagger|\Phi\rangle = |k\rangle \qquad E = E_k$$

$$|\mathrm{BCS}\rangle = \Pi_{k>0}\left(u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger\right)|-\rangle \quad =$$

$$\sum_{k>0}\frac{v_k}{u_k}a_k{}^+ a_{\bar{k}}{}^+ |0> + \frac{1}{2}\sum_{kk'>0}\frac{v_k v_{k'}}{u_k u_{k'}} a_k{}^+ a_{\bar{k}}{}^+ a_{k'}{}^+ a_{\bar{k}'}{}^+ + ...$$

- The BCS wave functions **breaks the particle number symmetry**.
- The u,v amplitudes are determined applying the **variational principle** by minimizing:

$$\langle \mathrm{BCS}|H - \lambda N|\mathrm{BCS}\rangle$$

with a **general Hamiltonian**:

$$H = T + V = \sum_{k_1 k_2}\langle k_1|t|k_2\rangle a_{k_1}^\dagger a_{k_2} + \frac{1}{4}\sum_{k_1 k_2 k_3 k_4}\langle k_1 k_2|\bar{v}|k_3 k_4\rangle a_{k_1}^\dagger a_{k_2}^\dagger a_{k_4} a_{k_3}$$

$$\lambda \equiv \frac{\partial E}{\partial N}$$

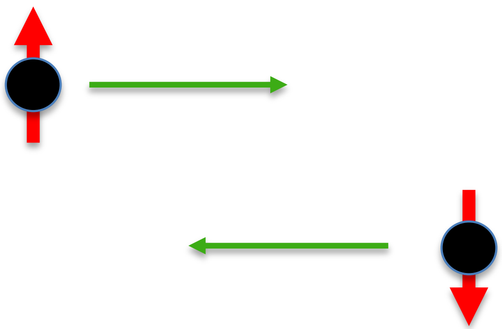
Fermi energy

Time-reversal states

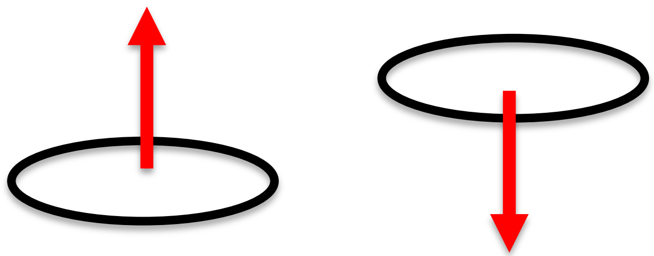
$$t \quad \rightarrow \quad -t$$

$$|k\rangle \quad \rightarrow \quad |\tilde{k}\rangle$$

$$\begin{cases} \mathbf{r} \rightarrow \mathbf{r} \\ \mathbf{p} \rightarrow -\mathbf{p} \\ \sigma_i \rightarrow -\sigma_i . \end{cases}$$



Electrons in time-reversal states: opposite momenta and spins.



$|jm\rangle$ $\qquad$ $|\widetilde{jm}\rangle = (-)^{j+m}|j-m\rangle$

Nucleons in time-reversal states.

$$|\mathrm{BCS}\rangle = \Pi_{k>0}\left(u_k + v_k a^\dagger_k a^\dagger_{\bar{k}}\right)|-\rangle.$$

Nucleons around the Fermi energy organize themselves in Cooper pairs, formed by quasiparticle states (superpositions of particles and holes) in time reversal.

The ground state of the even-even nucleus is a condensate of Cooper pairs.

To break a pair, costs an energy given by the energy gap $\boldsymbol{\Delta}$.

Nucleons around the Fermi energy organize themselves in Cooper pairs, formed by quasiparticle states (superpositions of particles and holes) in time reversal.
The ground state of the even-even nucleus is a condensate of Cooper pairs.
To break a pair, costs an energy given by the energy gap ***Δ***.

$$N = \sum_k v_k^2 = 2\sum_{k>0} v_k^2.$$

Number equation: the correct particle number is reproduced (on average)

$$\Delta_k = -\sum_{k'>0} \frac{\Delta_{k'}}{2E_{k'}} v_{k\bar{k}k'\bar{k}'}.$$

This quantity is the GAP.
No E_x is smaller than the gap.

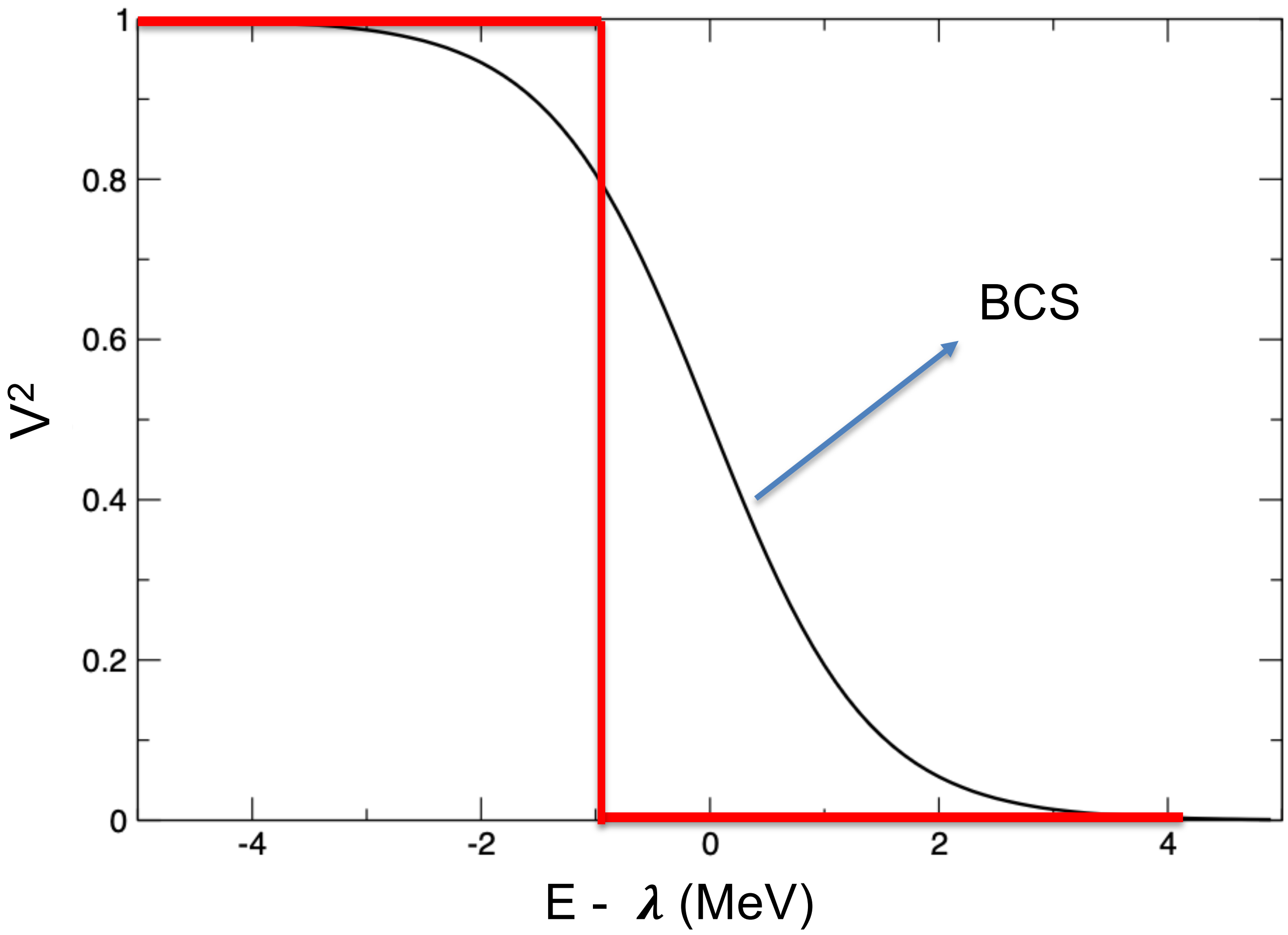
$$E_k = \sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}$$

Quasiparticle energy: to add or remove a particle one needs an extra energy which can be interpreted as the binding of the Cooper pair.

$$v_k^2 = \frac{1}{2} - \frac{\tilde{\varepsilon}_k}{2E_k} \qquad u_k^2 = \frac{1}{2} + \frac{\tilde{\varepsilon}_k}{2E_k}$$

$$v_k^2 + u_k^2 = 1$$

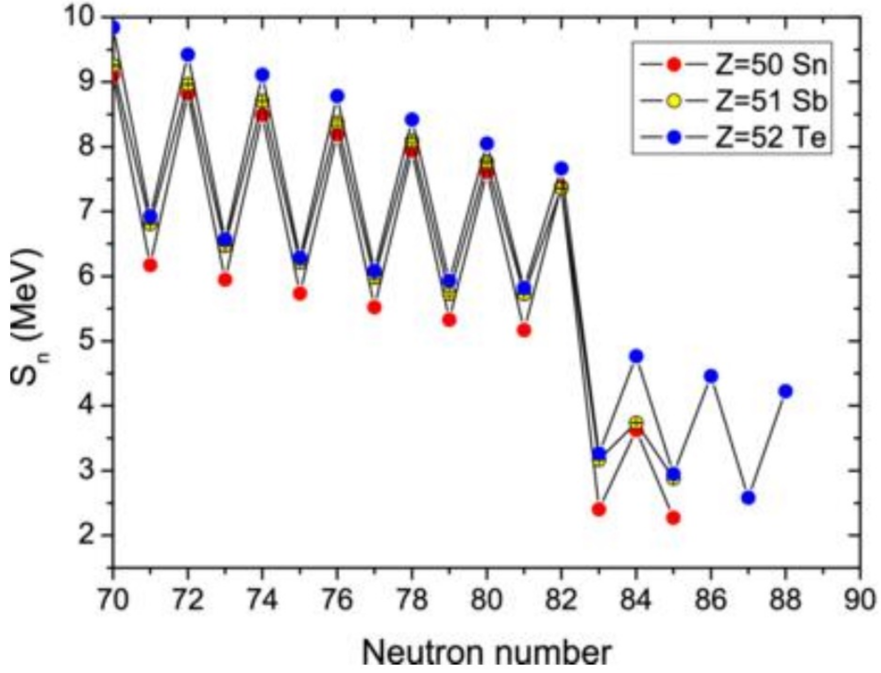
Pairing changes the occupation numbers of orbitals close to the Fermi energy

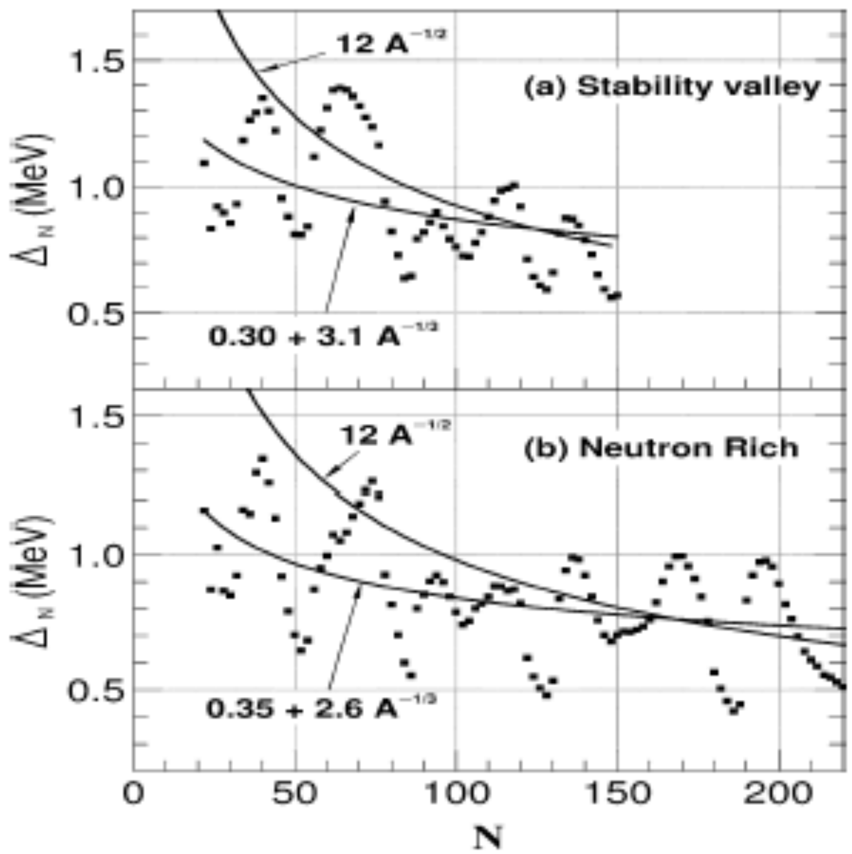


Odd-even staggering of separation energies

Global comparison with experiment

$$\Delta^{(3)}(N) = (-)^{A+1}\frac{S_n(A+1) - S_n(A)}{2}.$$



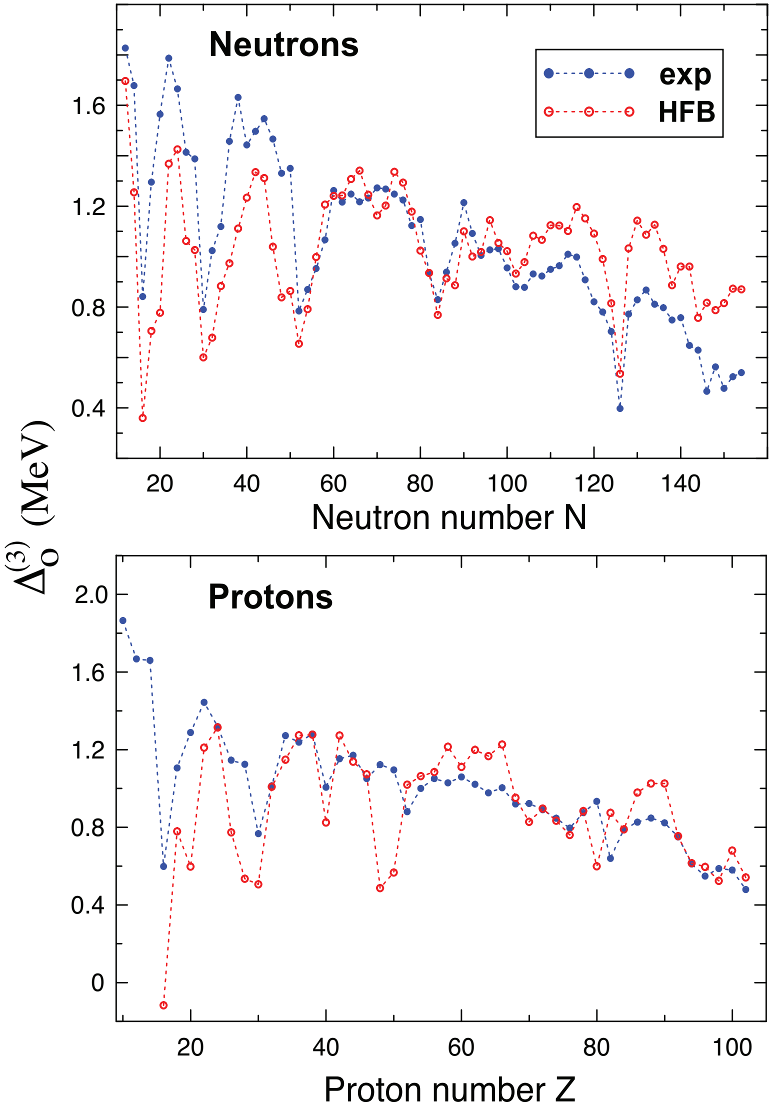


S. Hilaire, J.F. Berger, M. Girod, W. Satula, P. Schuck, Phys. Lett. B531(2002)61

Global analyses of odd-even mass differences

$$V(\mathbf{r}, \mathbf{r}') = V_0 \left(1 - \eta \frac{\rho(\mathbf{r})}{\rho_0}\right) \delta(\mathbf{r} - \mathbf{r}').$$

η = 0 -> Volume η = 0.5 -> Mixed η = 1 -> Surface



Theory	pairing	residual neutrons	residual protons	$V_0^{\text{eff}}(p)/V_0^{\text{eff}}(n)$
Constant		0.31	0.27	
c/A^α		0.24	0.22	
HF+BCS	volume	0.31	0.38	1.05
HF+BCS	mixed	0.30	0.36	1.08
HF+BCS	surface	0.27	0.35	1.12
HFB	mixed	0.27	0.32	1.11
HFB+LN	mixed	0.23	0.28	1.11
HFB-14		0.46	0.44	1.10

G.F. Bertsch et al. Phys. Rev. C 79, 034306 (2009)

The RPA equations to calculate collective excitations keep the same form

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega_{\mathrm{n}} \begin{pmatrix} X \\ Y \end{pmatrix},$$

But the phonons are expanded over a set of 2 quasiparticles:

$$|n\rangle = \Sigma_{ph} [\, X_{ph}\ |ph^{-1}\rangle - Y_{ph}\ |hp^{-1}\rangle \,]$$

$$\downarrow$$

$$|n\rangle = \Sigma_{ph} [\, X_{ph}\ |\alpha\beta\rangle - Y_{ph}\ |\alpha\beta\rangle \,]$$

The QRPA equations

$$\begin{pmatrix} A_{\alpha\beta,\gamma\delta} & B_{\alpha\beta,\gamma\delta} \\ -B^*_{\alpha\beta,\gamma\delta} & -A^*_{\alpha\beta,\gamma\delta} \end{pmatrix} \begin{pmatrix} X^\nu_{\gamma\delta} \\ Y^\nu_{\gamma\delta} \end{pmatrix} = E_\nu \begin{pmatrix} X^\nu_{\alpha\beta} \\ Y^\nu_{\alpha\beta} \end{pmatrix}.$$

$$\begin{aligned} A_{\alpha\beta,\gamma\delta} = & \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\delta}}} \\ & \times \left[(E_\alpha + E_\beta)\,\delta_{\alpha\gamma}\delta_{\beta\delta} + G_{\alpha\beta\gamma\delta}(u_\alpha u_\beta u_\gamma u_\delta + v_\alpha v_\beta v_\gamma v_\delta) \right. \\ & \left. + F_{\alpha\beta\gamma\delta}(u_\alpha v_\beta u_\gamma v_\delta + v_\alpha u_\beta v_\gamma u_\delta) - (-1)^{j_\gamma + j_\delta - J'} F_{\alpha\beta\delta\gamma}(u_\alpha v_\beta v_\gamma u_\delta + v_\alpha u_\beta u_\gamma v_\delta) \right], \\ B_{\alpha\beta,\gamma\delta} = & \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\delta}}} \\ & \times \left[-G_{\alpha\beta\delta\gamma}(u_\alpha u_\beta v_\gamma v_\delta + v_\alpha v_\beta u_\gamma u_\delta) - (-1)^{j_\delta + j_\gamma - J'} F_{\alpha\beta\delta\gamma}(u_\alpha v_\beta u_\gamma v_\delta + v_\alpha u_\beta v_\gamma u_\delta) \right. \\ & \left. + (-1)^{j_\alpha + j_\beta + j_\gamma + j_\delta - J - J'} F_{\alpha\beta\gamma\delta}(u_\alpha v_\beta v_\gamma u_\delta + v_\alpha u_\beta u_\gamma v_\delta) \right], \end{aligned}$$

$$G_{\alpha\beta\gamma\delta} = \sum_{m_\alpha m_\beta m_\gamma m_\delta} \langle j_\alpha m_\alpha j_\beta m_\beta | JM \rangle \langle j_\gamma m_\gamma j_\delta m_\delta | J'M' \rangle V^{pp}_{\alpha\beta,\gamma\delta},$$

$$F_{\alpha\beta\gamma\delta} = \sum_{m_\alpha m_\beta m_\gamma m_\delta} \langle j_\alpha m_\alpha j_\beta m_\beta | JM \rangle \langle j_\gamma m_\gamma j_\delta m_\delta | J'M' \rangle V^{ph}_{\alpha\bar{\delta}\bar{\beta}\gamma}.$$

$$\begin{pmatrix} A_{\alpha\beta,\gamma\delta} & B_{\alpha\beta,\gamma\delta} \\ -B^*_{\alpha\beta,\gamma\delta} & -A^*_{\alpha\beta,\gamma\delta} \end{pmatrix} \begin{pmatrix} X^\nu_{\gamma\delta} \\ Y^\nu_{\gamma\delta} \end{pmatrix} = E_\nu \begin{pmatrix} X^\nu_{\alpha\beta} \\ Y^\nu_{\alpha\beta} \end{pmatrix}.$$

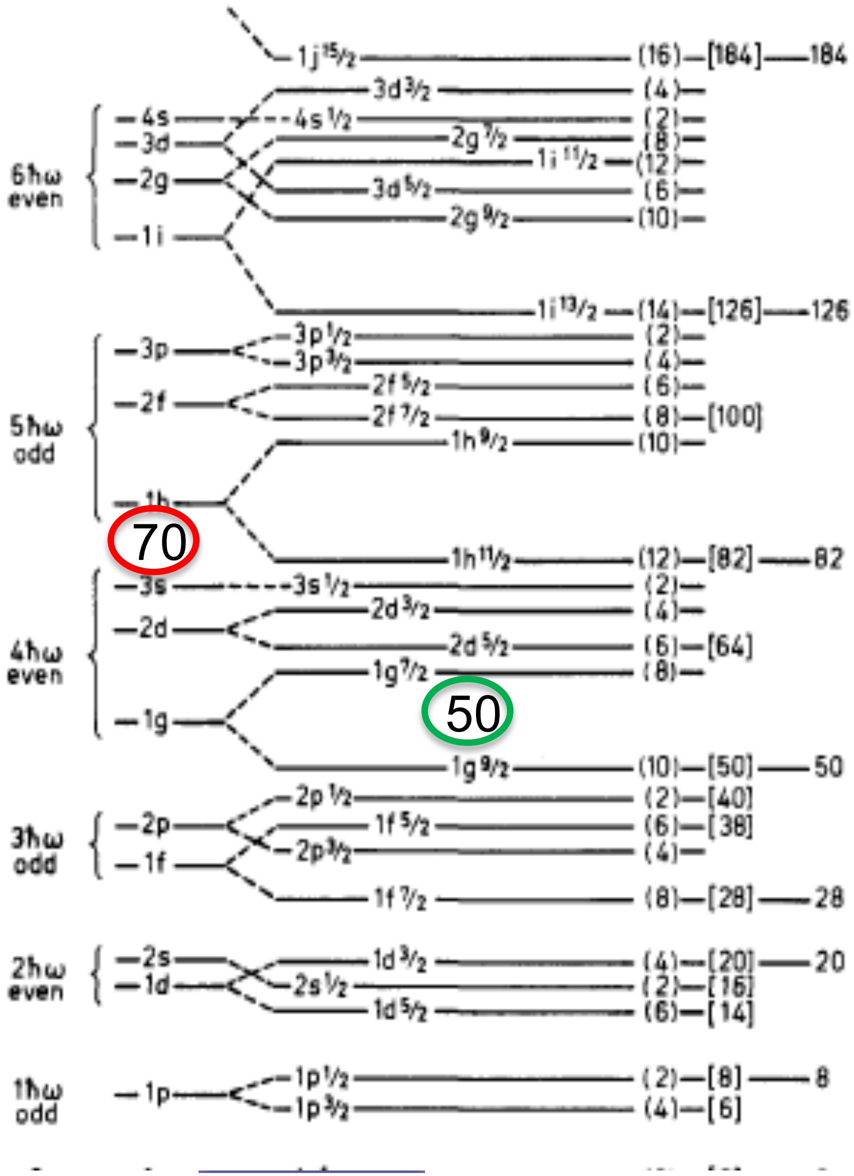
= 0, 1 without pairing

$$\begin{aligned} A_{\alpha\beta,\gamma\delta} = & \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\delta}}} \\ & \times \left[(E_\alpha + E_\beta)\,\delta_{\alpha\gamma}\delta_{\beta\delta} + G_{\alpha\beta\gamma\delta}(u_\alpha u_\beta u_\gamma u_\delta + v_\alpha v_\beta v_\gamma v_\delta) \right. \\ & \left. + F_{\alpha\beta\gamma\delta}(u_\alpha v_\beta u_\gamma v_\delta + v_\alpha u_\beta v_\gamma u_\delta) - (-1)^{j_\gamma + j_\delta - J'} F_{\alpha\beta\delta\gamma}(u_\alpha v_\beta v_\gamma u_\delta + v_\alpha u_\beta u_\gamma v_\delta) \right], \\ B_{\alpha\beta,\gamma\delta} = & \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\delta}}} \\ & \times \left[-G_{\alpha\beta\delta\gamma}(u_\alpha u_\beta v_\gamma v_\delta + v_\alpha v_\beta u_\gamma u_\delta) - (-1)^{j_\delta + j_\gamma - J'} F_{\alpha\beta\delta\gamma}(u_\alpha v_\beta u_\gamma v_\delta + v_\alpha u_\beta v_\gamma u_\delta) \right. \\ & \left. + (-1)^{j_\alpha + j_\beta + j_\gamma + j_\delta - J - J'} F_{\alpha\beta\gamma\delta}(u_\alpha v_\beta v_\gamma u_\delta + v_\alpha u_\beta u_\gamma v_\delta) \right], \end{aligned}$$

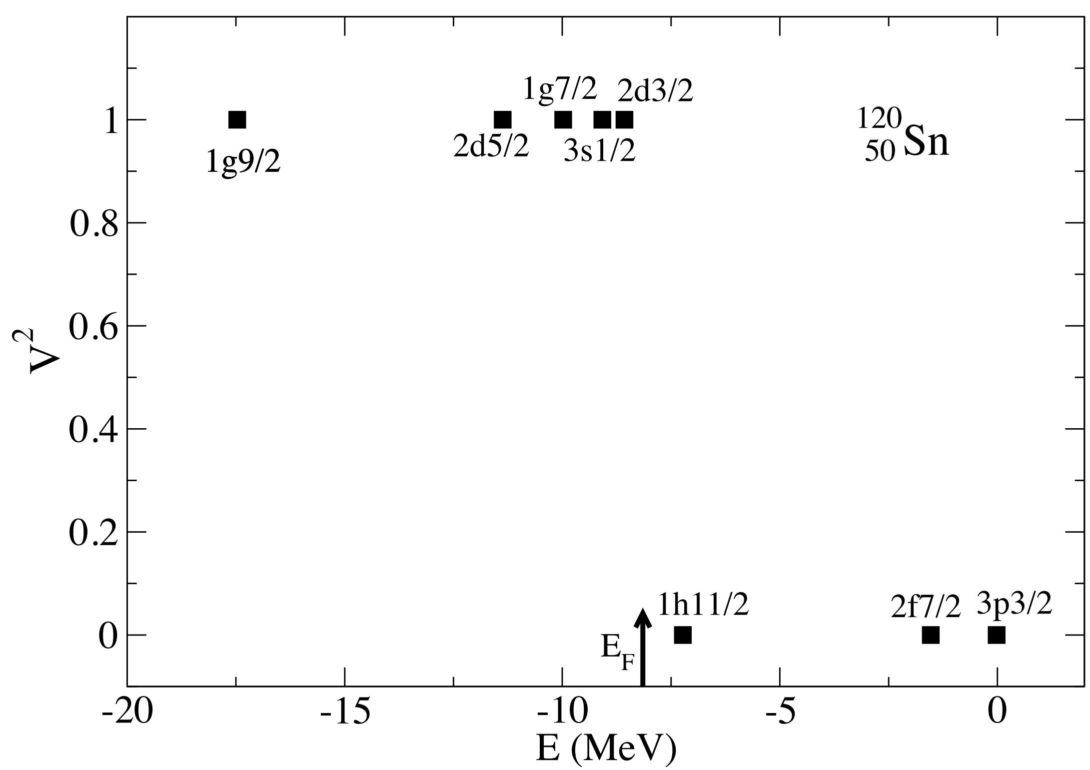
$$G_{\alpha\beta\gamma\delta} = \sum_{m_\alpha m_\beta m_\gamma m_\delta} \langle j_\alpha m_\alpha j_\beta m_\beta | JM \rangle \langle j_\gamma m_\gamma j_\delta m_\delta | J'M' \rangle V^{pp}_{\alpha\beta,\gamma\delta},$$

$$F_{\alpha\beta\gamma\delta} = \sum_{m_\alpha m_\beta m_\gamma m_\delta} \langle j_\alpha m_\alpha j_\beta m_\beta | JM \rangle \langle j_\gamma m_\gamma j_\delta m_\delta | J'M' \rangle V^{ph}_{\alpha\bar{\delta}\bar{\beta}\gamma}.$$

Back to $^{120}_{50}Sn$

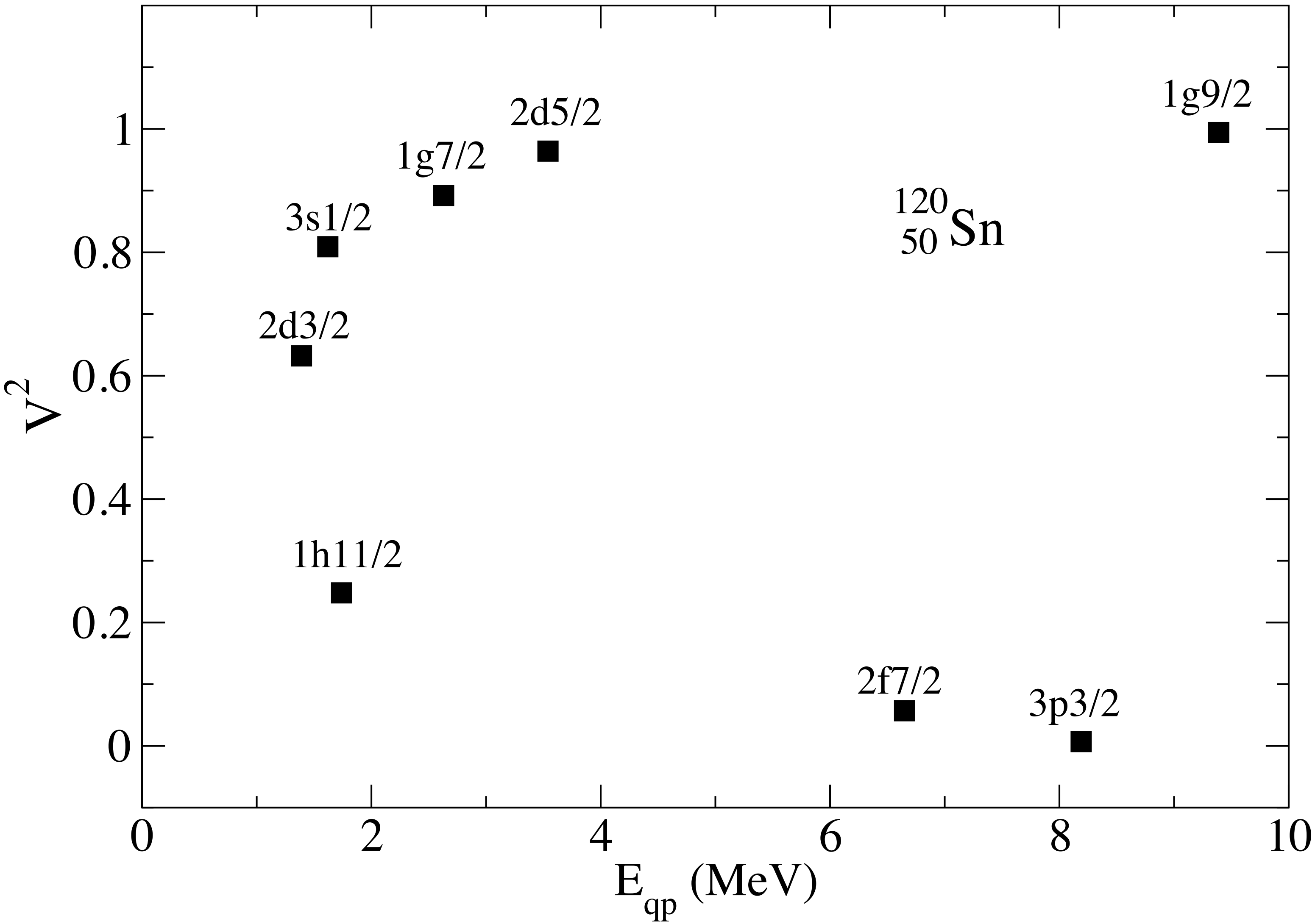


No pairing,empty 1h11/2



With pairing correlations

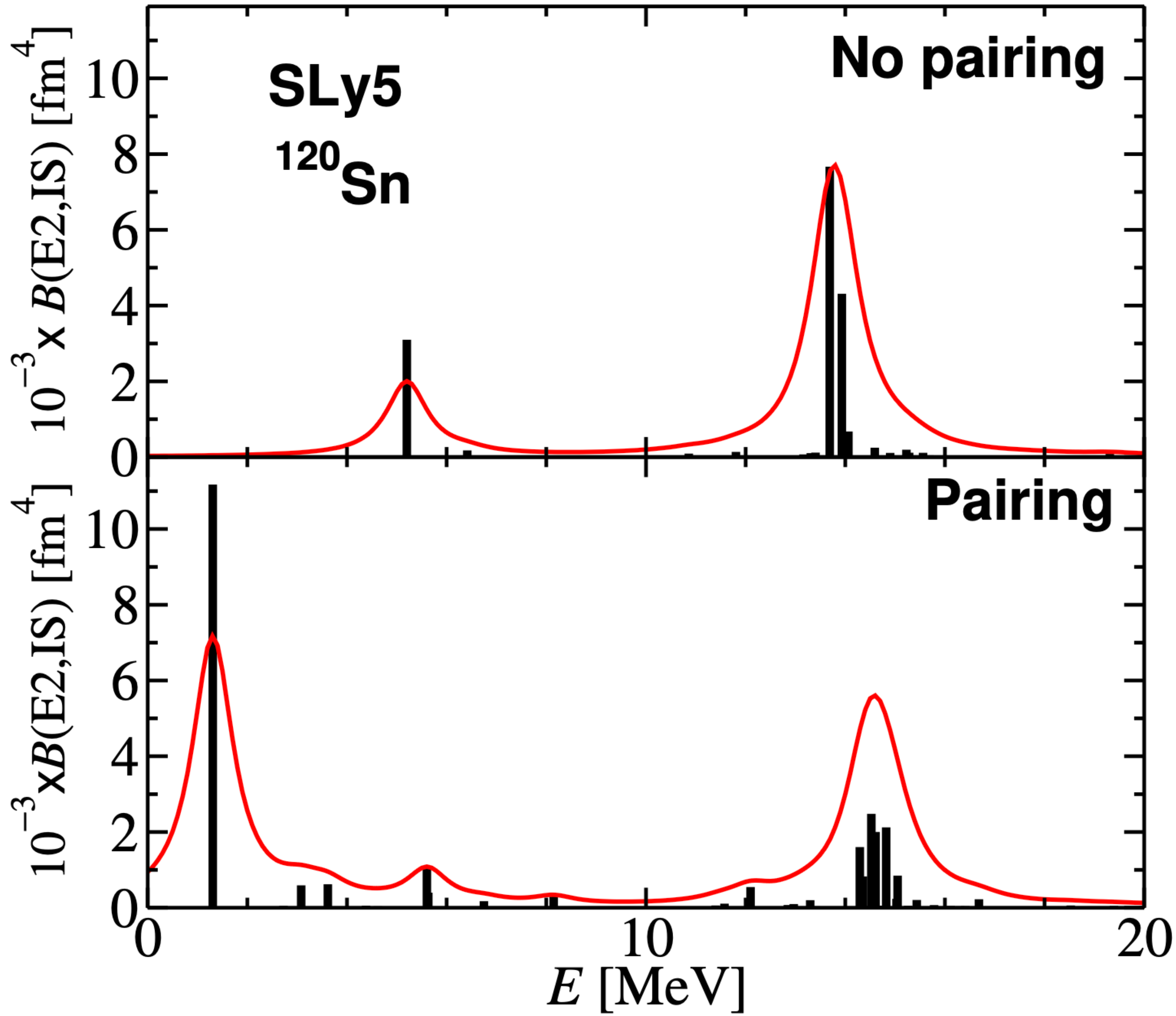
Occupation of quasiparticle levels (neutrons) $E^2_{qp} = (\boldsymbol{\varepsilon} - E_F)^2$



The pairing contribution to the total energy is small …

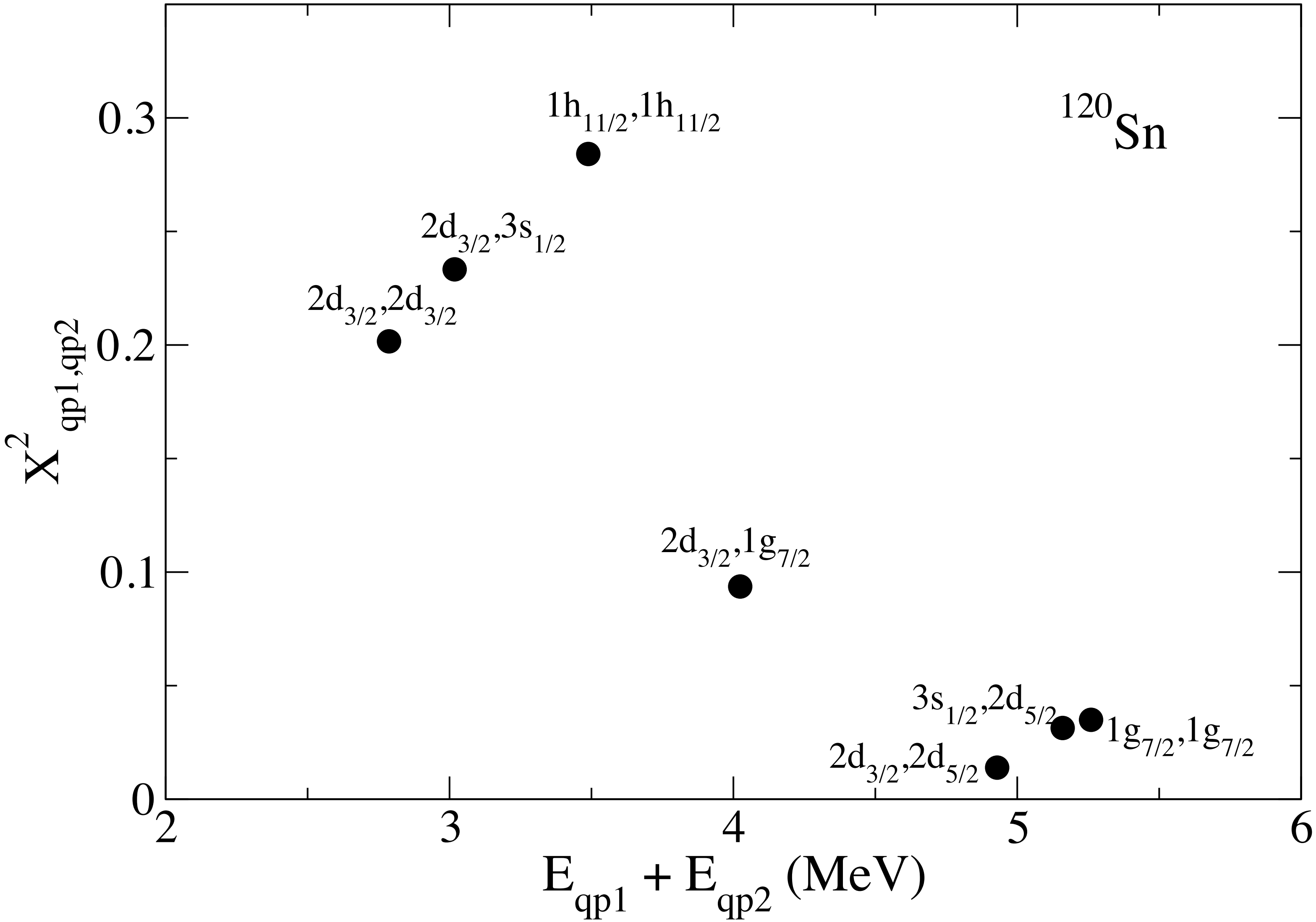
```
-INTEGRAL OF THE ENERGY DENSITY:
 E(KIN) =             0.21769E+04
 E(SKYRME) =         -0.34793E+04
  |___E(t0) =        -0.12698E+05
  |___E(t3) =         0.82849E+04
  |___E(t1,t2) =      0.93408E+03
 E(SO) =             -0.54885E+02
 E(CD) =              0.36706E+03
 E(CE) =             -0.19131E+02
 E(pair) =           -0.99067E+01
 E(TOT) =            -0.10193E+04
```

... but the change in 2+ excitations is substantial



024

2qp neutron admixtures in low-lying 2+ state

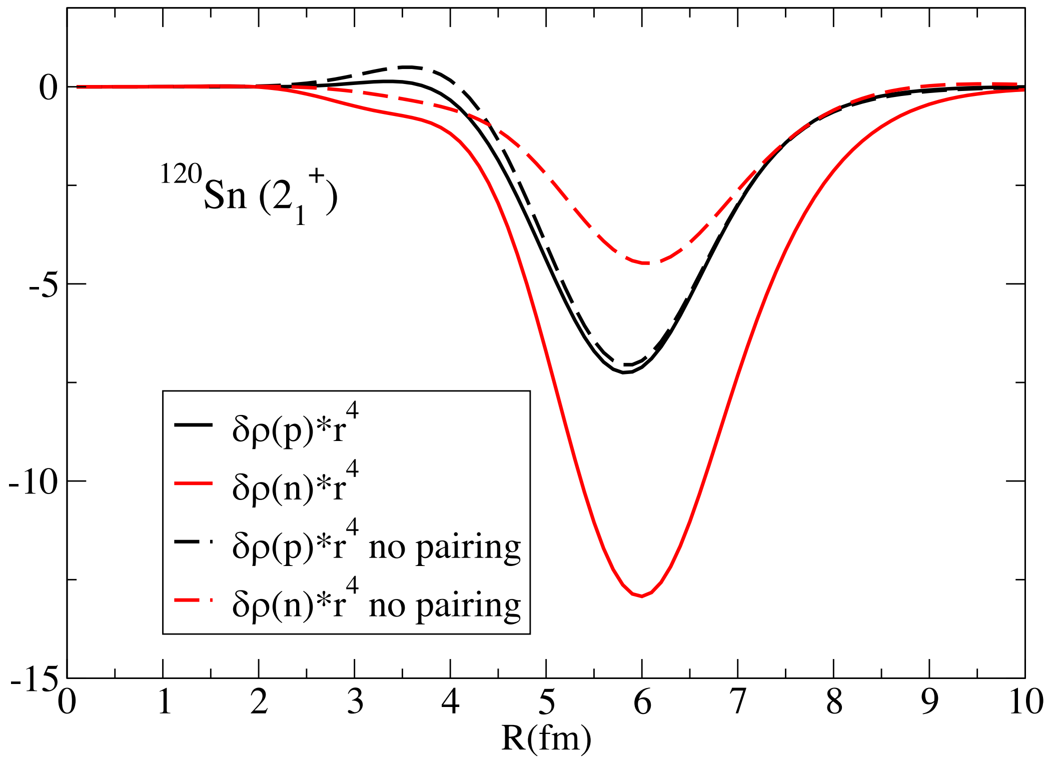


Transition densities and strengths

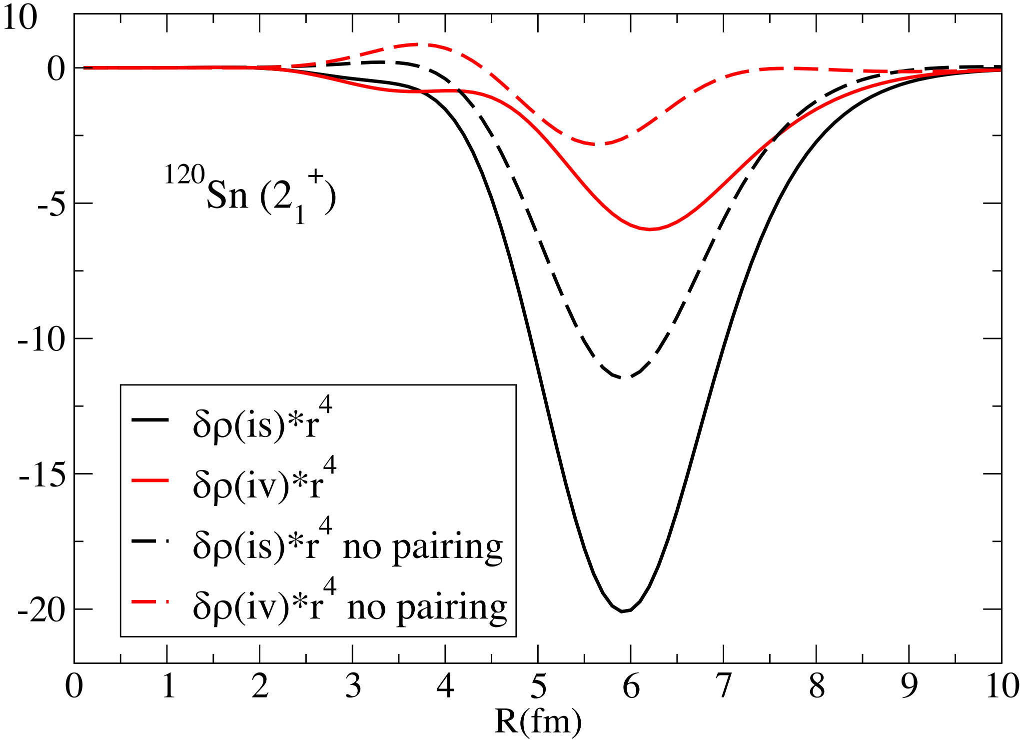
$$S(E) = \sum_k | < k|F|0 > |^2 \delta(E - E_k)$$

$$B(L,k) = | < k| \sum_i r_i^L Y_{LM}(\hat{r}_i)|0 > |^2 = | \frac{\sqrt{2J_f + 1}}{\sqrt{2J_i + 1}} \int dr \quad \delta\rho_k^L(r)\, r^{L+2}|^2$$

$$\delta\rho_k^L(r) = \sum_{\alpha\beta} [X_{\alpha\beta}^k + Y_{\alpha\beta}^k][u_\alpha v_\beta + v_\alpha u_\beta] \frac{< j_\alpha||Y_L||j_\beta >}{\sqrt{2L+1}} R_\alpha(r) R_\beta(r)$$



^{120}Sn (2_1^+)
δρ(p)*r^4
δρ(n)*r^4
δρ(p)*r^4 no pairing
δρ(n)*r^4 no pairing
0
-5
-10
-15
0 1 2 3 4 5 6 7 8 9 10
R(fm)



^{120}Sn (2_1^+)
δρ(is)*r^4
δρ(iv)*r^4
δρ(is)*r^4 no pairing
δρ(iv)*r^4 no pairing
0
-5
-10
-15
-20
0 1 2 3 4 5 6 7 8 9 10
R(fm)

Some issues / limitations

Ome must be careful about the presence of low-lying strength caused by spurious states associated with symmetry breaking
(1- -> translational invariance)
(0+ -> number conservation in BCS calculations)

BCS pairs are built only out of states in time reversal.
A more general ansatz (HFB), coupling states with different number of nodes, is better to treat weakly bound nuclei and their coupling with the continuum. There are a number of available HFB codes, like HFODD, HFBTHO, HFBRAD.

Depending on the specific properties one is looking for, there may be an important dependence of the results on the chosen functional

	E (MeV)				$B(EL, 0 \to L)$ (e^2 fm^{2L})			
Phonons	Expt.	SAMi	SGII	SkM*	Expt.	SAMi	SGII	SkM*
2^+	1.171	2.708	1.941	1.420	2.016×10^3	1.463×10^3	1.766×10^3	2.632×10^3
3^-		3.595	3.313	3.297		1.880×10^5	1.396×10^5	1.089×10^5
4^+		4.029	3.757	3.230		2.496×10^6	1.568×10^6	1.453×10^6
5^-		4.603	3.669	3.536		4.454×10^7	2.555×10^7	3.103×10^7