Two quasiparticle k-isomers within the covariant density functional theory

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Main goal
Study of the single particle excitations - extension of the relativistic mean field theory
Evaluation of the method - comparison with experimental data

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Isomer nuclei
Preliminaries

"Isomers"-"Isomerism": chemical term- states with diff. properties from same constituents.

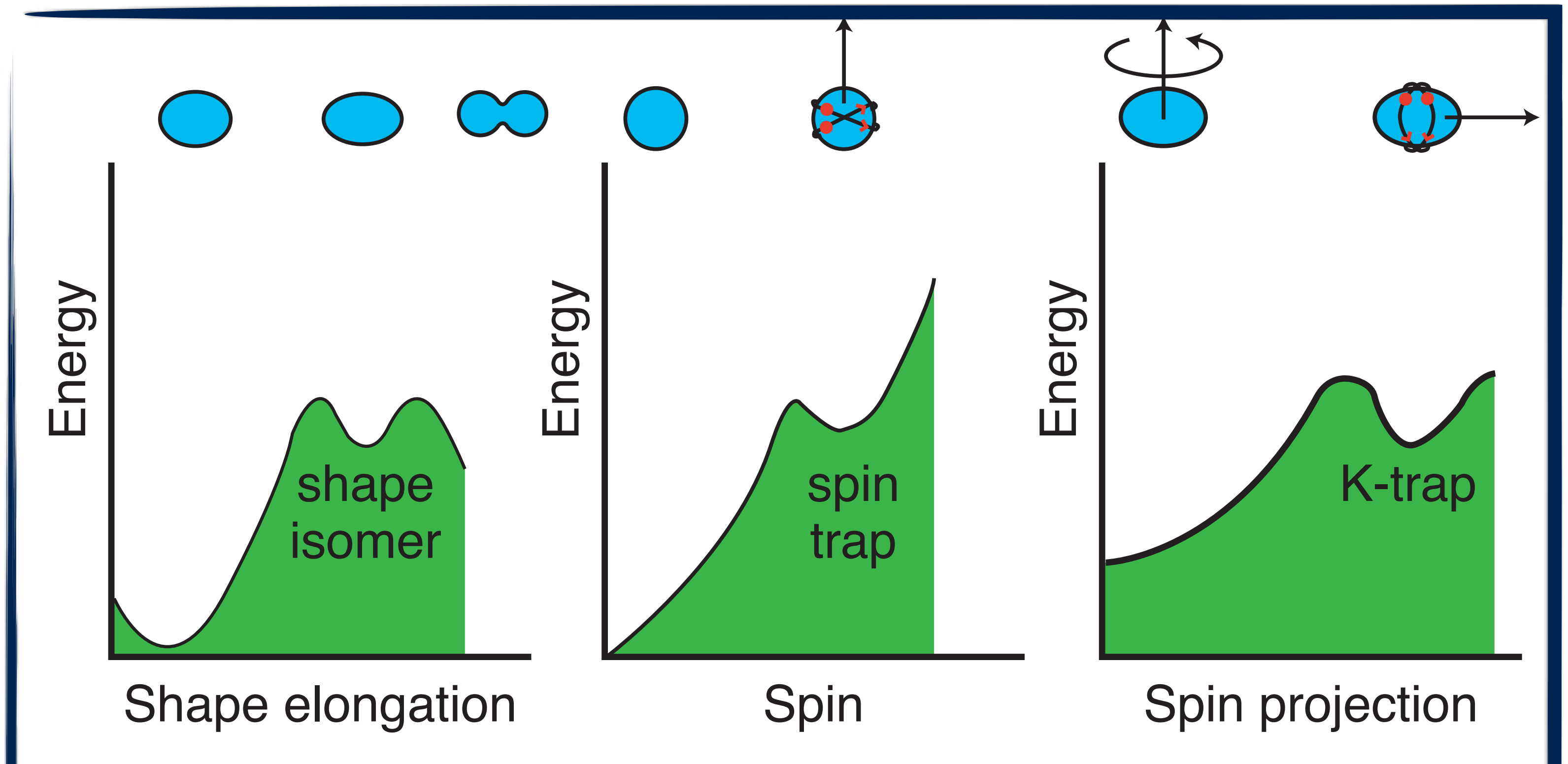
Nuclear physics:

- Metastable-excited states with measurable life-time
- Small overlap bt. initial and final state
- reduced transition

$$\tau \propto |\langle f \mid T_\lambda \mid i \rangle|^2 / (\Delta E)^{2\lambda+1}$$

T_λ :Transition operator from *f* to *i*

λ :multipolarity of the transition -> change in quantum numbers



Philip Walker & George Dracoulis NATURE | VOL 399 | 6 MAY 1999 | www.nature.com

Specific nuclear structure phenomena can lead to an increased lifetime of an excited state

Shape isomers

Second minimum in energy surface for larger deformation

Example: 242Am, lifetime 14ms, energy 2.2MeV, large to small axis ratio 2:1.

Spin trap-isomers

De-excitation requires large spin change -> electromagnetic transition of large λ very small probability

Appearance in nuclei near shell closure, spherical shape

Example: 180mTa, "natural" isomer, lifetime 10^{15} years, energy 75keV, spin $9\hbar$ $\lambda = 8$

Isomer nuclei
Preliminaries

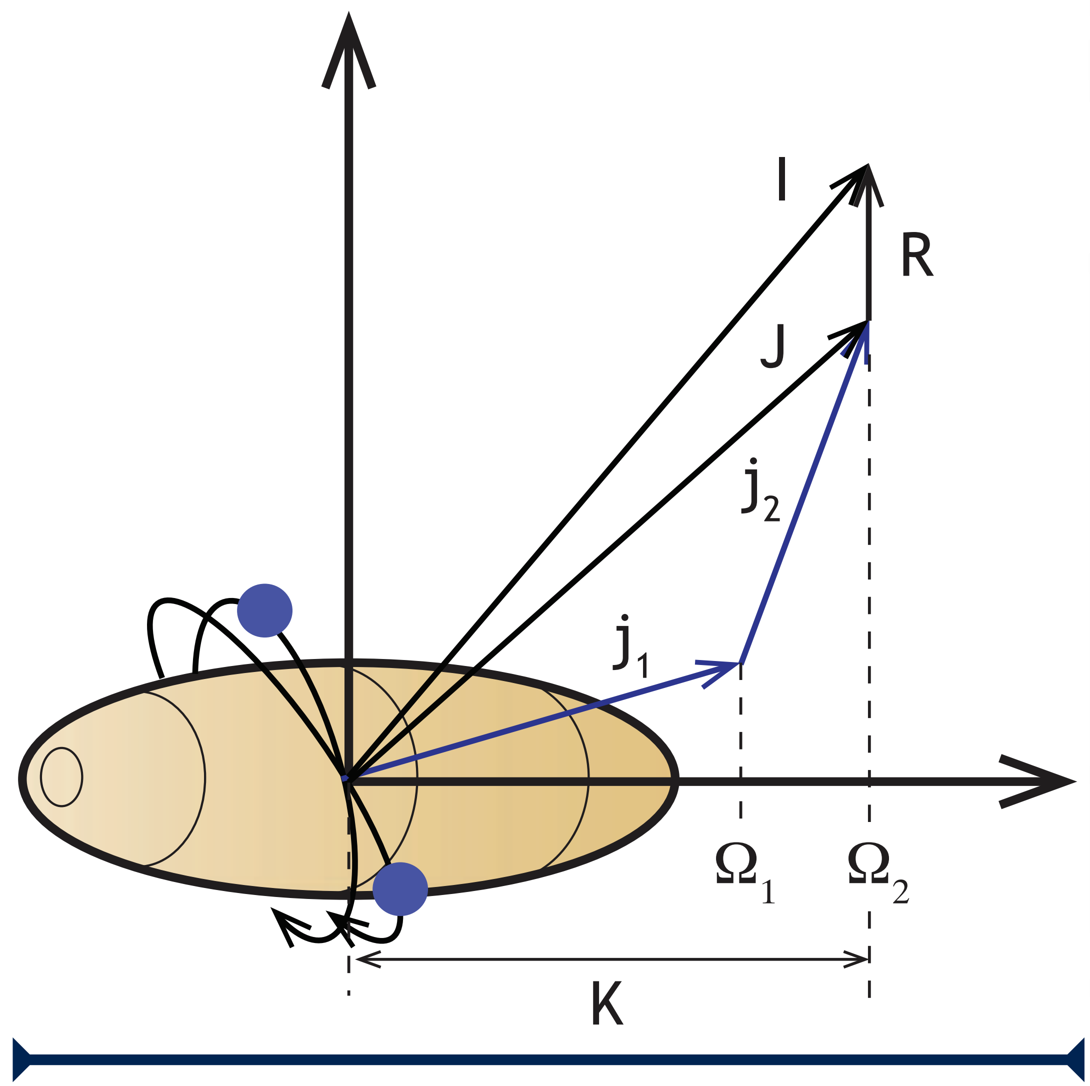


Illustration of a 2 particle coupling into a high-*K* in a axially deformed nuclei.

G D Dracoulis *et. al.*, Rep. Prog. Phys. **79** (2016) 07631

***K*-isomers**

- Heavy nuclei near the middle of nuclear shells
- Axially deformed shape - Prolate type
- *qu. number* K: projection of the total angular momentum onto the symmetry axis
- Single particle states with high-Ω near the Fermi surface

$$J^\pi = K^\pi = \sum_i \Omega_i^{\Pi(\pi_i)}$$

Excitation energy ~ breaking of a nucleon pair

$$E^* \approx \sum_k \sqrt{(\epsilon_k - \epsilon_{\mathrm{F}})^2 + \Delta^2}$$

Selection rule of an electromagnetic transition

$$\lambda \geqslant \Delta K \qquad \text{(Not strict)}$$

Example:
180mHf $I = 8$, $K = 8$, E*=1.1MeV
ground state: $I = 0$, $K = 0$
Most probable transition -> $I = 8$, $K = 0$ with $\lambda = 1$, 55keV

Covariant DFT
Relativistic mean field - RHB in brief

- Map the nuclear many body to a s.p. problem — nucleons treated as Dirac spinors in a mean field
- EDF is defined by an effective Lagrangian describing the interaction bt nucleon DDME2, DDPC1

The ground state is constructed as a slater determinant $|\Phi\rangle = \prod_i^A c_i^\dagger |0\rangle$

The single particle density is $\hat{\rho}_{kk'} = \langle\Phi|c_{k'}^\dagger c_k|\Phi\rangle$ and the EDF $E_{RMF}(\hat{\rho},\phi) = \langle\Phi|\mathcal{H}|\Phi\rangle$

__Introduce pairing correlation in the generalised framework of Hartree-Bogolyubov__

Basic concept: quaiparticles from the transformation $\alpha_k^+ = \sum_n U_{nk} c_n^+ + V_{nk} c_n$

Nuclear ground state now defines the quasiparticle vacuum

$$\alpha_k|\Phi_0\rangle = 0 \quad \text{for} \quad E_k > 0 \quad \text{or} \quad |\Phi_0\rangle = \prod_{E_k>0} \alpha_k|-\rangle$$

Along with the single particle density — pairing tensor

$$\hat{\rho}_{nn'} = \langle\Phi|c_{n'}^\dagger c_n|\Phi\rangle \Big/ \hat{\kappa}_{nn'} = \langle\Phi|c_{n'} c_n|\Phi\rangle \longrightarrow E_{\text{RHB}}[\hat{\rho},\hat{\kappa}] = E_{\text{RMF}}[\hat{\rho}] + E_{\text{pair}}[\hat{\kappa}]$$

$$E_{\text{pair}}[\hat{\kappa}] = \frac{1}{4}\sum_{n_1 n_1'}\sum_{n_2 n_2'} \hat{\kappa}^*_{n_1 n_1'} \langle n_1 n_1'|V^{pp}|n_2 n_2'\rangle \hat{\kappa}_{n_2 n_2'}$$

Defined by the pairing interaction Vpp
1. Constant Gap approximation - cutoff
2. TMR ~ Gogny like finite range

Solution of the RHB equations — U,V Bogoliubov wave functions, qp energies —> canonical s.p.

$$\begin{pmatrix} \hat{h}_D - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D^* + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

Mean Field $\quad \hat{h}_D = \dfrac{\delta E}{\delta\hat{\rho}},$

Pairing Field $\quad \hat{\Delta} = \dfrac{\delta E}{\delta\hat{\kappa}}$

K-Isomers
Common building blocks

Neutrons	Protons
$Z \sim 70 - 74$ $N \sim 100 - 108$	
$6^- : 5/2^-[512], 7/2^+[633]$	
$6^+ : 5/2^-[512], 7/2^-[514]$	$6^+ : 5/2^+[402], 7/2^+[404]$
$8^- : 9/2^+[624], 7/2^-[514]$	$8^- : 9/2^-[514], 7/2^+[404]$
$Z \sim 76$ $N \sim 110 - 116$	
$10^- : 9/2^-[505], 11/2^+[615]$	
$10^+ : 9/2^+[624], 11/2^+[615]$	$10^+ : 9/2^-[514], 11/2^-[505]$
$12^+ : 11/2^+[615], 13/2^+[606]$	
$Z \sim 102 - 108$ $N \sim 150 - 164$	
$8^- : 7/2^+[624], 9/2^-[734]$	$8^- : 7/2^-[514], 9/2^+[624]$
$8^- : 7/2^+[613], 9/2^-[734]$	
$10^- : 9/2^+[615], 11/2^-[725]$	$10^- : 9/2^-[505], 11/2^+[615]$

2 quasiparticle K-isomers and the most common orbital configurations with high-Ω

Axially deformed nuclei

Good quantum numbers:
Total ang. momentum projection - Parity

Nilsson model/ Anisotr. HO+*ls*+*l*^2
Nilsson labels

$$\Omega\pi[Nn_z m_l]$$

$$\Omega = m_l + m_s = m_l \pm \frac{1}{2} \qquad \pi = (-1)^N$$

$$N = n_z + 2n_\rho + m_l = n_x + n_y + n_z$$

$[Nn_z m_l]$ Approximate quan. numbers valid for large deformations

K-isomers
Construction of Nilsson diagrams

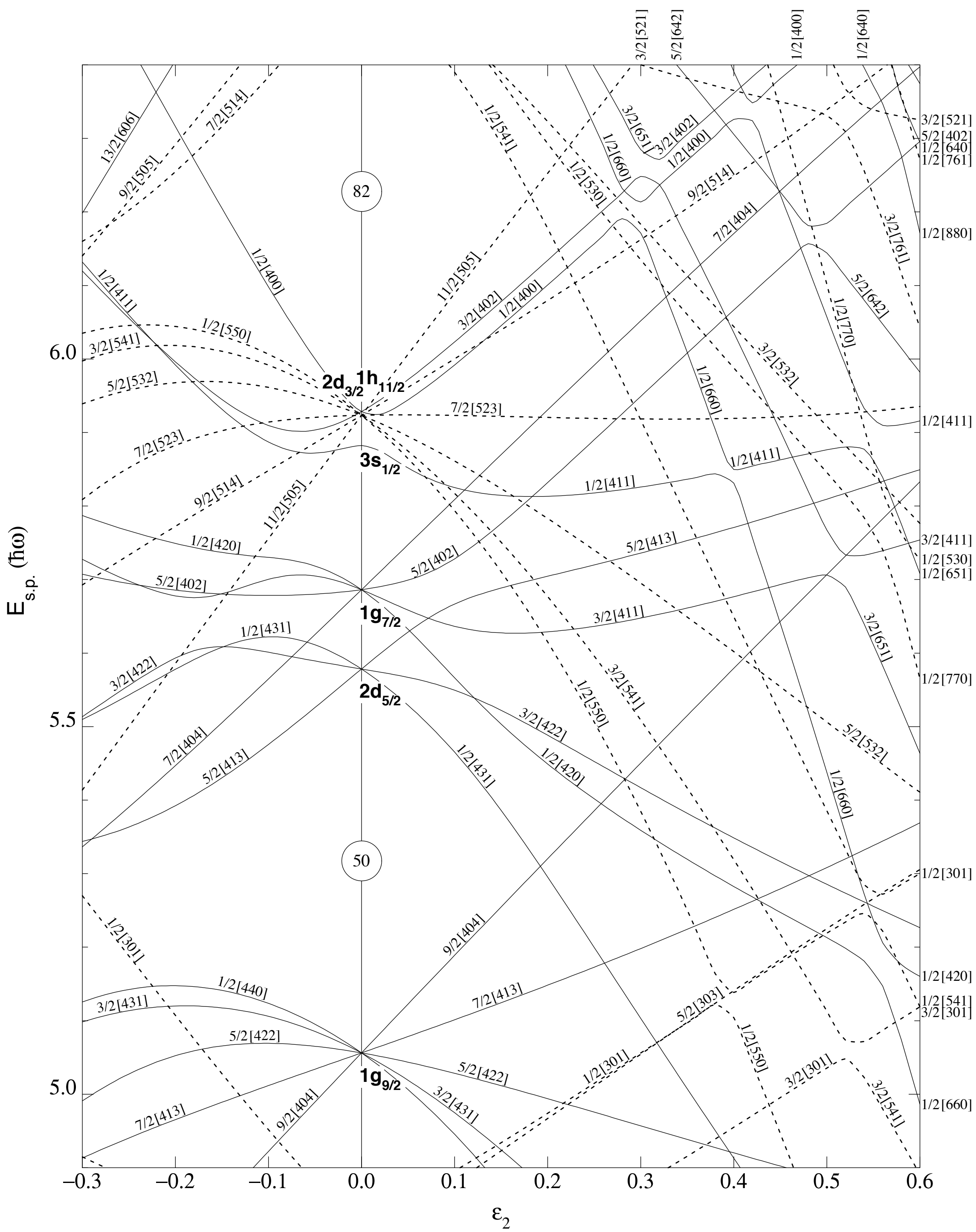


Figure 7. Nilsson diagram for neutrons, 82 ≤ N ≤ 126

Change of the single particle states with respect to quadrupole deformation β2

- Spherical shells defined by *j* , break into (2*j*+1)/2 states.
- For β2>0 -prolate shapes, orbits with low *Ω* shift downwards
- Orbits from diff. shells but with same *Ωπ* repel.

<u>In the RHB framework</u>

We solve the equations with the additional constraint of minimising the function with respect to $q_{2\mu}$

$$\langle \hat{H} \rangle + \sum_{\mu=0,2} C_{2\mu}(\langle \hat{Q}_{2\mu} - q_{2\mu})^2$$

$\hat{Q}_{2\mu}$:Expectation value of the quadrupole moment

$q_{2\mu}$:Wanted value

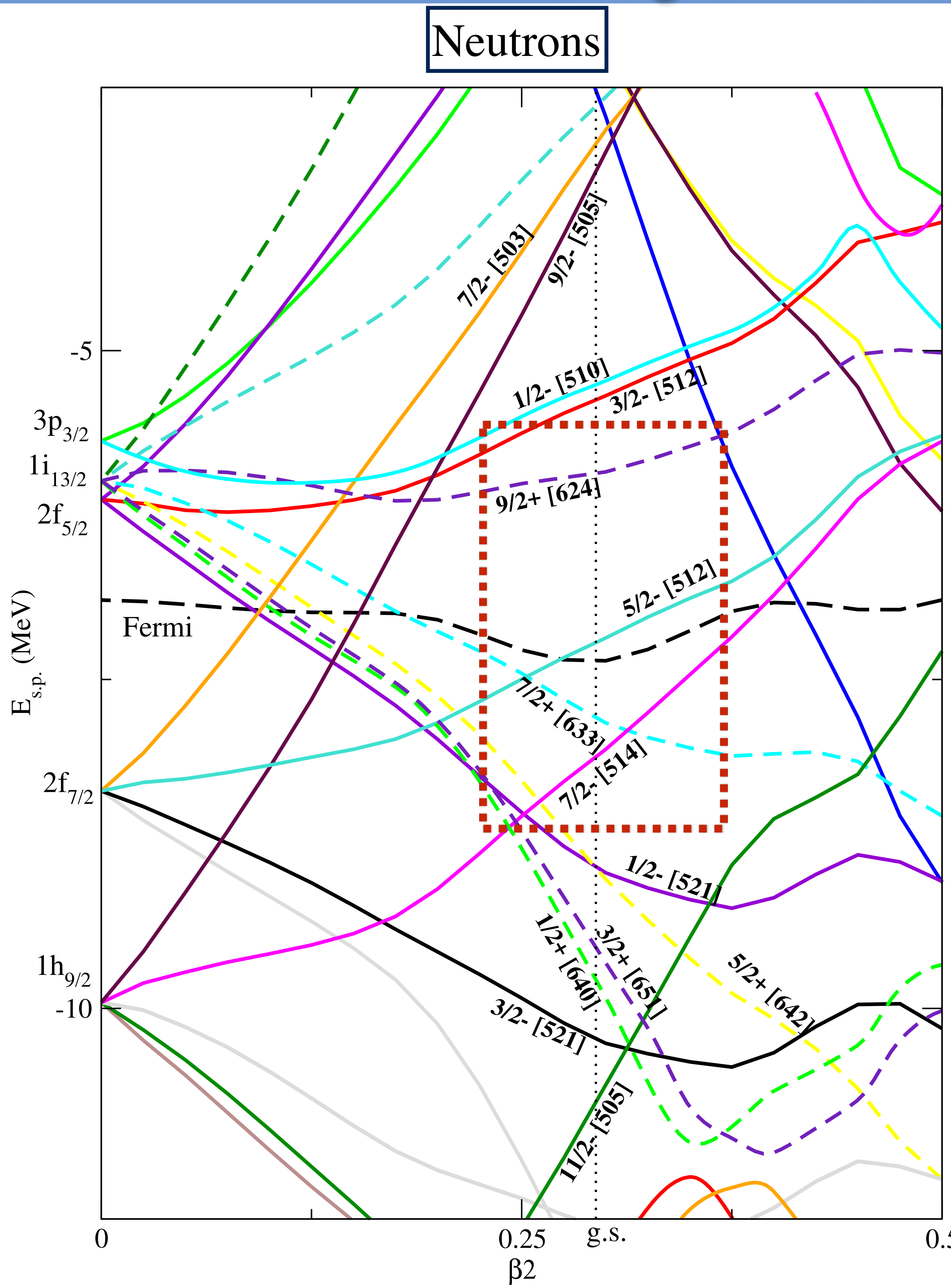
Use the relation $Q_{20} = \sqrt{\frac{9}{5\pi}} A R_0^2 \beta_2$

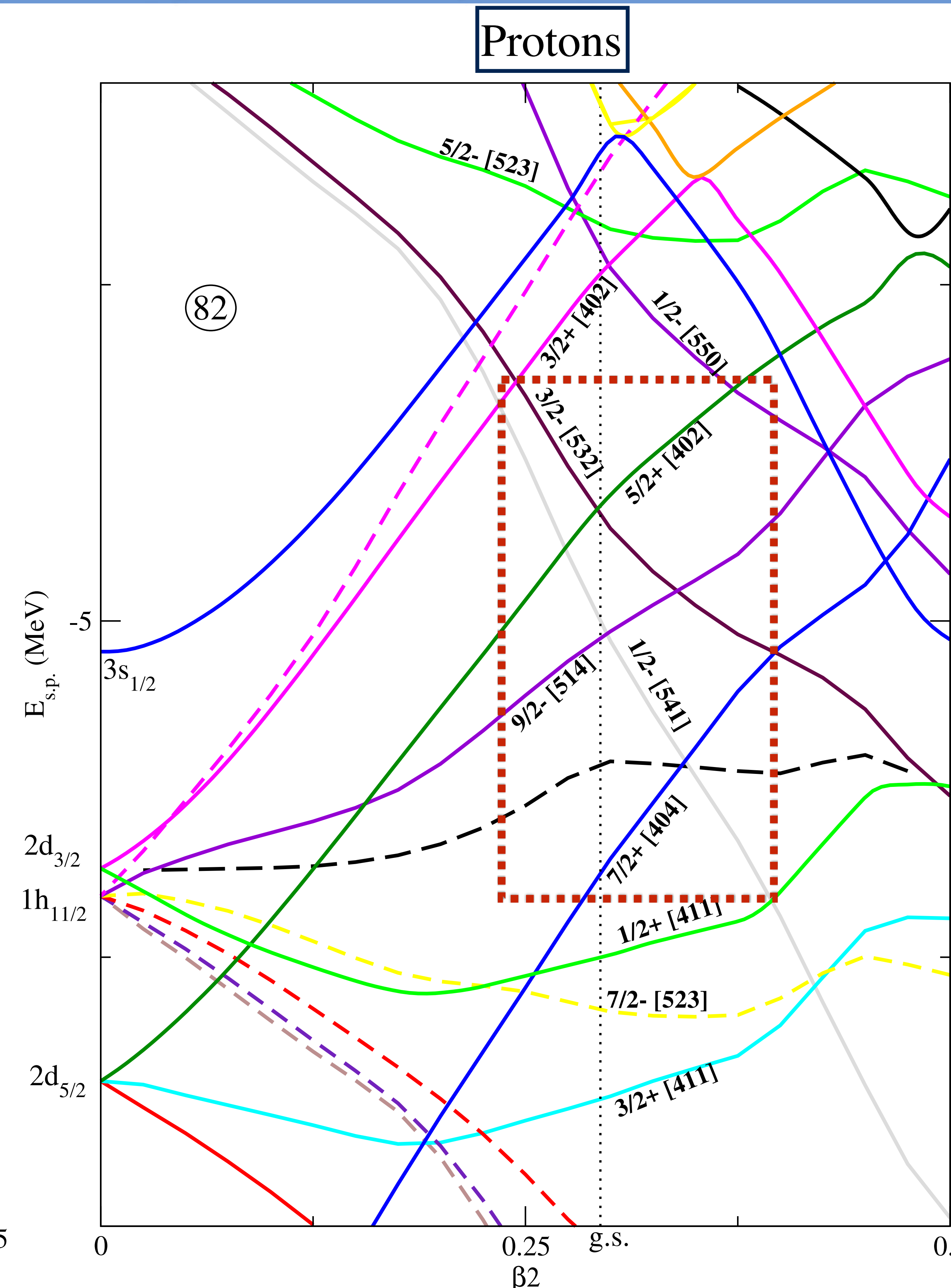
(coming from Liquid drop model)

For the evaluation of the deformation parameter $\beta 2$

K-isomers

Nilsson Diagram for Z = 72, N = 104, 176Hf





K-isomers within RHB
Theoretical construction

From the ground state - quasiparticle vacuum

$$\alpha_k|\Phi_0\rangle = 0 \quad \text{for} \quad E_k > 0 \quad \text{or} \quad |\Phi_0\rangle = \prod_{E_k>0} \alpha_k|-\rangle$$

Create 2-qp. states

$$|\Phi_2\rangle = \alpha_1^\dagger \alpha_2^\dagger |\Phi_0\rangle$$

The set $(\alpha'_1, \alpha'_2, \ldots, \alpha'_N)$ defines a new vacuum

$$\alpha'_1 = \alpha_1^\dagger,\ \alpha'_2 = \alpha_2^\dagger,\ \ldots,\ \alpha'_N = \alpha_N$$

Essentially a new quasiparticle basis with the exchange of the operators $\alpha_1^\dagger \leftrightarrow \alpha_1,\ \alpha_2^\dagger \leftrightarrow \alpha_2$

or the columns $(U_{l1}, V_{l1}) \leftrightarrow (V_{l1}^*, U_{l1}^*)$ and $U_{l2}, V_{l2}) \leftrightarrow (V_{l2}^*, U_{l2}^*)$

Typically blocking of these orbits breaks time reversal symmetry
Formally we would also have to solve RHB eqs. for the -*K* subspace
and have to deal with the creation of currents.

Instead we use the Equal Filling Approximation (EFA)
which conserves time reversal symmetry
Replace the old densities with the following (k_b denotes the blocked state)

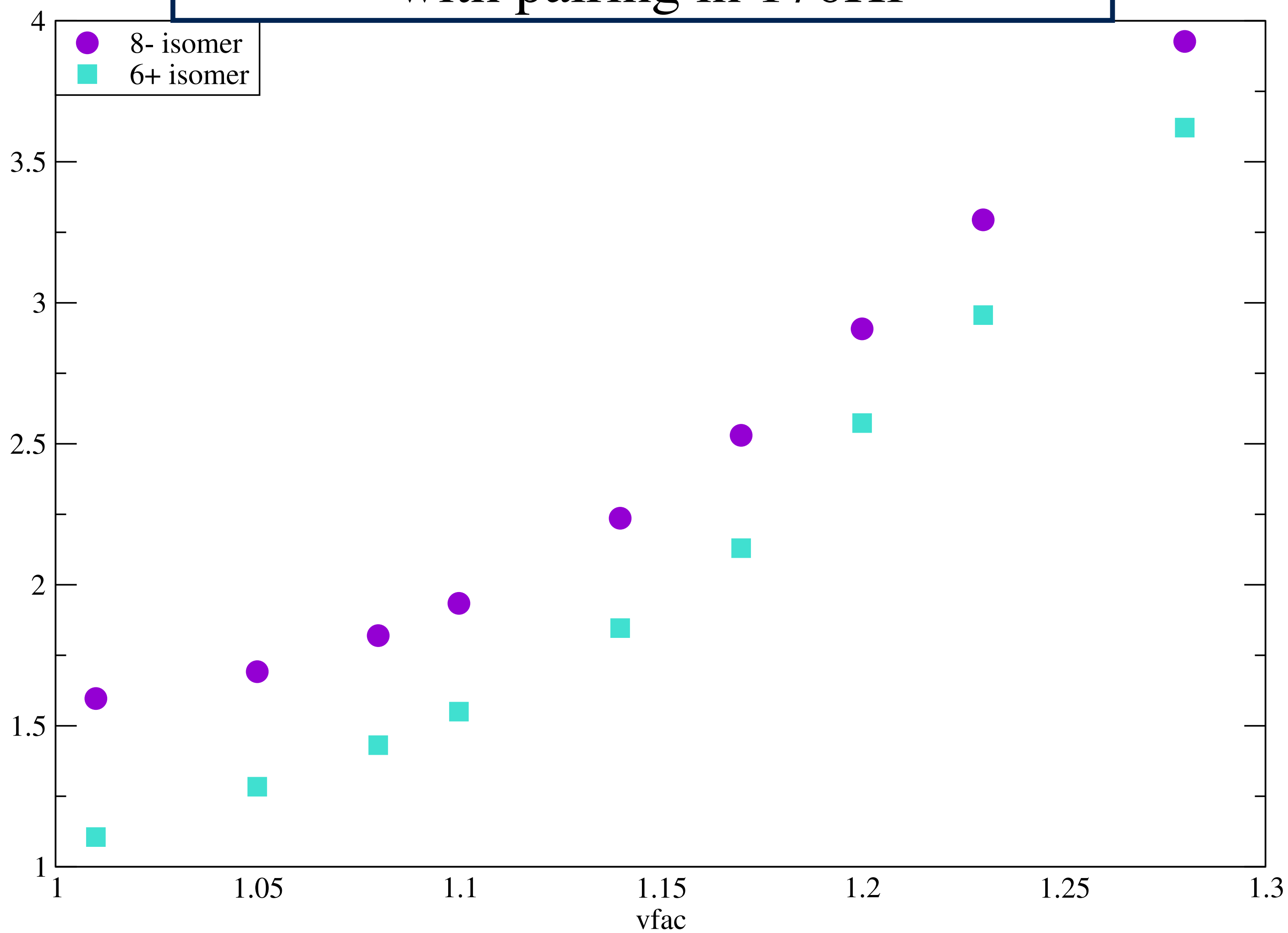
$$\begin{aligned} \rho' &= \rho_{M\times M} + \frac{1}{2}(U_{k_b}U_{k_b}^{*T} - V_{k_b}^* V_{k_b}^T) \\ \kappa' &= \kappa_{M\times M} - \frac{1}{2}(U_{k_b}V_{k_b}^{*T} + V_{k_b}^* U_{k_b}^T) \end{aligned}$$

S. Perez-Martin and L. M. Robledo, Phys. Rev. C **78**, 014304 (2008).

K-isomers within RHB

176Hf test example - change with pairing

Energy of the 8- and 6+ isomer change with pairing in 176Hf



Energy of the isomers increases wt pairing
Expected since more energy required to break the pair

1. First we solve the RHB eqs. for the g.s.
2. Then we block the quasiparticle states that lead to the creation of the isomer we want to examine
3. We calculate the excitation energy from the difference bt the two calculated energies

In the application of the method we used the functionals DD-ME2 and DD-PC1

For pairing correlations we used the TMR force:

- Two body force similar to Gogny
- Finite range - no need for cutoff parameter
- Separable in momentum space
- Vfac enhancement parameter

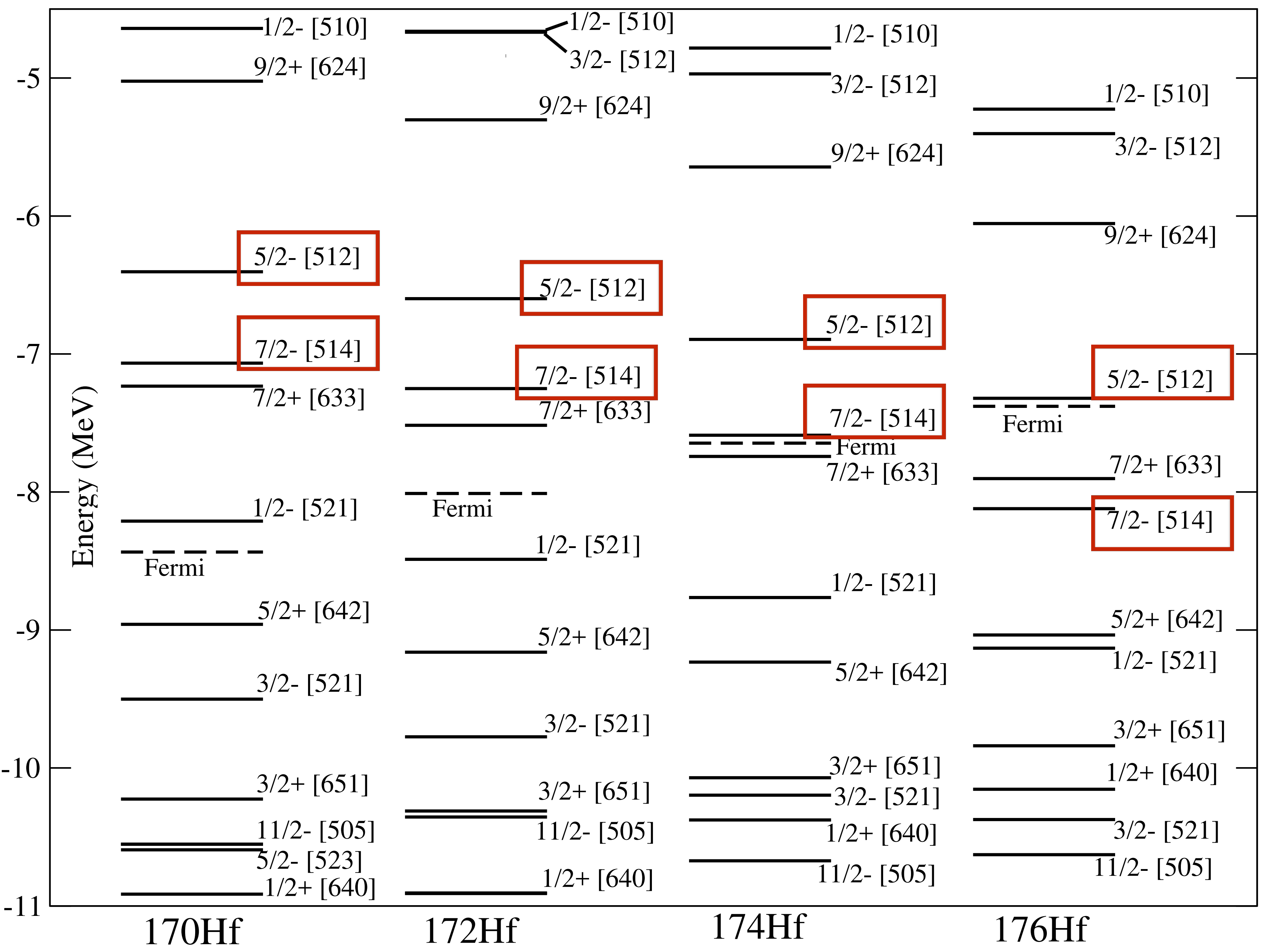
Adjust pairing strength in the g.s. of 176Hf nucleus via the the 3pt OES gap formula

$$\Delta^{(3)}(N) = \frac{1}{2}[B(N-1,Z) + B(N+1,Z) - 2B(N,Z)]$$

K-isomers

6+ isomer in Z=72 isotopes of Hf

Neutron single particle spectrum for 170-176Hf



6+ isomer 170-176Hf:

coming from 2qp configuration

$$\nu 5/2^{-}[512]\ \nu 7/2^{-}[514]$$

With the increase in N:

Neutron orbits shifted downwards

Fermi surface moves up

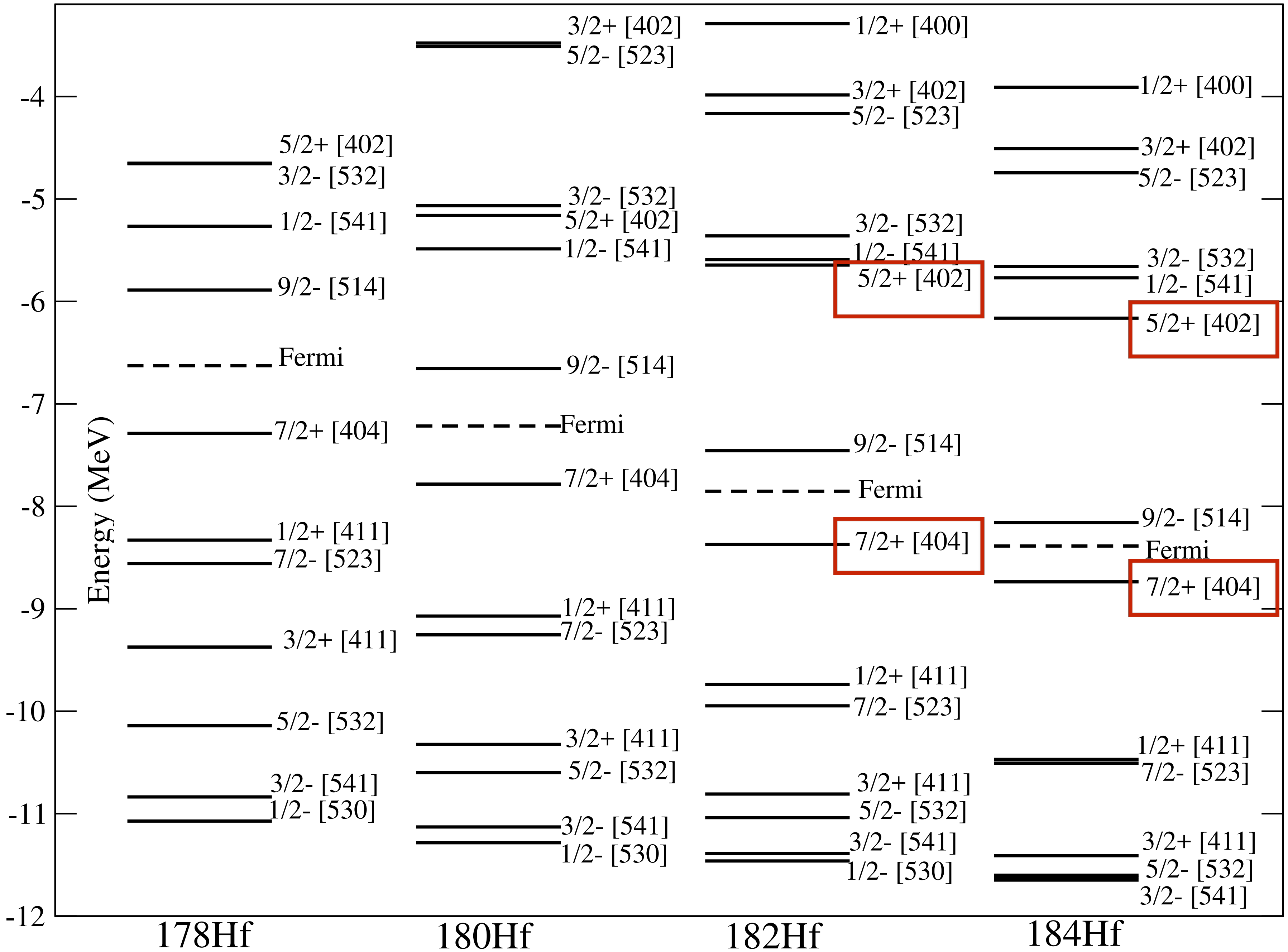
in 174Hf and 176Hf

States of interest closer to Fermi -> lower qp energy

K-Isomers

6+ isomer in Z=72 isotopes of Hf

Proton single particle spectrum for 178-184Hf



<u>6+ isomer in 182-184Hf:</u>

arising from 2qp configuration

$\pi 5/2^{+}[402]\ \pi 7/2^{+}[404]$

<u>With the increase in N</u>

P orbitals shifted downwards

Relative position of Fermi stable

<u>In 182Hf and 184Hf</u>

Relative position of the

$\pi 5/2^{+}[402]\ \pi 7/2^{+}[404]$

stays the same

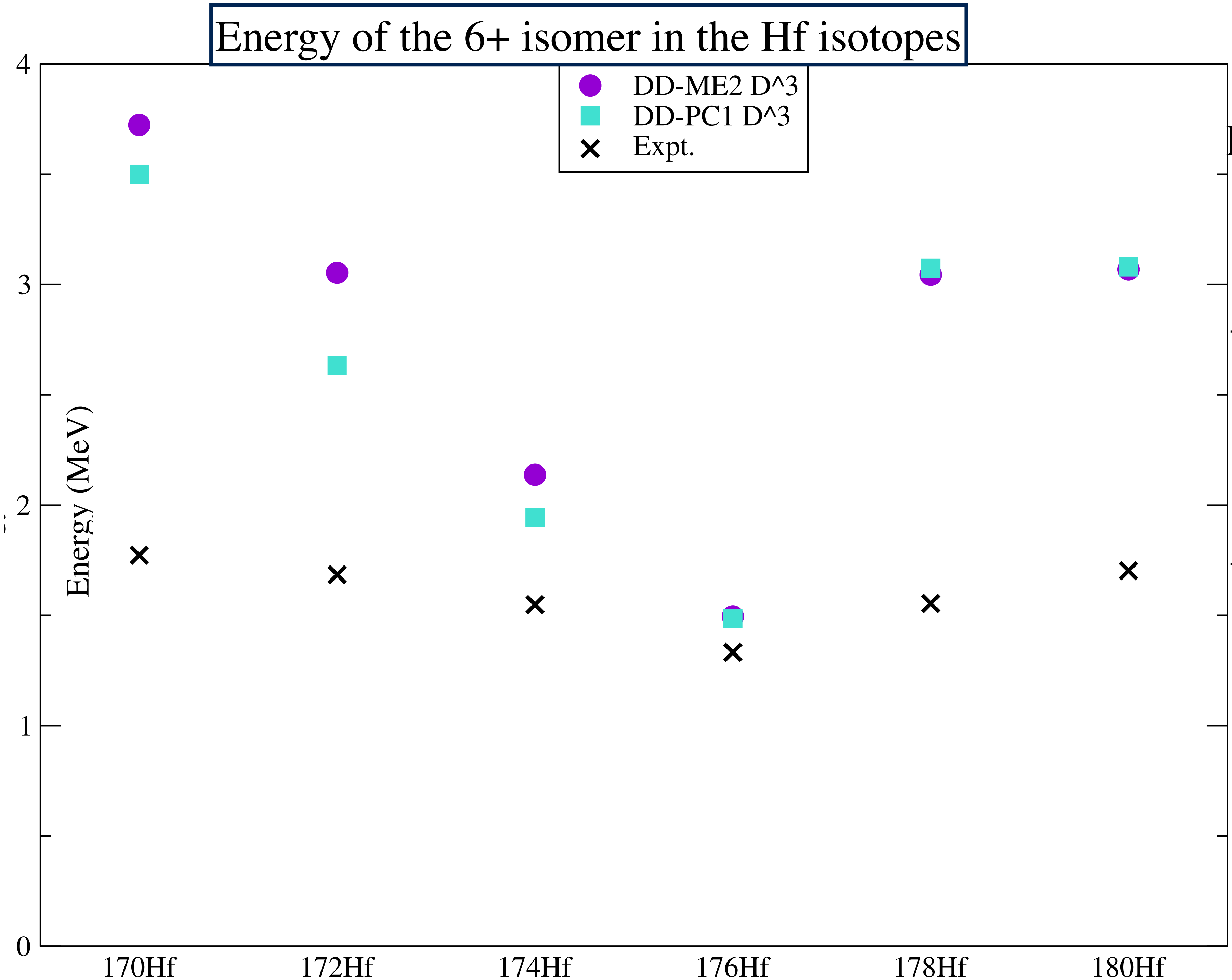
$\pi 7/2^{+}[404]$

Is the state with the

lowest qp energy

K-Isomers

6+ isomer in Z=72 isotopes of Hf



Expt. values | G. D. Dracoulis *et. al.* , Rep. Prog. Phys. **79** (2016) 07631
F. G. Kondev *et.al.* , At. Data & Nucl. Tables, April (2015)

<u>In general</u>

Fluctuation of the isomer energy
Result of the relative pos. of Fermi
Lowest value 176Hf ~ 1.3MeV
Greater change for theory

<u>Theoretical prediction 170-176Hf:</u>

Difference wt expt. starts ~ 2MeV
Gradually decreases
176Hf very close to expt. value

<u>Theoretical prediction 178-180Hf:</u>

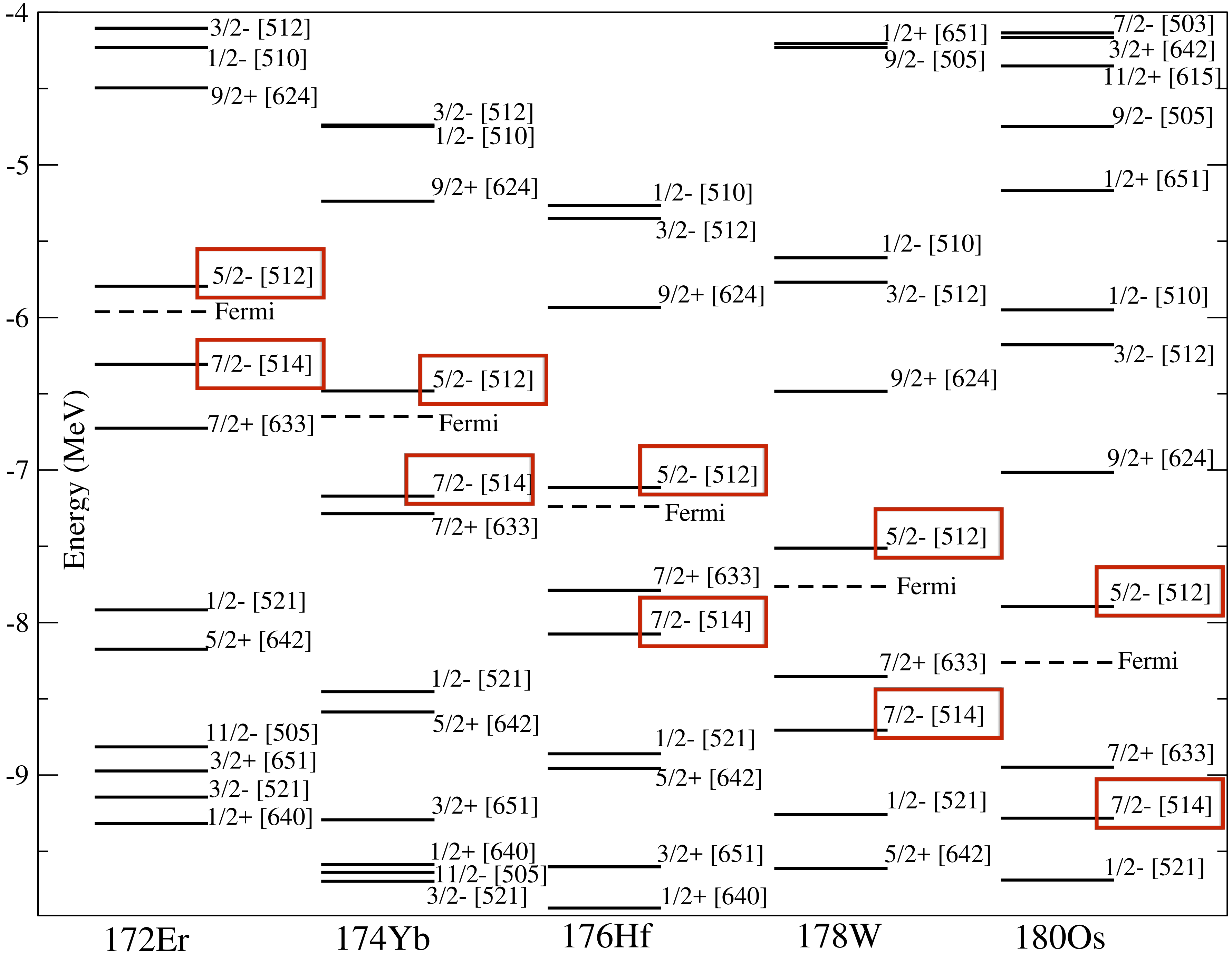
Diff. with expt. stable ~ 1.2MeV
Isomer energy very small increase
similarly with expt.

Results show similar pattern for the two functionals

K-isomers

6+ isomer at N=104 isotones

Neutron Single particle spectrum for N=104 isotones



<u>6+ isomers for N=104:</u>

arising from 2qp configuration

$\nu 5/2^{-}[512]\ \nu 7/2^{-}[514]$

<u>With the increase in Z</u>

Neutron orbits shift downwards

Relative position of Fermi stable

Orbit $\nu 5/2^{-}[512]$

Closest particle state to F.S.

Orbit $\nu 7/2^{-}[514]$

Closest hole state to F.S.

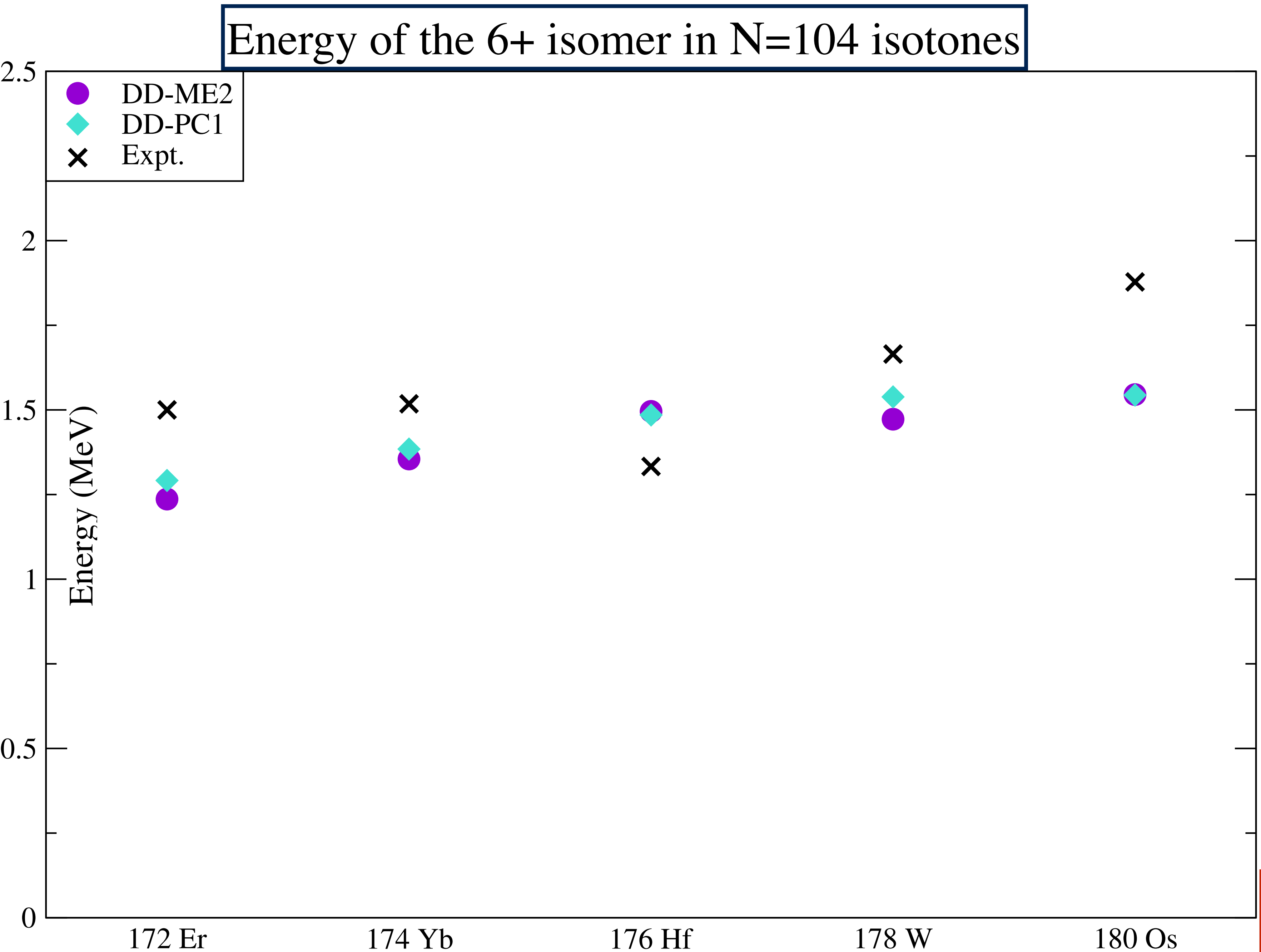
for 172Er, 174Yb

2nd closest hole state for 176Hf, 178W, 180Os

The gap between them gradually increases.

K-isomers

6+ isomer in N=104 isotones



Expt: G. D. Dracoulis *et. al.* , Phys. Let. B **635** (2006)

In General

Flat or small increase in isomer energy ~ 1.25->1.5MeV

Better description of the expt. values compared with Hf results

We don't get the small kink in 176Hf

Theor. prediction for 172Er-178W:

Difference wt expt. < 0.2 MeV

Theor. prediction for 180Os:

Slightly larger

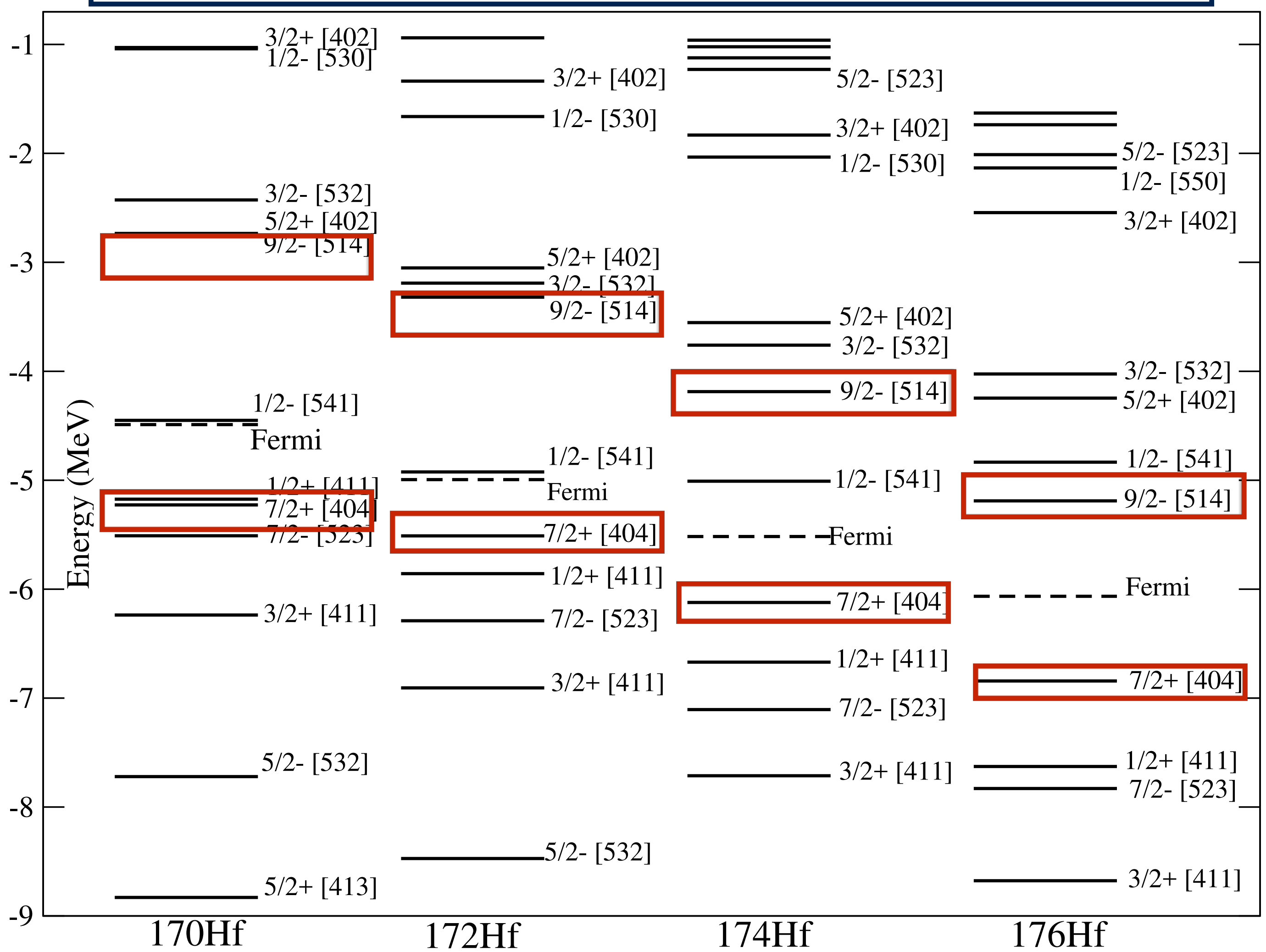
Energy difference ~ 0.5MeV

Here the two functionals are almost equivalent

K-Isomers

8- isomer in Hf isotopes

Proton Single particle spectrum for Hf isotopes



Same general properties with previous spectra

Gap bt the two states gets smaller

Relative position of the states w.r.t. Fermi

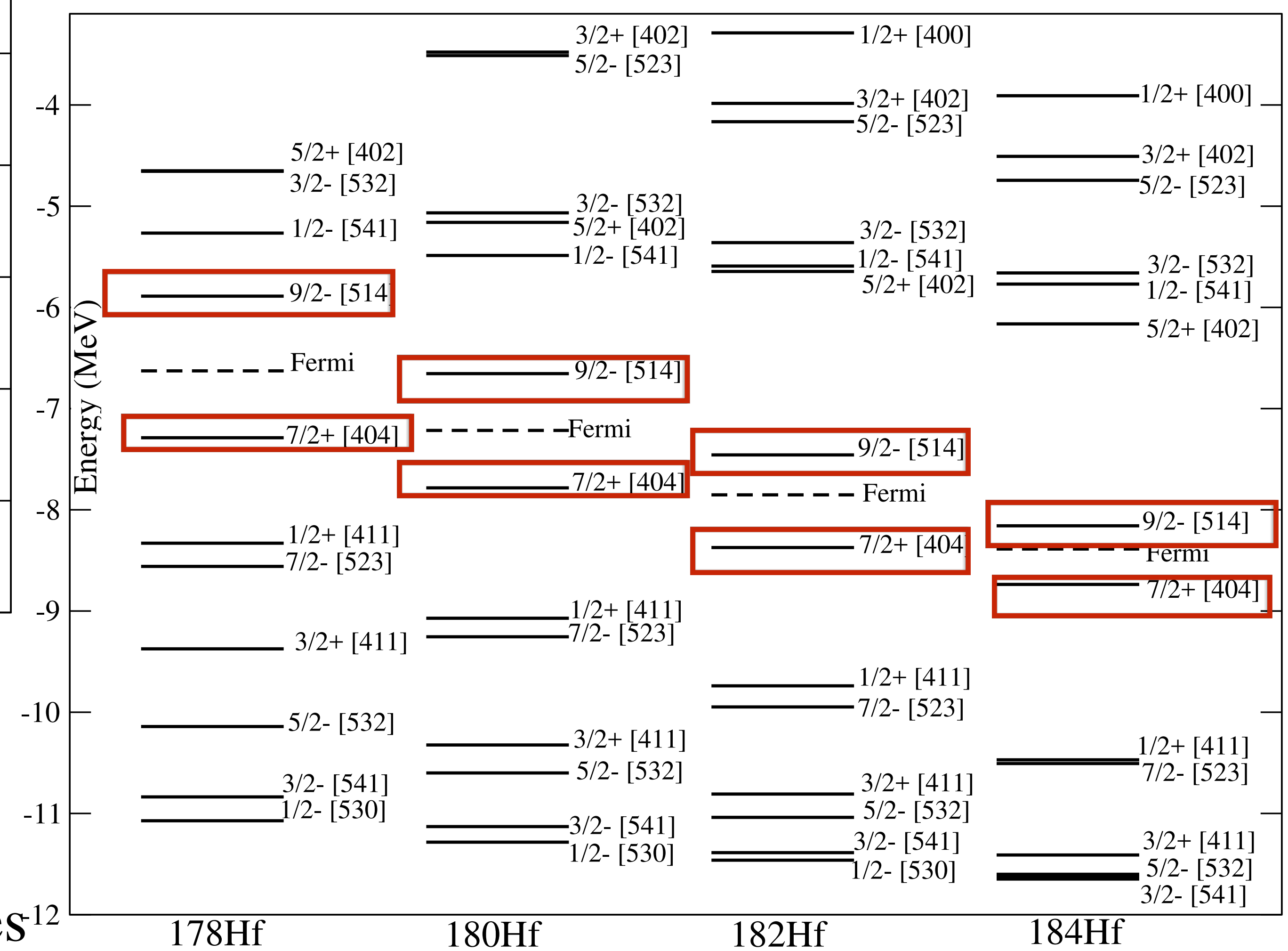
$\pi 9/2^-[514]$ Closest particle state for all the isotopes

$\pi 7/2^+[404]$
- Initially for 170Hf 2nd closest hole state
- Gradually moving closer to Fermi
- For 172Hb - 184Hf the closest hole state

8- isomer for Z=72:

arising from the 2qp configuration

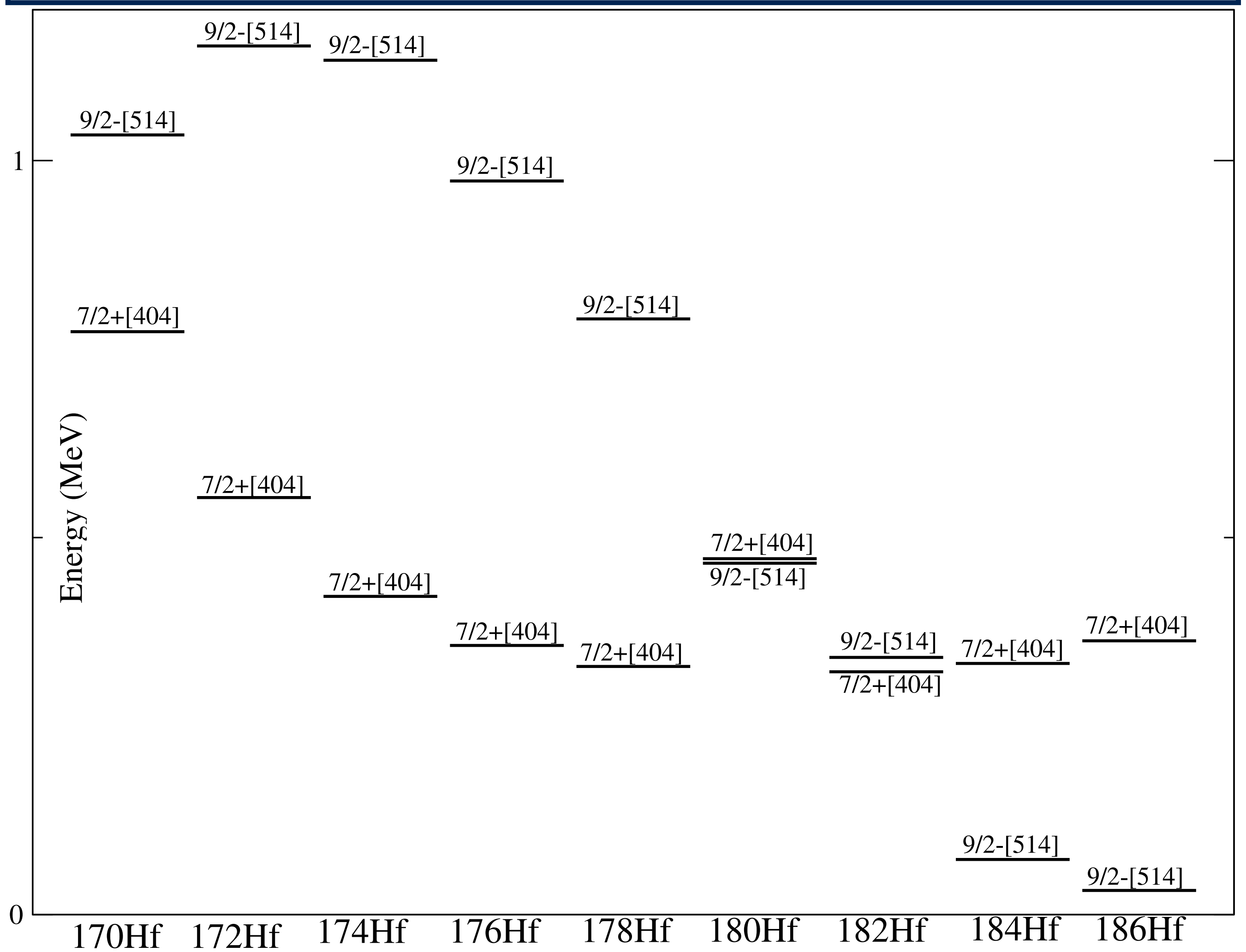
$\pi^2 9/2^-[514] \otimes 7/2^+[404]$



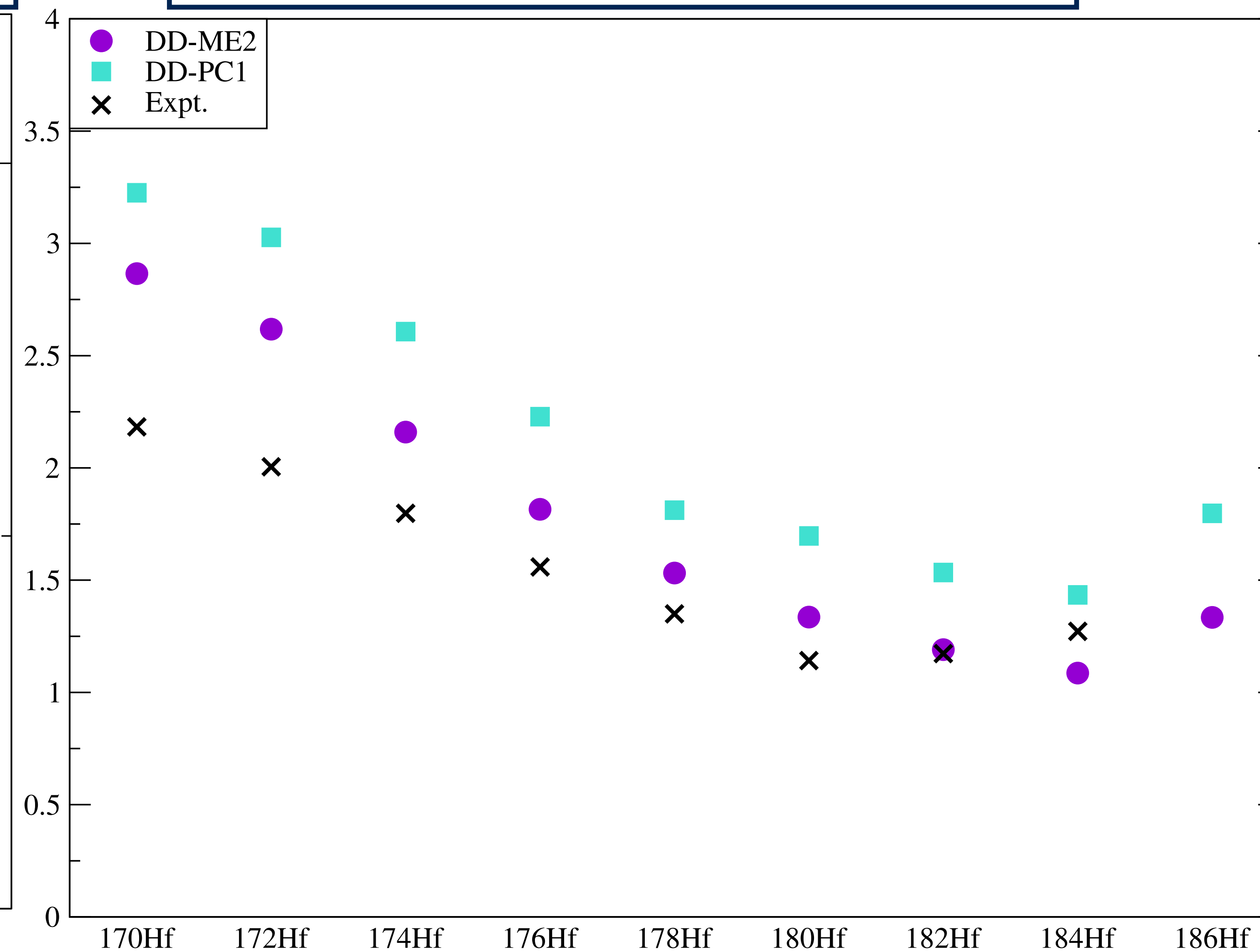
K-Isomers

8- isomer in Hf isotopes

Quasiparticle spectrum for Hf is. after blocking.



Energy of the 8- isomer in Hf isotopes



F. G. Kondev *et.al.* , At. Data & Nucl. Tables, April (2015)

Both states move to lower energies leading
The sum of the two qp energies to decrease.
There is a crossing bt the two states in 180Hf

$\pi 7/2^{+}[404]$ Lowest qp energy up to 178Hf

$\pi 9/2^{-}[514]$ Lowest qp energy from 180Hf

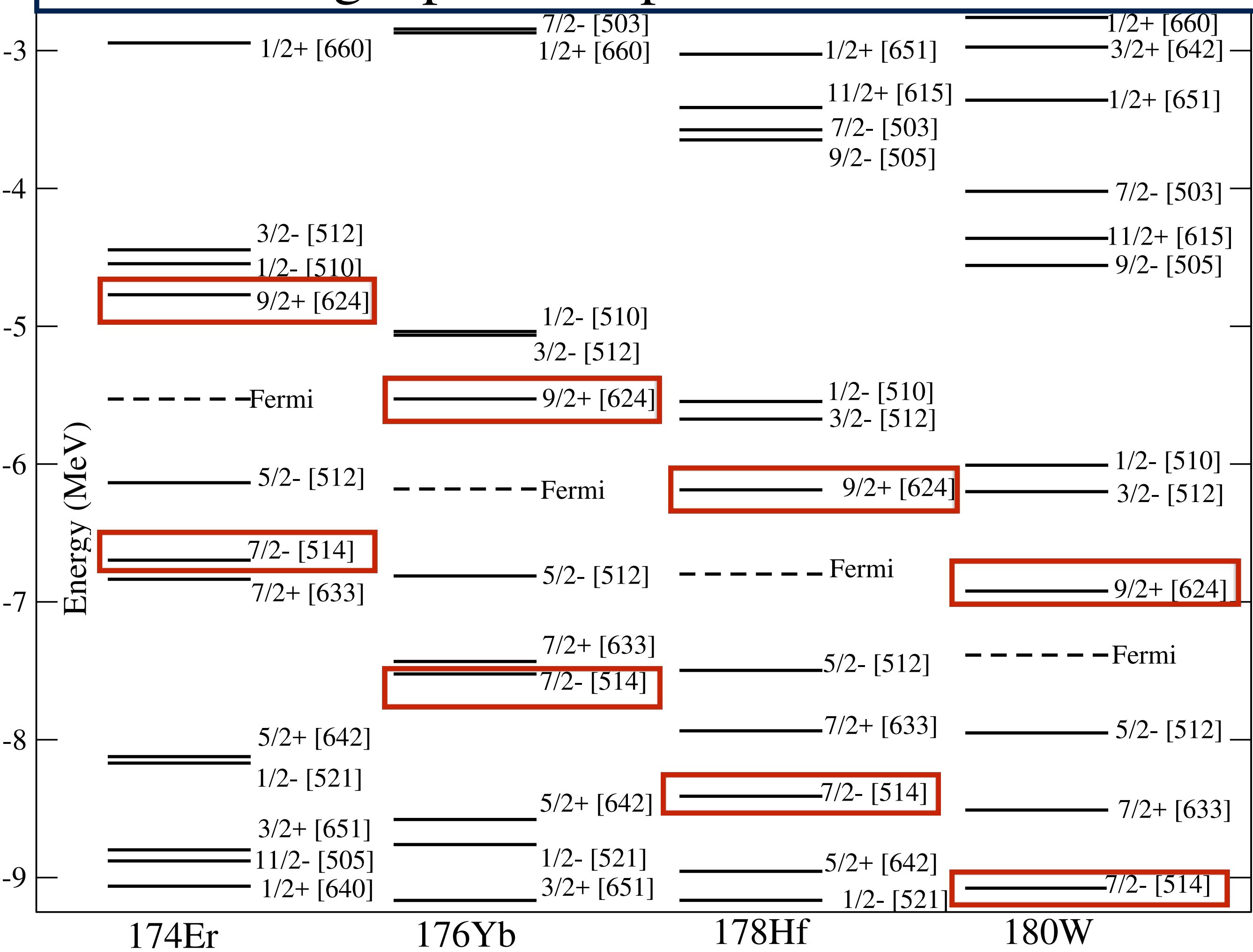
Isomeric energy

- Theor. prediction following sum of the qp energies decreasing gradually until 184Hf neq. to expt.
- Closer to expt. values for heavier isotopes.
- DDPC1 slightly larger than DDME2 ~ 0.5 MeV

K-Isomers

8- isomer in N=106 isotones

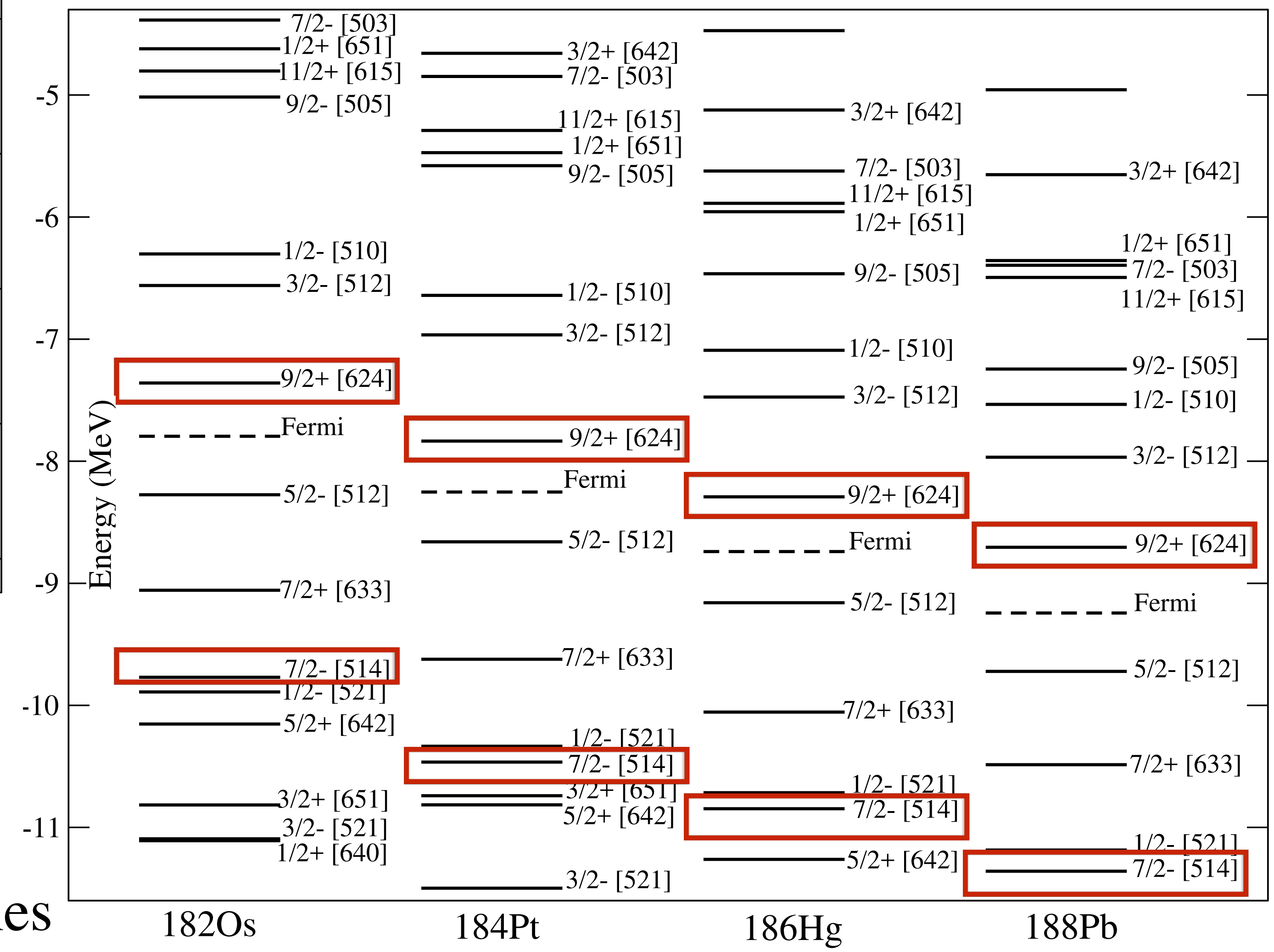
Neutron Single particle spectrum for N=106 isotones



8- isomer for N=106:

arising from the 2qp configuration

$\nu^2 7/2^-[514] \otimes 9/2^+[624]$



Now the gap bt the two states gradually increases

Relative position of the states w.r.t. Fermi

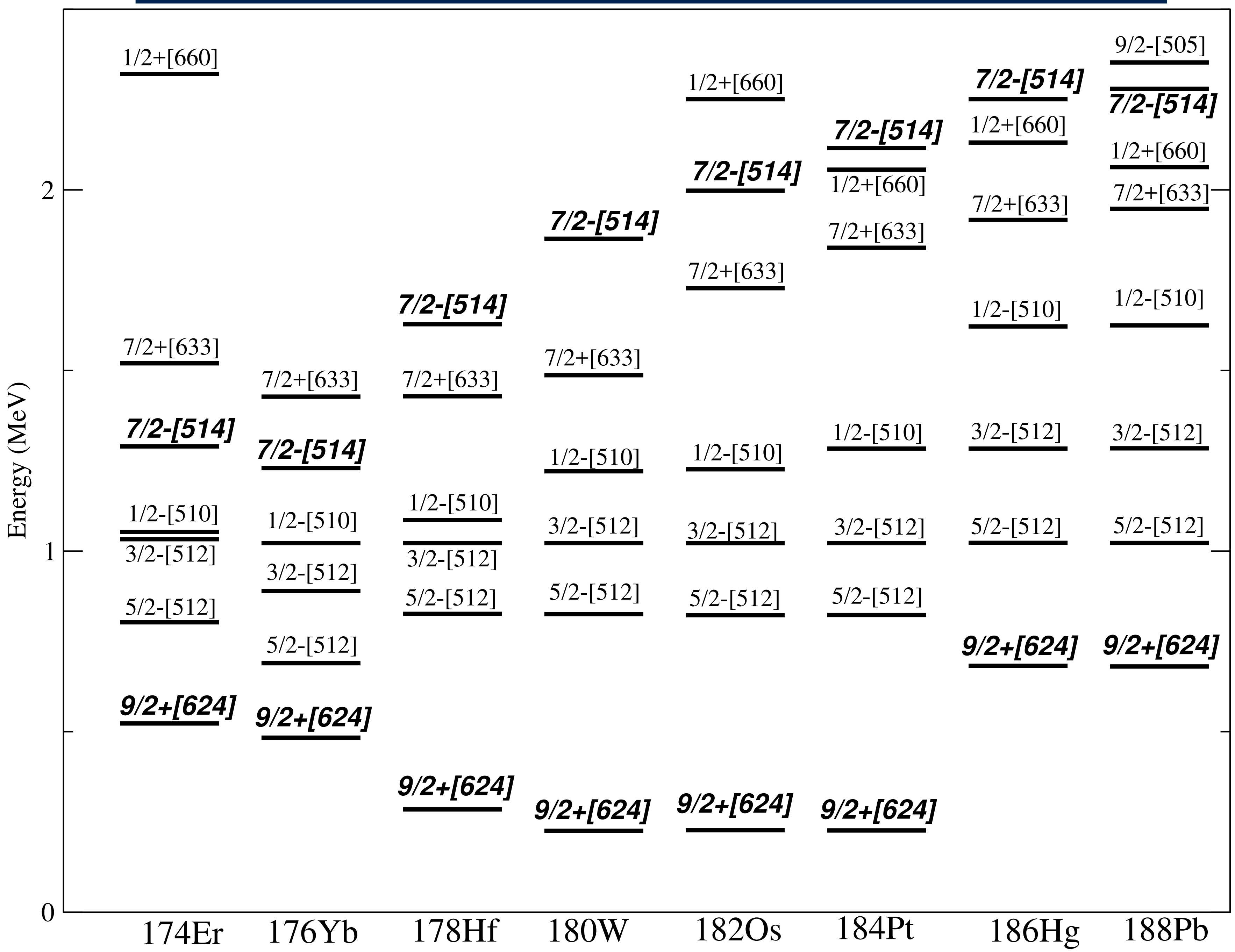
$\nu 9/2^+[624]$ Closest particle state for all the isotones

$\nu 7/2^-[514]$
- Initially for 174Er 2nd closest hole state
- Gradually moving further down in energy
- For 176Yb - 184Pt two intermediate s.p. orbits
- For 186Hg & 188Pb three intermediate s.p. orbits

K-Isomers

8- isomer in N=106 isotones

Quasiparticle spectrum for N=106 after blocking.



Reproduction of previous structure at the qp spectrum of the isomer

$\nu 9/2^{+}[624]$

Lowest qp energy For all the isotones

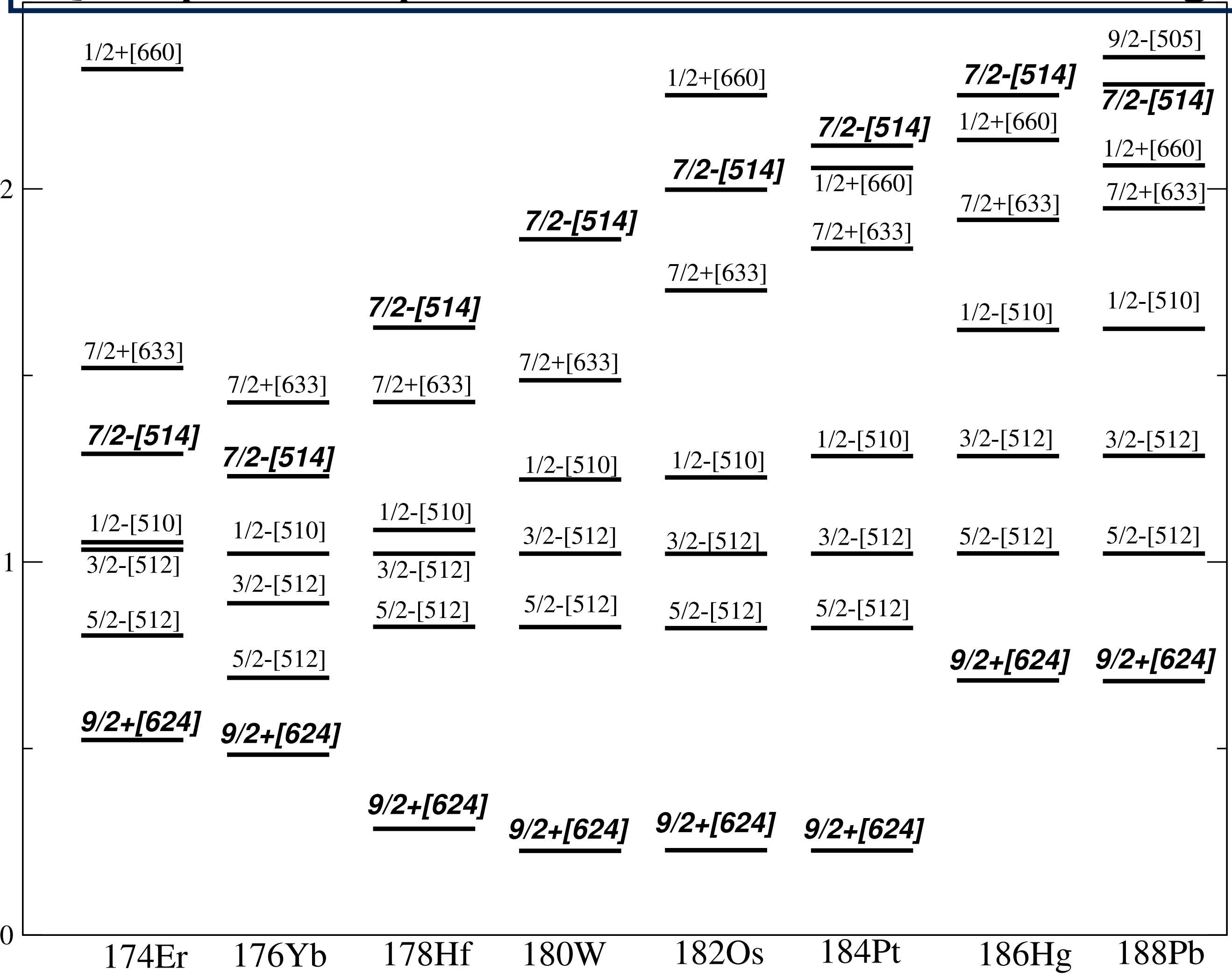
$\nu 7/2^{-}[514]$

Increase of the qp energy for heavier isotones

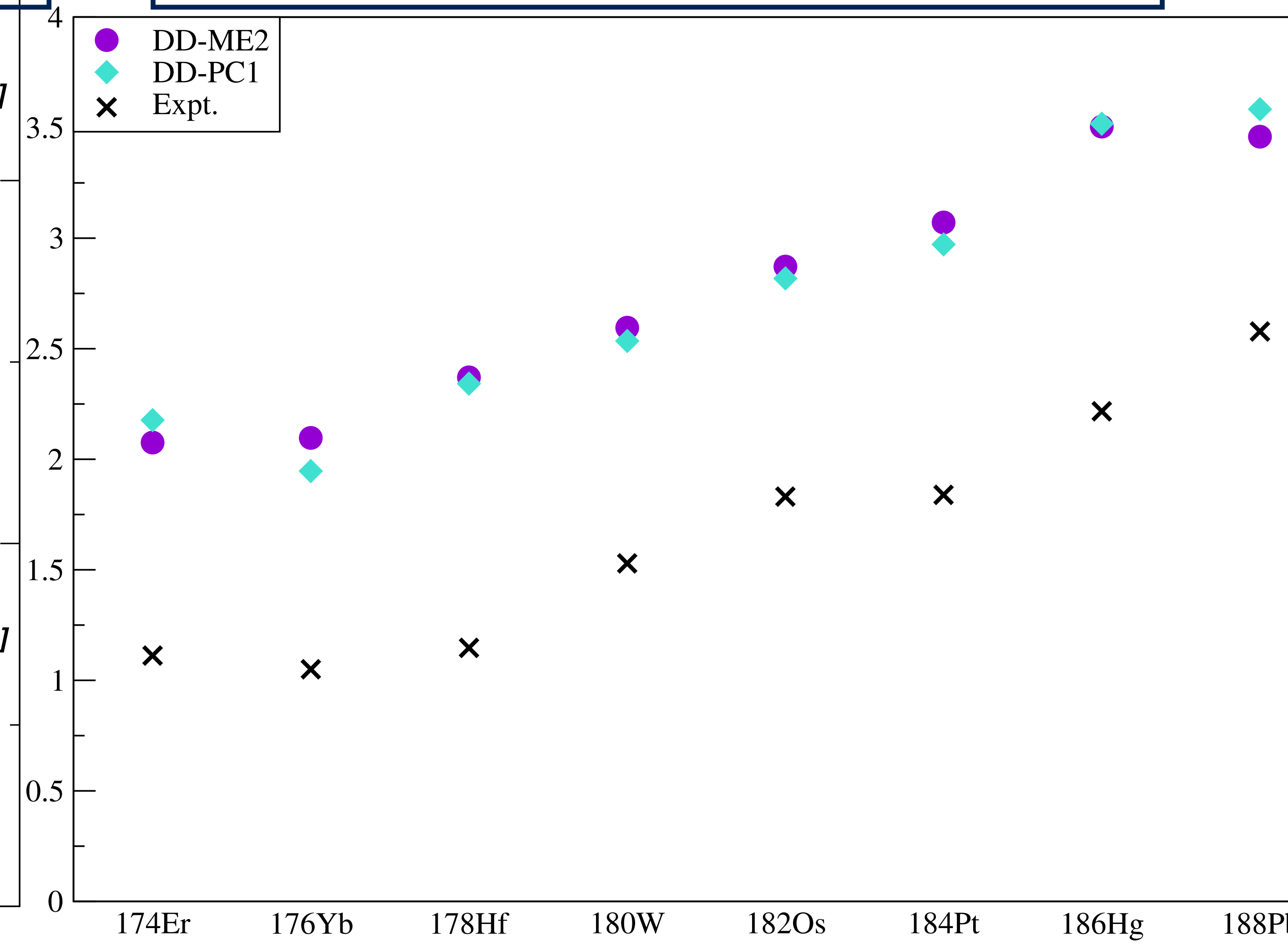
K-Isomers

8- isomer in N=106 isotones

Quasiparticle spectrum for N=106 after blocking.



Energy of the 8- isomer in N=106 isotones



Expt: G. D. Dracoulis *et. al.* , Phys. Let. B **635** (2006)

Reproduction of previous structure at the qp spectrum of the isomer

$\nu 9/2^+[624]$ Lowest qp energy for all the isotones

$\nu 7/2^-[514]$ Increase of its qp energy for heavier isotones

Isomeric energy

- Direct effect of the qp structure in the evolution of the excitation energy
- Increase of the isomer energy-irregular pattern
- Remarkable agreement bt expt. and theoretical evolution pattern
- Albeit for constant diff. wt expt. value ~1MeV

K-Isomers
Summary-Outlook

- Confirmation of the existence of the required single particle states - Nilsson diagrams
- Application of the blocking effect within the Equal Filling Approximation.
- Calculation of energy of the 2 quasiparticle states.
- Reproduction of the qualitative picture on the systematic appearance of the 6+ and 8- isomers.
- Equivalent results for DDME2 and DDPC1.
- Important ingredients for the calculation of isomeric energies:
    1. Relative position of the s.p. states with the Fermi surface.
    2. The energy gap bt the states and the existence of other states in between.
    3. The absolute value of the quasiparticle energy and its sum
- Best agreement with experimental values in cases where the 2 states are indeed the closest to the Fermi surface i.e. having the lowest qp energy
- Significant difference between theory and experiment for the rest of the cases.
- Application of the full blocking scheme with currents
- Extending to superheavy region
- Suggestion to study k-isomers including further correlations such as
    1. Particle Vibration Coupling or Tensor forces that modify the s.p. spectrum.
    2. The effect of the unpaired nucleons in the mean field.

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