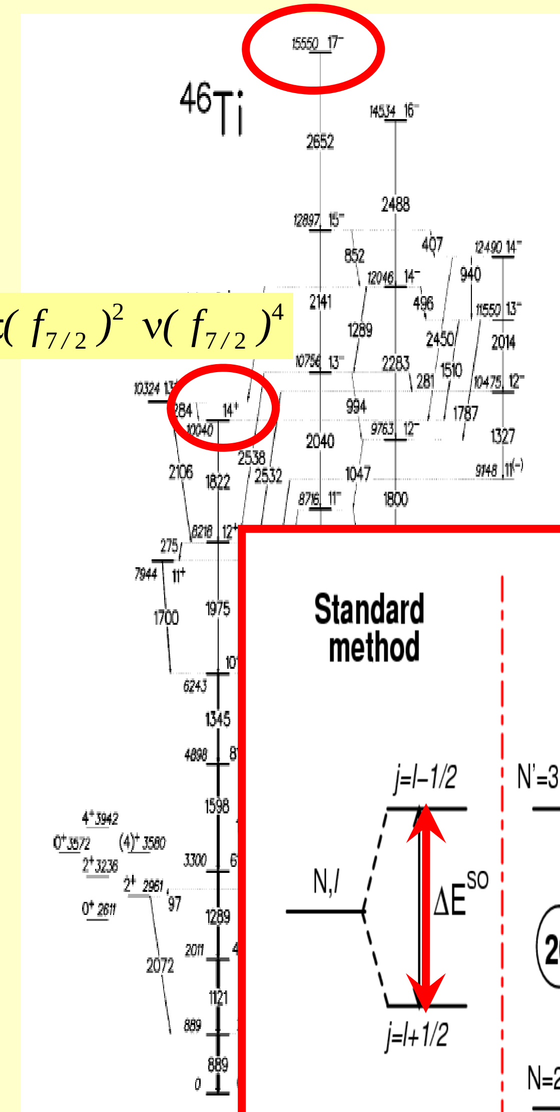
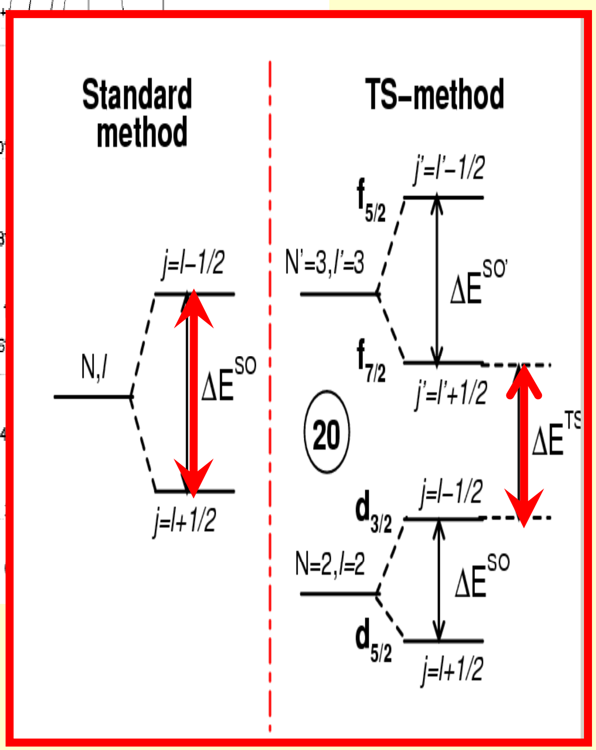
Terminating states: can they be used to constraint DFT?

$\pi(d_{3/2})^{-1}(f_{7/2})^{3}\ \nu(f_{7/2})^{4}$

$\pi(f_{7/2})^{2}\ \nu(f_{7/2})^{4}$





Energy difference $\Delta E^{TS} = E(d^{-1}_{3/2}\, f^{n+1}_{7/2}) - E(f^{n}_{7/2})$

provides unique and reliable constraints on time-odd mean fields and the strength of spin-orbit interaction

(red – exact quote from H.Zdunczuk et al, PRC 71(05)024305) – let call it as "TS-method"

In self-consistent models

$$\Delta E^{TS-SC} = E_{binding}(d^{-1}_{3/2}\, f^{n+1}_{7/2}) - E_{binding}(f^{n}_{7/2}) =$$
$$= f(N, l, j, N', j', l', TO, m^*(k_F)/m, pol.)$$

Function of:

- spin-orbit
- orbital motion
- time-odd mean fields (TO)
- energy scale (effective mass $m^*(k_F)/m$)
- polarization effects in time-even mean fields

Answer: NO.

Basis of the TS-method

$$\hat{H}_{Nilsson} - \frac{3}{2}\hbar\omega_0 = \hbar\omega_0\left\{N - k\left[2\vec{l}\vec{s} + \mu(\vec{l}^{\,2} - <\vec{l}^{\,2}>_N\right]\right\}$$

$$\left[E\left(d_{3/2}^{-1} f_{7/2}^{n+1}\right) - E\left(f_{7/2}^{n}\right)\right]_{Nilsson} = \hbar\omega_0\left(1 - 6\kappa - 2\kappa\mu\right)$$

disregard the flat-bottom effects on potential $\mu \sim 0$

$$\left[E\left(d_{3/2}^{-1} f_{7/2}^{n+1}\right) - E\left(f_{7/2}^{n}\right)\right]_{Nilsson} = \hbar\omega_0\left(1 - 6\kappa\right)$$

Energy difference is defined by
- $\hbar\omega_0$ - energy scale
- κ - spin-orbit strength

BUT, in realistic Nilsson potential

$$\hat{H}_{Nilsson} - \frac{3}{2}\hbar\omega_0 = \hbar\omega_0\left\{N - k_N\left[2\vec{l}\vec{s} + \mu_N(\vec{l}^{\,2} - <\vec{l}^{\,2}>_N\right]\right\}$$

$$\left[E\left(d_{3/2}^{-1} f_{7/2}^{n+1}\right) - E\left(f_{7/2}^{n}\right)\right]_{Nilsson} = \hbar\omega_0\left(1 - 3\left[\kappa_2 + \kappa_3\right] - 3\kappa_3\mu_3 - \kappa_2\mu_2\right)$$

	Protons		Neutrons	
N	κ	μ	κ	μ
2	0.105	0.0	0.105	0.0
3	0.090	0.30	0.090	0.25

"standard" parametrization of the Nilsson potential, 1986, T.Bengtsson, I. Ragnarsson

$$\left[E\left(d_{3/2}^{-1} f_{7/2}^{n+1}\right) - E\left(f_{7/2}^{n}\right)\right]_{Nilsson} = 0.415\hbar\omega_0$$ --The $\mu = 0$ case (TS-method)

$$\left[E\left(d_{3/2}^{-1} f_{7/2}^{n+1}\right) - E\left(f_{7/2}^{n}\right)\right]_{Nilsson} = 0.334\hbar\omega_0$$ -- Standard parameters

$$\left[E\left(d_{3/2}^{-1} f_{7/2}^{n+1}\right) - E\left(f_{7/2}^{n}\right)\right]$$

Explicit dependence on the orbital angular momentum cannot be ignored