Nuclear DFT electromagnetic moments in heavy deformed open-shell odd nuclei

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Seminarium Fizyki Jądra Atomowego, Warszawa, 16 listopada 2023

The bottom line

The nuclear electromagnetic moments of odd nuclei are all about:

1. **Polarization**
2. **Self-consistency**
3. **Symmetry restoration**

About half of the nuclides in nature are odd

Basic definitions

The electric and magnetic moments are defined as

$$Q_{\lambda\mu} = \langle\Psi|\hat{Q}_{\lambda\mu}|\Psi\rangle = \int q_{\lambda\mu}(\vec{r})\, d^3\vec{r},$$

$$M_{\lambda\mu} = \langle\Psi|\hat{M}_{\lambda\mu}|\Psi\rangle = \int m_{\lambda\mu}(\vec{r})\, d^3\vec{r},$$

where $|\Psi\rangle$ is a many-body state, and $q_{\lambda\mu}(\vec{r})$ and $m_{\lambda\mu}(\vec{r})$ are the corresponding electric and magnetic-moment densities:

$$q_{\lambda\mu}(\vec{r}) = e\rho(\vec{r})Q_{\lambda\mu}(\vec{r}),$$

$$m_{\lambda\mu}(\vec{r}) = \mu_N\left[g_s\vec{s}(\vec{r}) + \tfrac{2}{\lambda+1}g_l\left(\vec{r}\times\vec{j}(\vec{r})\right)\right]\cdot\vec{\nabla}Q_{\lambda\mu}(\vec{r}),$$

and e, g_s, and g_l are the elementary charge, and the spin and orbital gyromagnetic factors, respectively. The multipole functions (solid harmonics) have the standard form: $Q_{\lambda\mu}(\vec{r}) = r^\lambda Y_{\lambda\mu}(\theta,\phi)$.

Schmidt limits

The magnetic operator $\bar{\mu}$ is a one-body operator and the magnetic dipole moment μ is the expectation value of $\bar{\mu}_z$. The M1 operator acting on a composed state $|\mathrm{Im}\rangle$ can then be written as the sum of single particle M1 operators $\bar{\mu}_z(j)$ acting each on an individual valence nucleon with total momentum j:

$$\mu = g_L\, \mathbf{L} + g_s\, \mathbf{s}$$

$$\mu(I) \equiv \left\langle I(j_1, j_2, \ldots, j_n), m = I \left| \sum_{i=1}^{n} \bar{\mu}_z(i) \right| I(j_1, j_2, \ldots, j_n), m = I \right\rangle \qquad (2.1)$$

The single particle magnetic moment $\mu(j)$ for a valence nucleon around a doubly magic core is uniquely defined by the quantum numbers l and j of the occupied single particle orbit [22]:

$$\text{for an odd proton:} \begin{cases} \mu = j - \frac{1}{2} + \mu_{\mathrm{p}} & \text{for } j = l + \frac{1}{2} \\ \mu = \dfrac{j}{j+1}\left(j + \dfrac{3}{2} - \mu_{\mathrm{p}}\right) & \text{for } j = l - \frac{1}{2} \end{cases} \qquad (2.2)$$

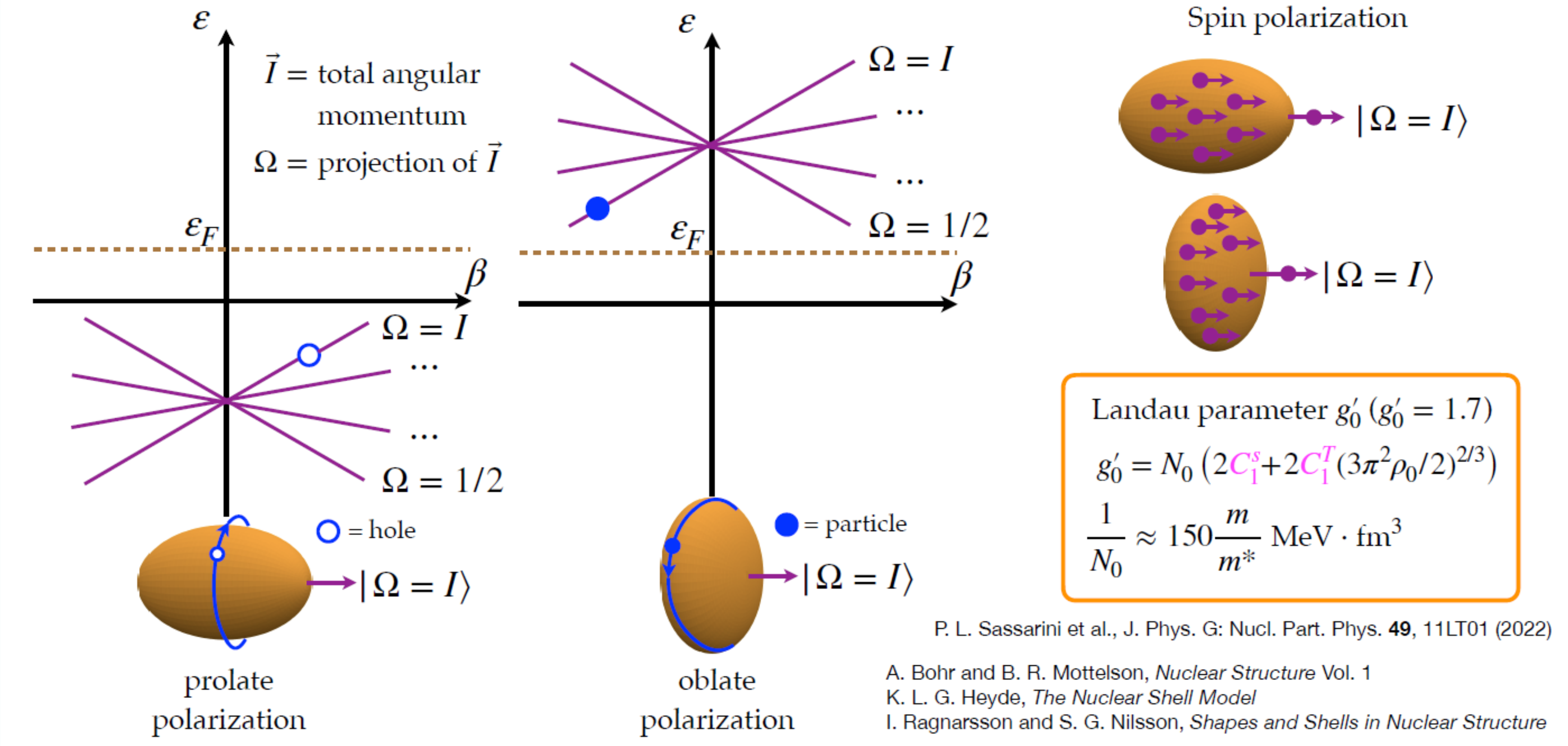
$$\text{for an odd neutron:} \begin{cases} \mu = \mu_{\mathrm{n}} & \text{for } j = l + \frac{1}{2} \\ \mu = -\dfrac{j}{j+1}\mu_{\mathrm{n}} & \text{for } j = l - \frac{1}{2} \end{cases} \qquad (2.3)$$

Schmidt limits

These single particle moments calculated using the free proton and free neutron moments ($\mu_{\mathrm{p}} = +2.793$, $\mu_{\mathrm{n}} = -1.913$) are called the Schmidt moments. In a nucleus, the magnetic

Gerda Neyens, Rep. Prog. Phys. 66 (2003) 633–689

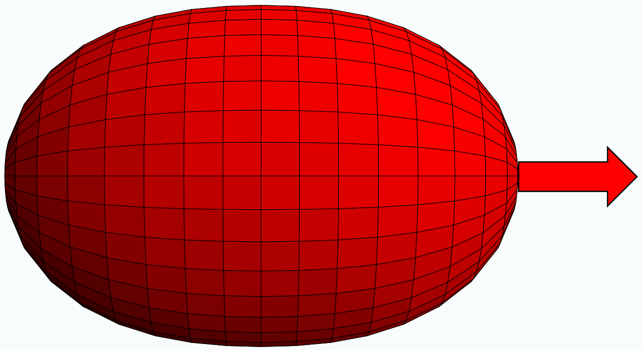
Shape and spin polarization

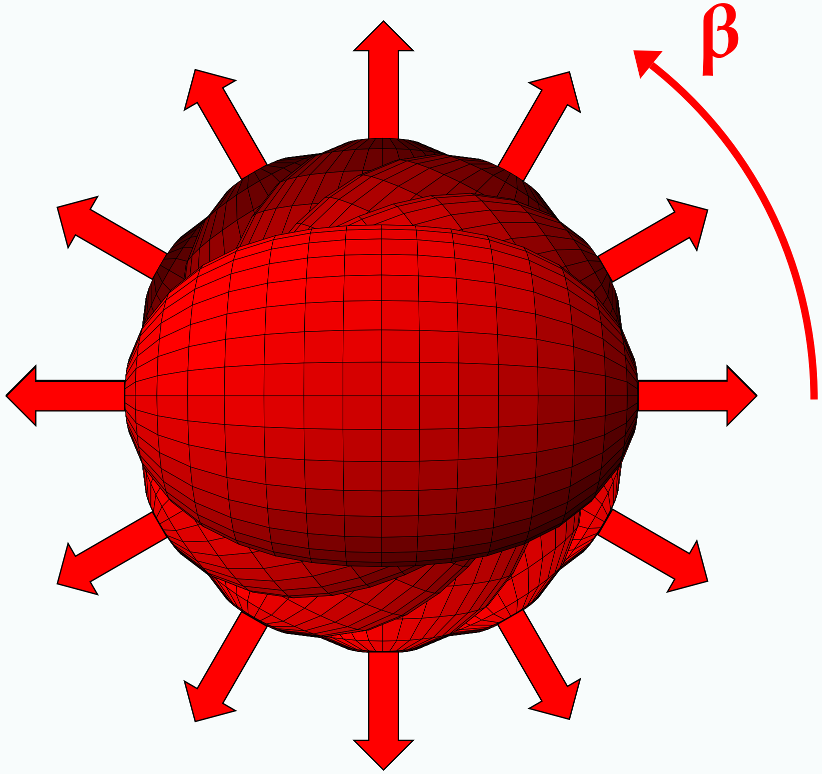


Picture: courtesy H. Wibowo

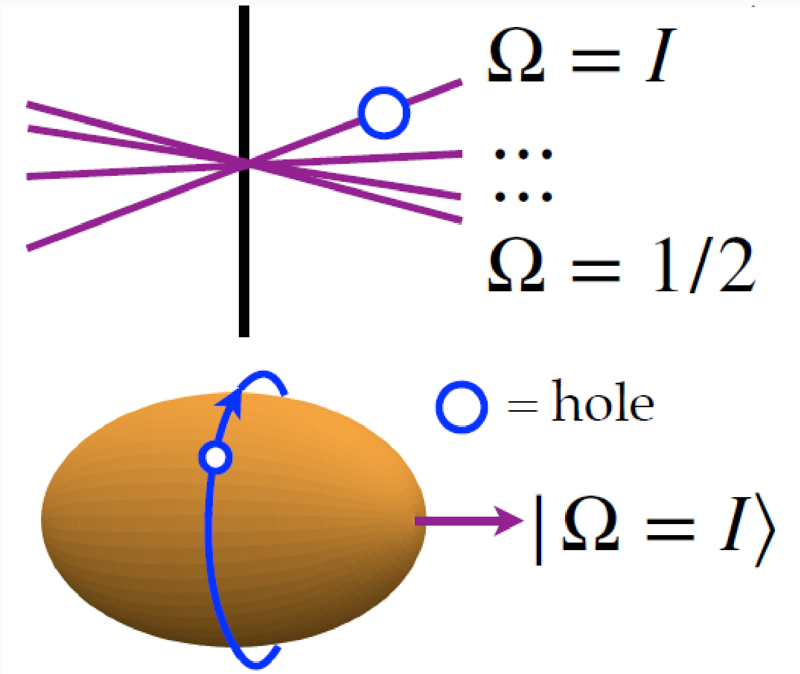
Time-odd spin alignment & symmetry restoration

"Intrinsic"
Symmetry broken





"Laboratory"
Symmetry restored



$$|IM\rangle = \mathcal{N}_I \int_{\beta=0}^{\pi} \mathrm{d}\beta \, d^I_{M\Omega}(\beta) |\Omega, \beta\rangle$$

J. A. Sheikh et al., J. Phys. G48, 123001 (2021)

Nuclear quadrupole & dipole moments

Spectroscopic electric quadrupole Q and magnetic dipole μ moments are :

$$Q = \sqrt{\frac{16\pi}{5}}\langle II\,|\,\hat{Q}_{20}\,|\,II\rangle \quad \text{and} \quad \mu = \sqrt{\frac{4\pi}{3}}\langle II\,|\,\hat{M}_{10}\,|\,II\rangle\,.$$

P. Ring and P. Schuck, *The Nuclear Many-Body Problem*

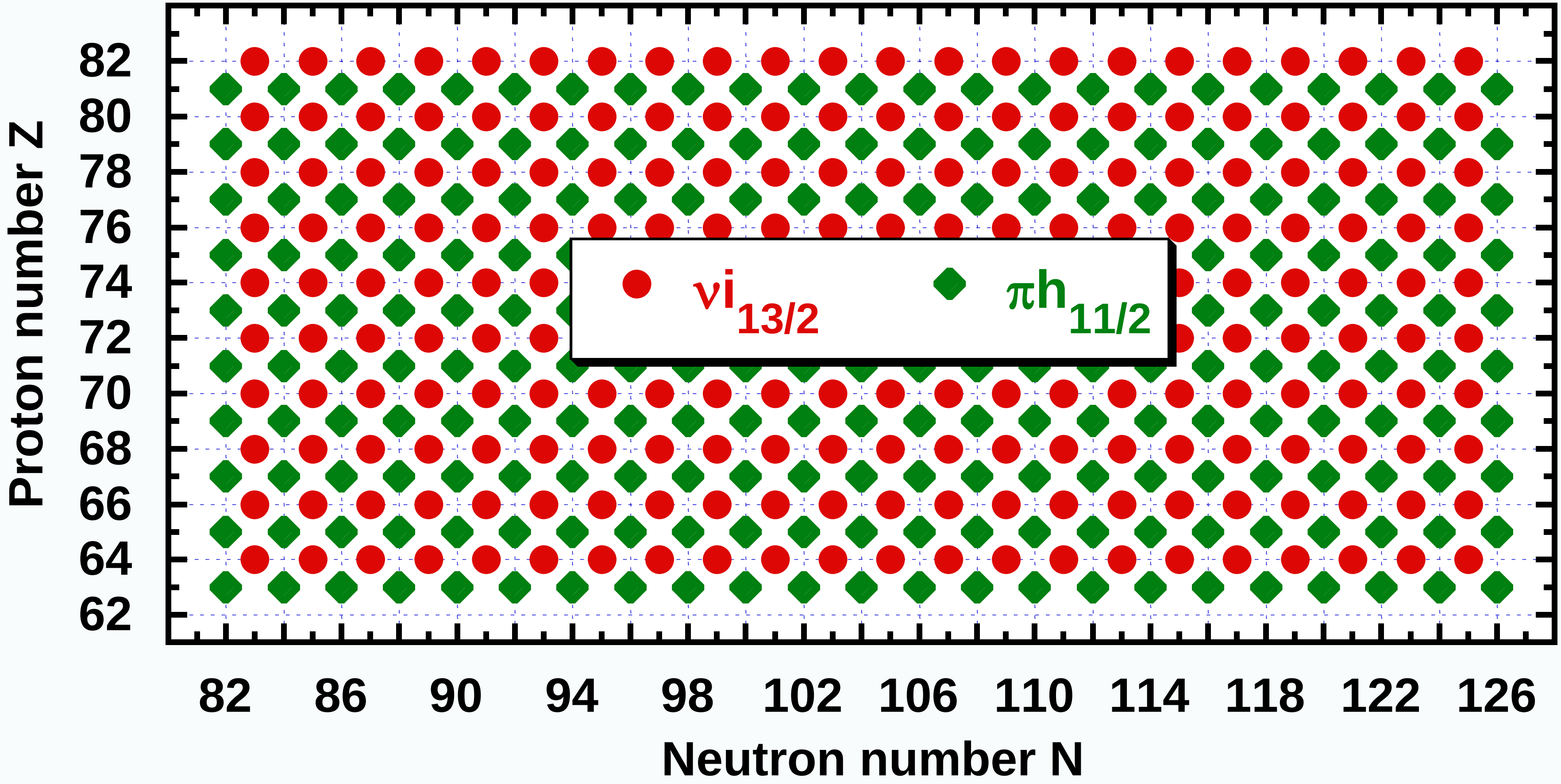
$$\hat{Q}_{20} = \sqrt{\frac{5}{16\pi}}e\sum_{i=1}^{A}\left(\frac{1}{2}-t_3^{(i)}\right)\left\{3z_i^2 - r_i^2\right\};\quad \hat{M}_{10} = \sqrt{\frac{3}{4\pi}}\mu_N\sum_{i=1}^{A}\left\{g_s^{(i)}s_{zi}+g_\ell^{(i)}\ell_{zi}\right\};$$

$$g_s^{(i)} = g_p(g_n) = 5.59(-3.83)$$
$$g_\ell^{(i)} = 1(0)$$

Intrinsic moments = moments of the symmetry-broken state
Spectroscopic moments = moments of the symmetry-restored state

Spectroscopic moments = moments measured experimentally

The first systematic nuclear-DFT analysis of the electromagnetic moments in heavy deformed open-shell odd nuclei



Blocked quasiparticles were tagged by the neutron $i_{13/2}$ (Ω=+13/2) or proton $h_{11/2}$ (Ω=+11/2) single-particle orbitals

J. Bonnard *et al.*, Phys. Lett. B 843 (2023) 138014

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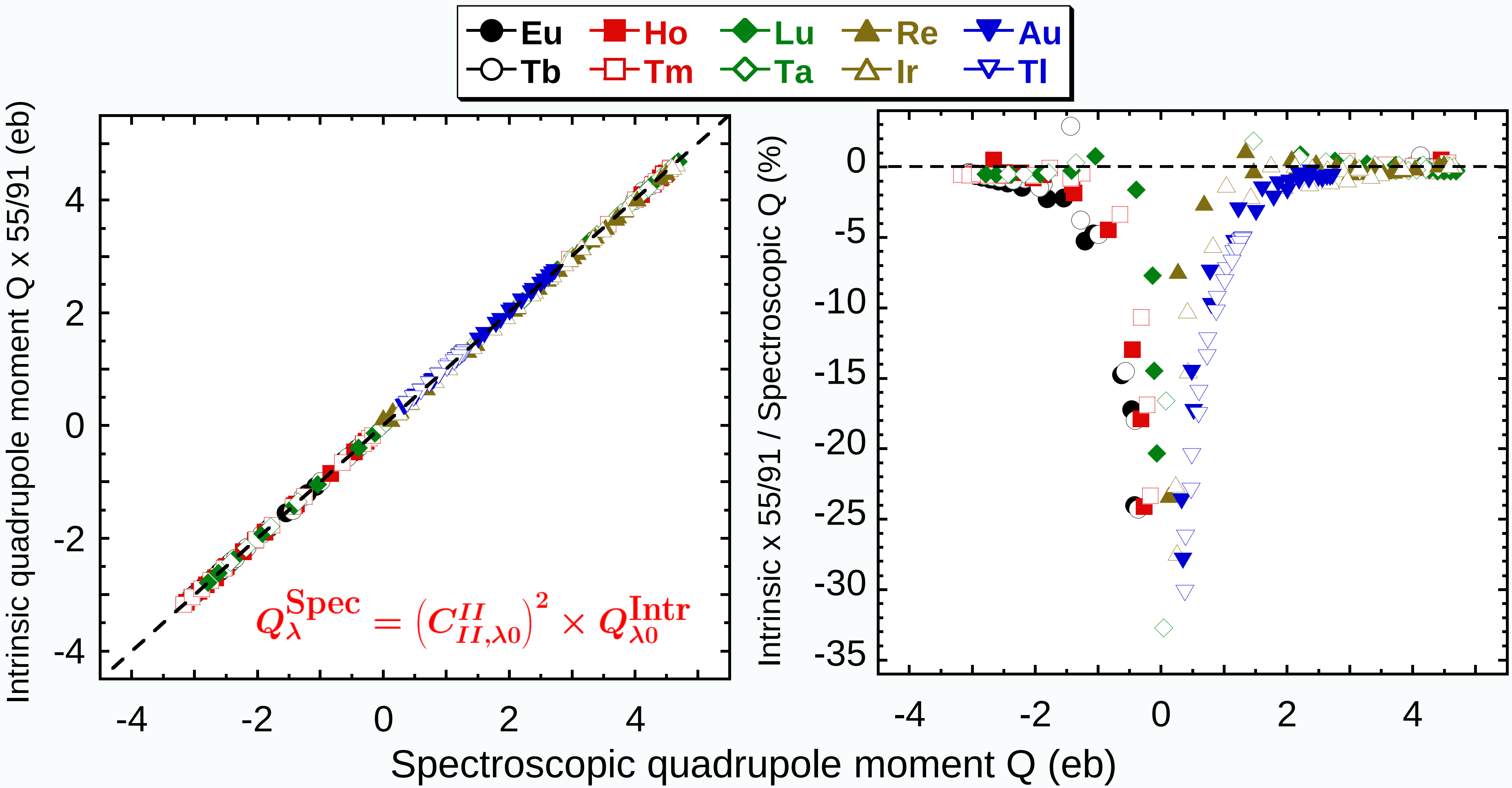
Heavy deformed π11/2⁻ odd-Z nuclei



Conclusion:

Spectroscopic electric quadrupole moments can be inferred from the intrinsic ones at ~5% precision only at |Q|>1b)

J. Bonnard *et al.*, Phys. Lett. B 843 (2023) 138014

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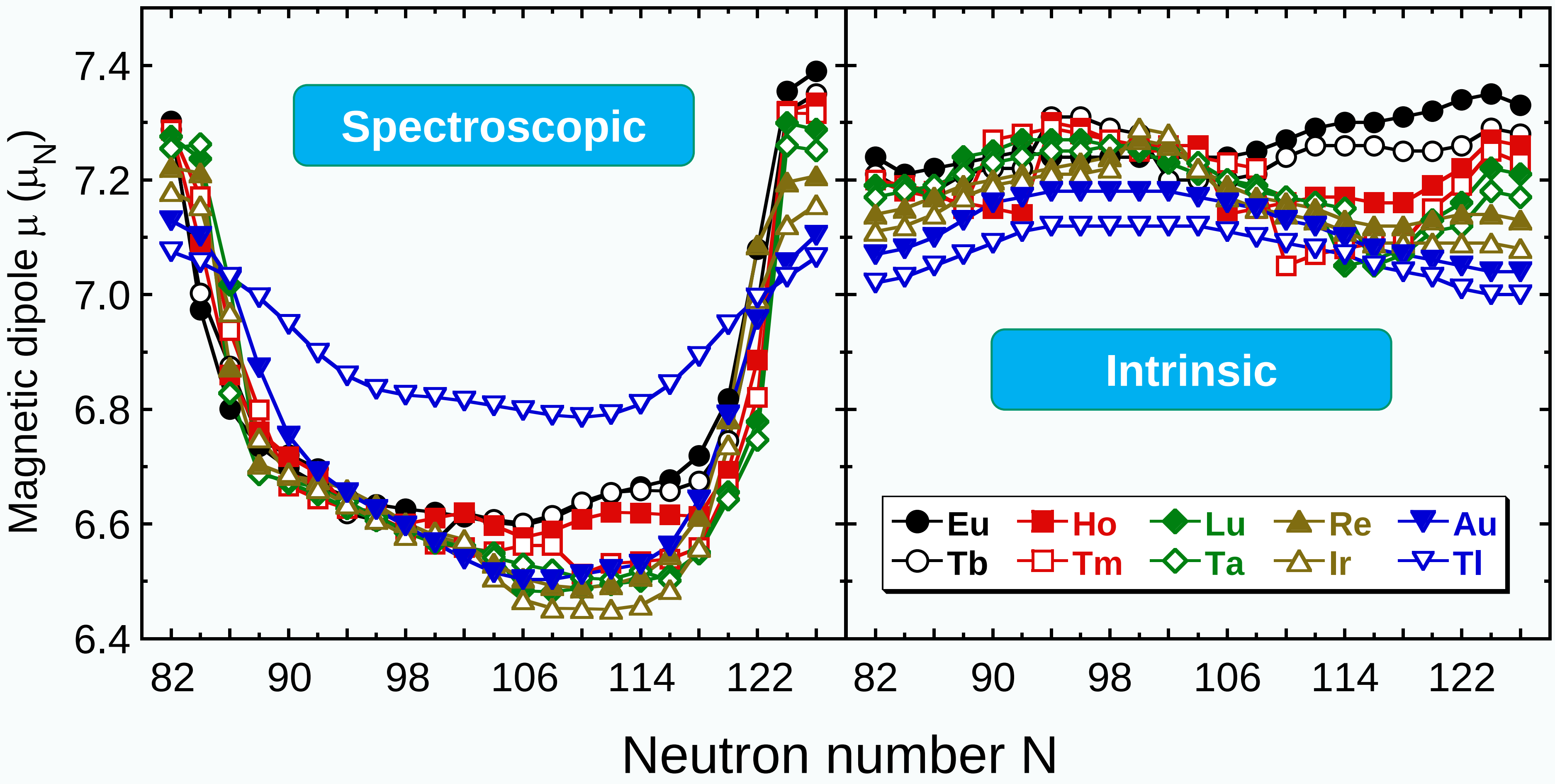
Heavy deformed $\pi 11/2^-$ odd-Z nuclei

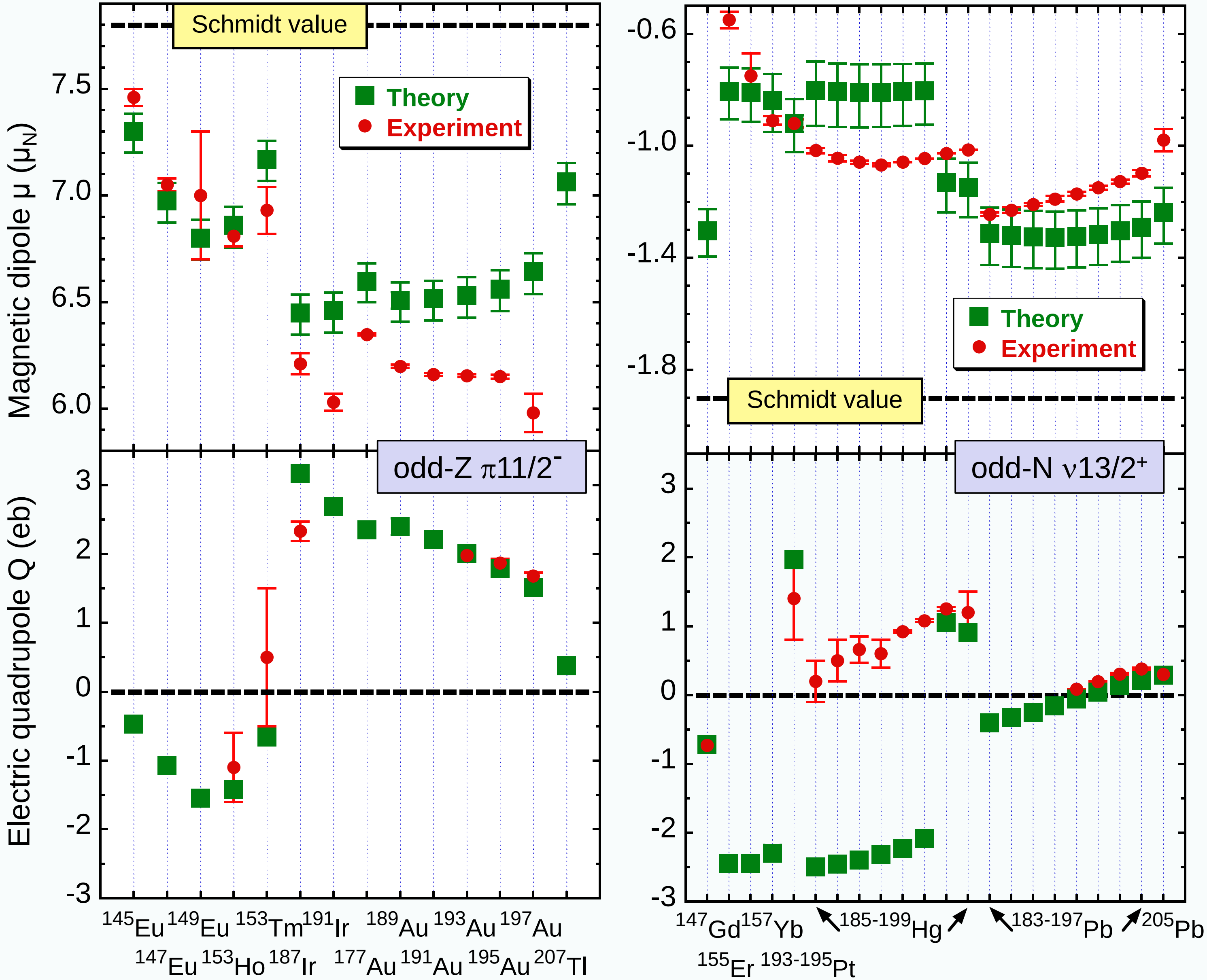


J. Bonnard *et al.*, Phys. Lett. B 843 (2023) 138014

Conclusion:

Spectroscopic magnetic dipole moments cannot be inferred from the intrinsic ones

Spectroscopic moments: theory vs. experiment



J. Bonnard *et al.*, Phys. Lett. B 843 (2023) 138014

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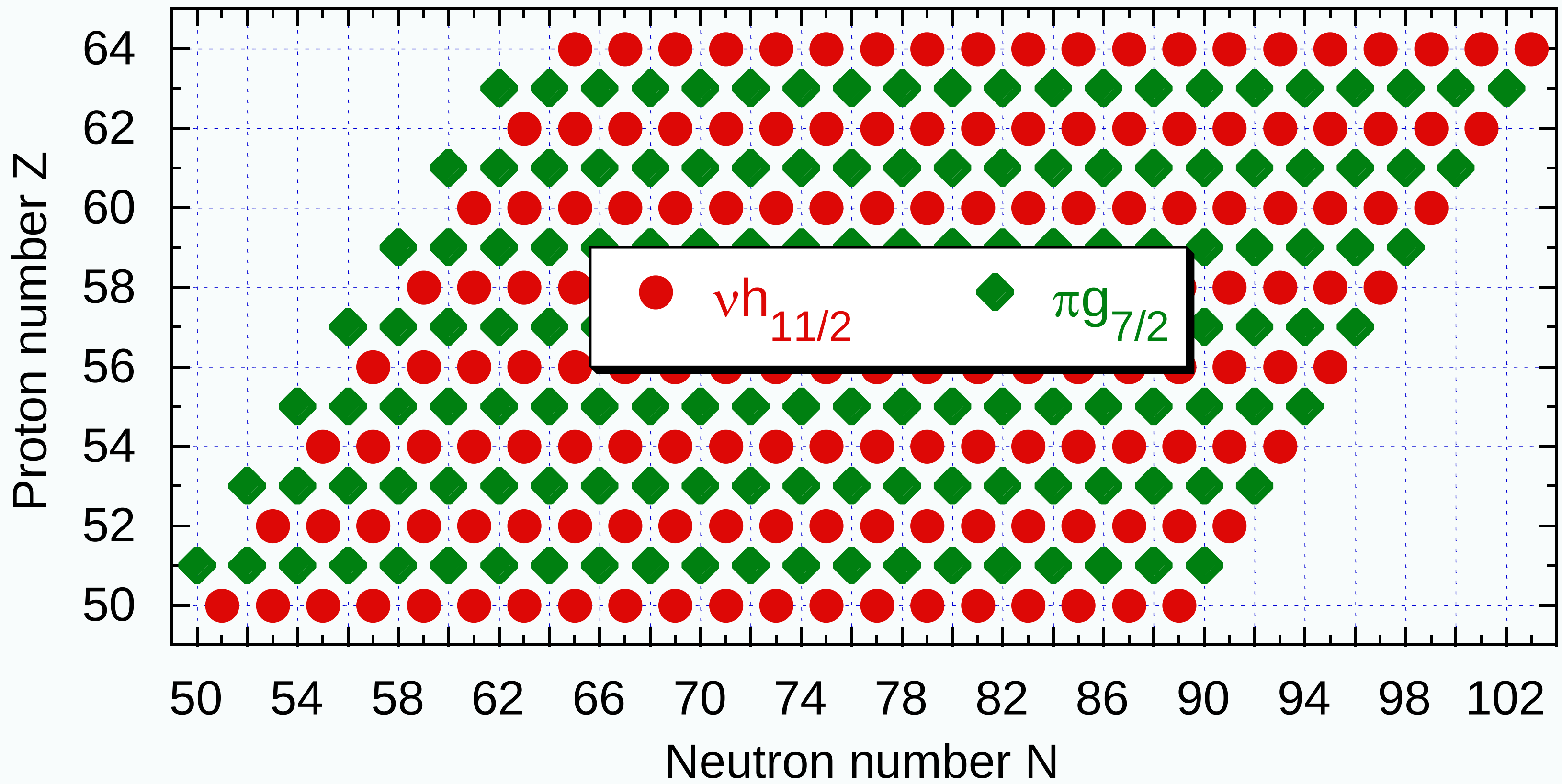
Nuclear-DFT analysis of electromagnetic moments between the Sn and Gd isotopes



H. Wibowo *et al.*, to be published

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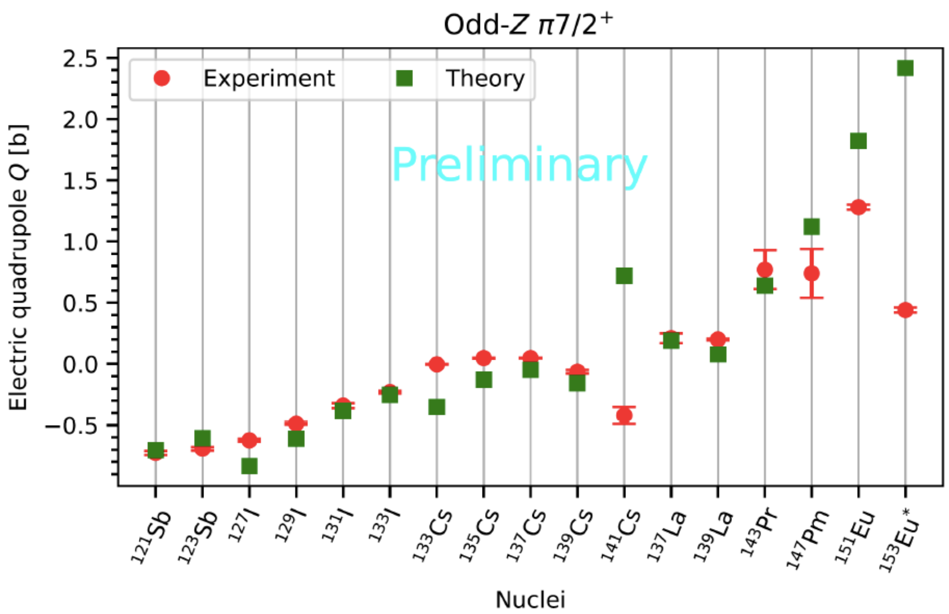
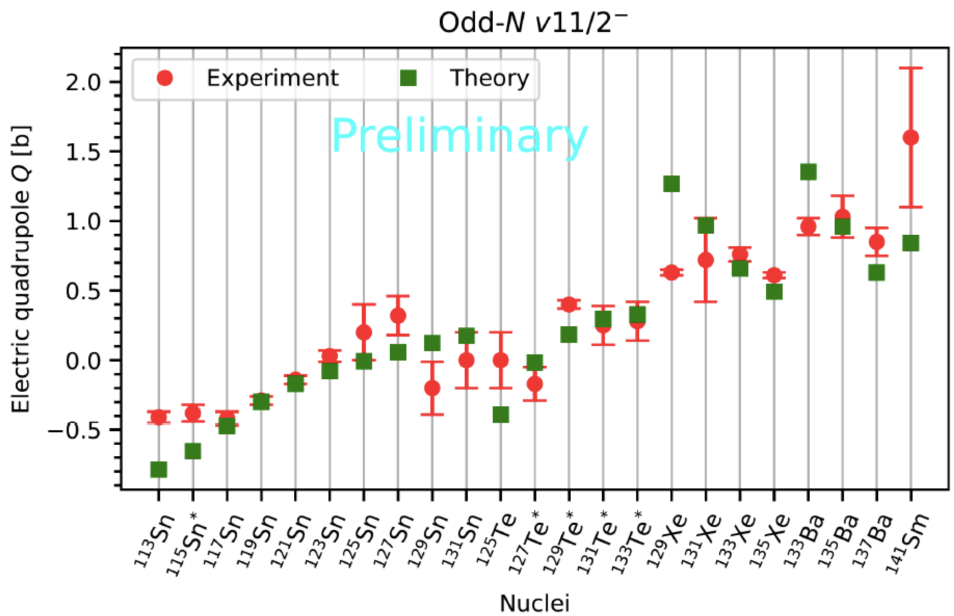
Quadrupole moments: theory vs. experiment



N. J. Stone, *Table of nuclear magnetic dipole and electric quadrupole moments* (2014), INDC, report INDC(NDS)-0658

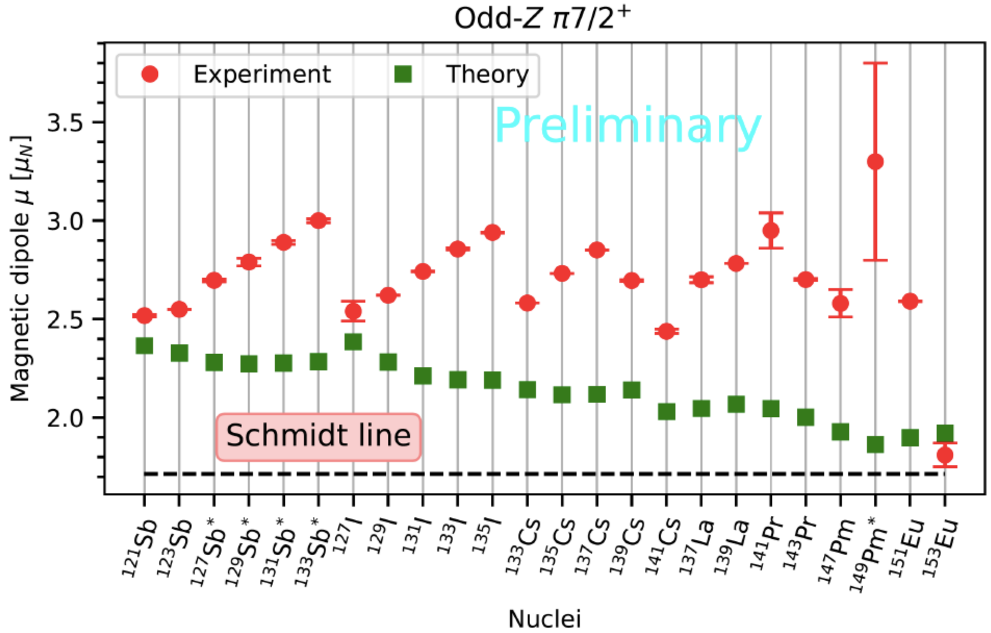
N. J. Stone, *Table of nuclear electric quadrupole moments, ADNDT 111-112*, 1 (2016)



Picture: courtesy H. Wibowo

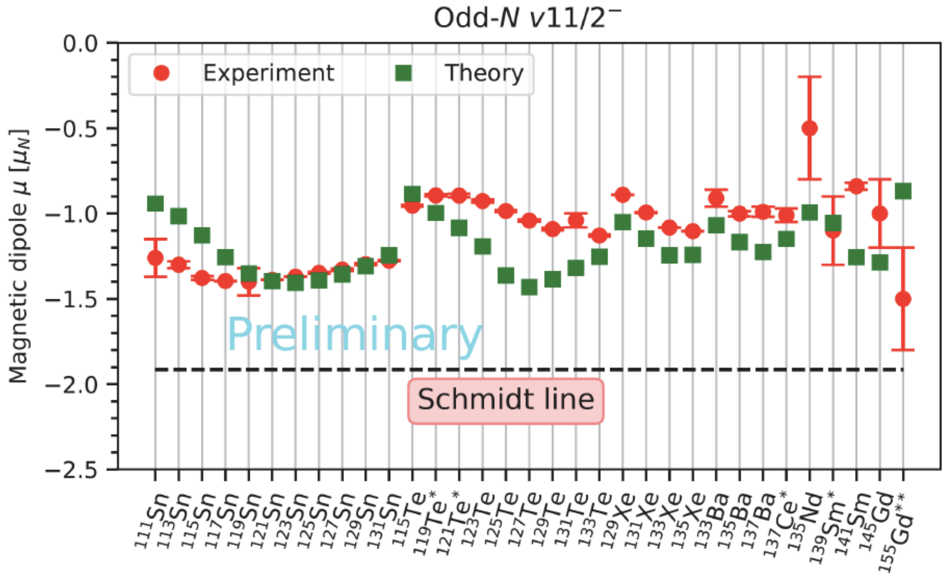
H. Wibowo *et al.*, to be published

Magnetic dipole moments: theory vs. experiment



N. J. Stone, *Table of nuclear magnetic dipole and electric quadrupole moments* (2014), INDC, report INDC(NDS)-0658

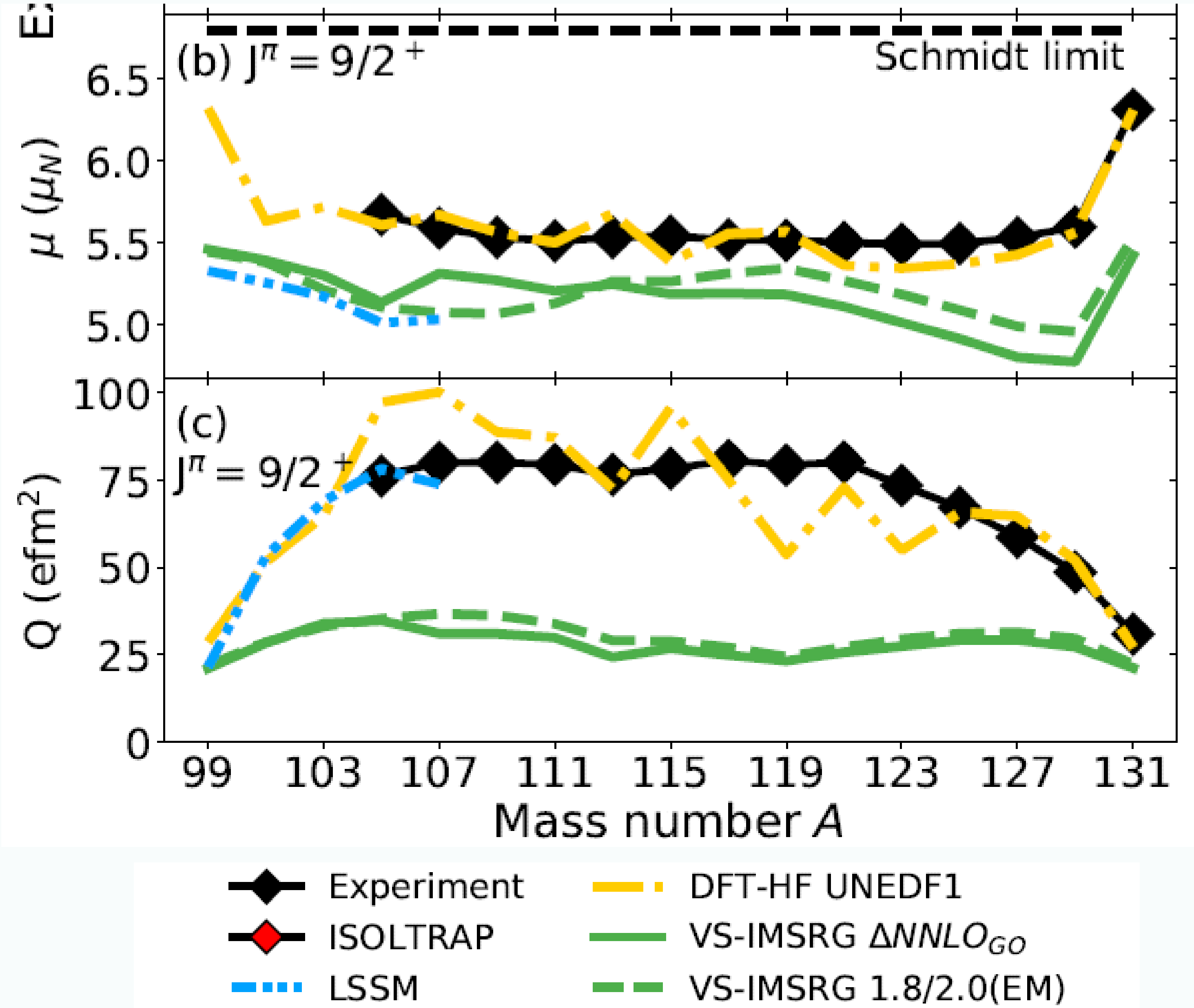
Schmidt lines represent the value of magnetic dipole moment of an odd-mass nucleus which is completely determined by the ℓ and j values of the unpaired nucleon (single-particle model).



Picture: courtesy H. Wibowo

H. Wibowo *et al.*, to be published

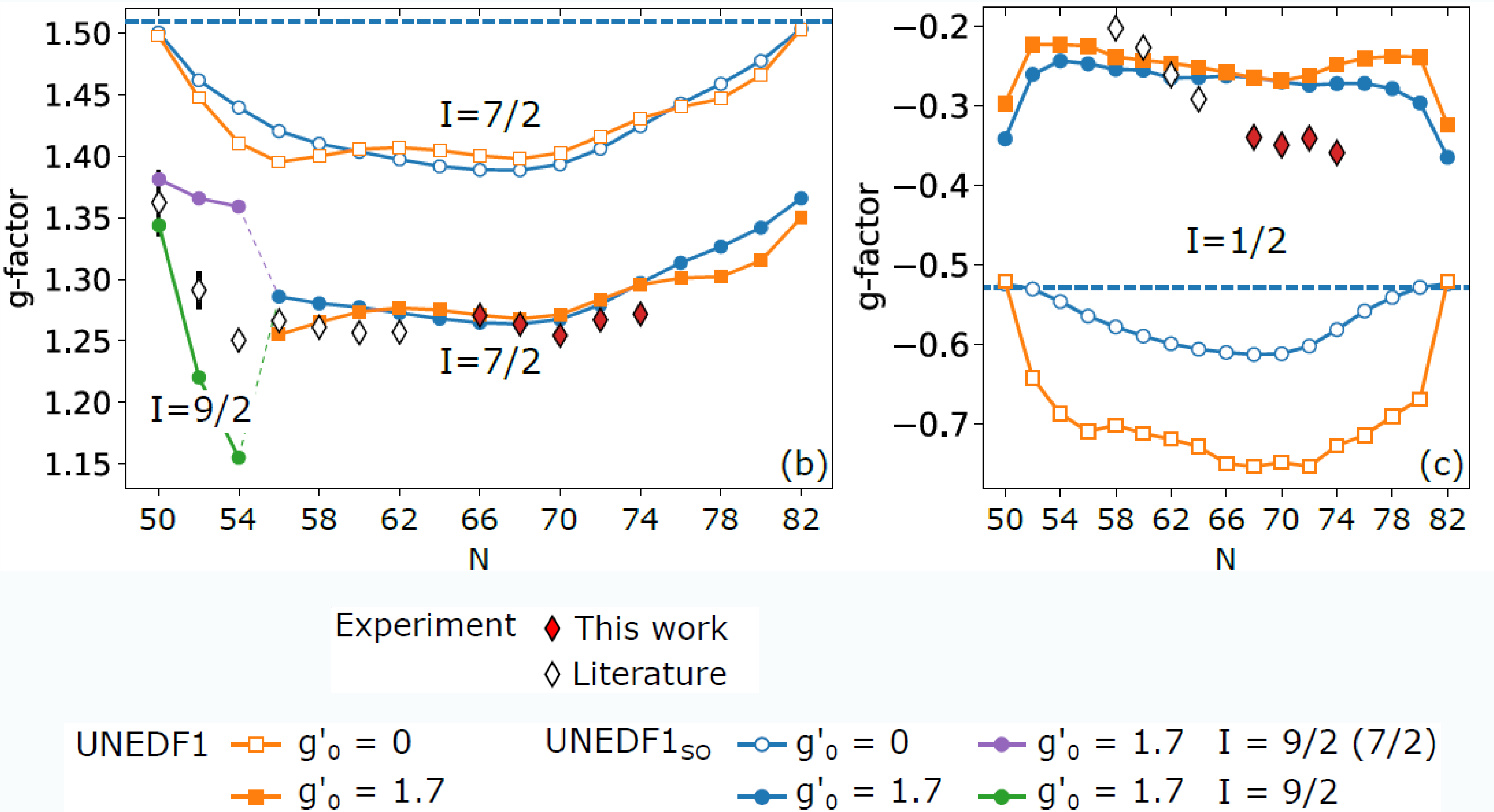
Moments of the 9/2 states in In



A.R. Vernon *et al.*, Nature 607, 260 (2022)

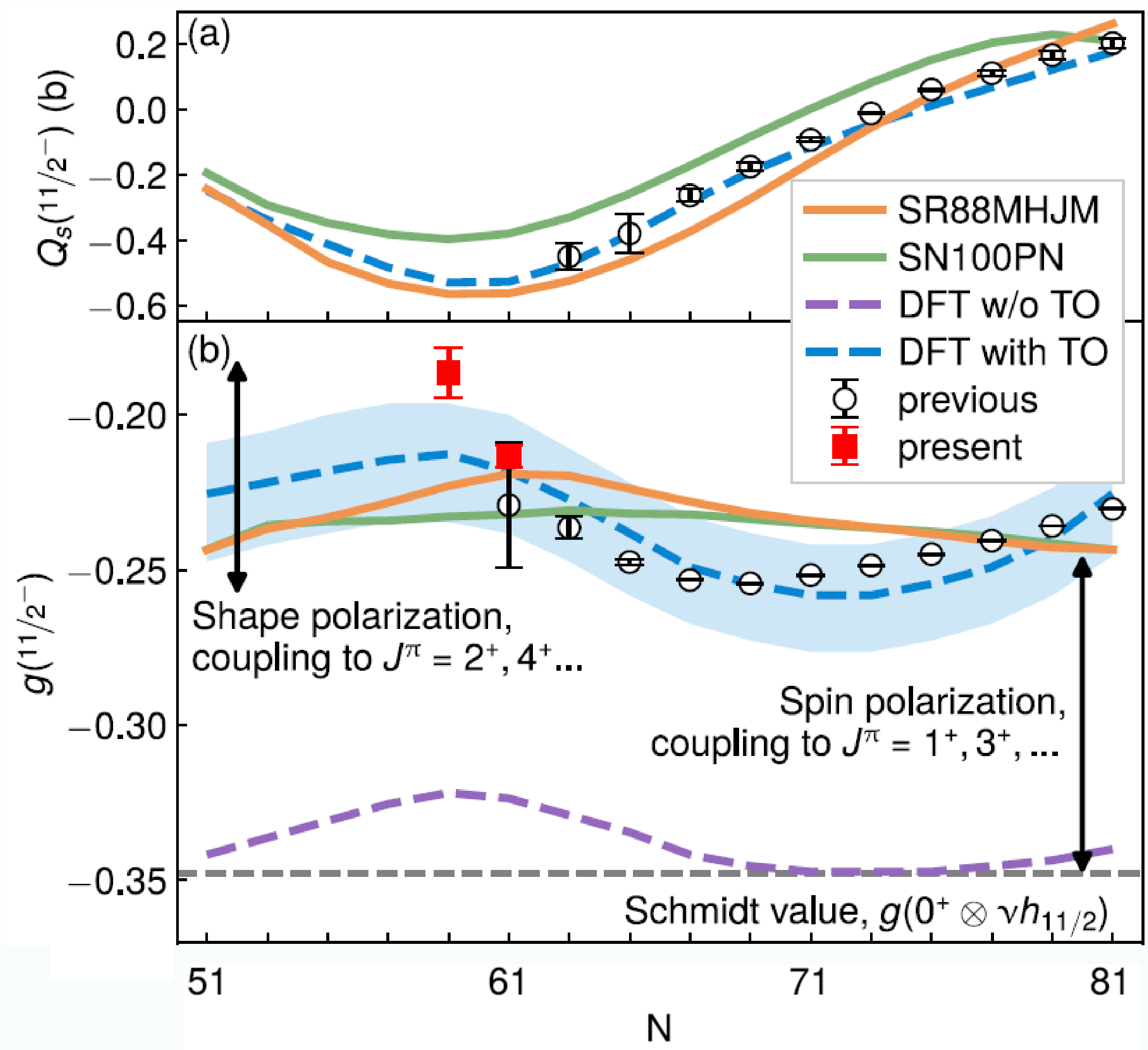
L. Nies *et al.*, Phys. Rev. Lett. 131, 022502 (2023)

Moments of the 1/2, 7/2 & 9/2 states in Ag



R. P. de Groote *et al.*, submitted to Phys. Lett. B

Moments of the $\nu h_{11/2}$ isomers in Sn



$g = \mu/I$

T.J. Gray *et al.*, Phys. Lett. B 847 (2023) 138268

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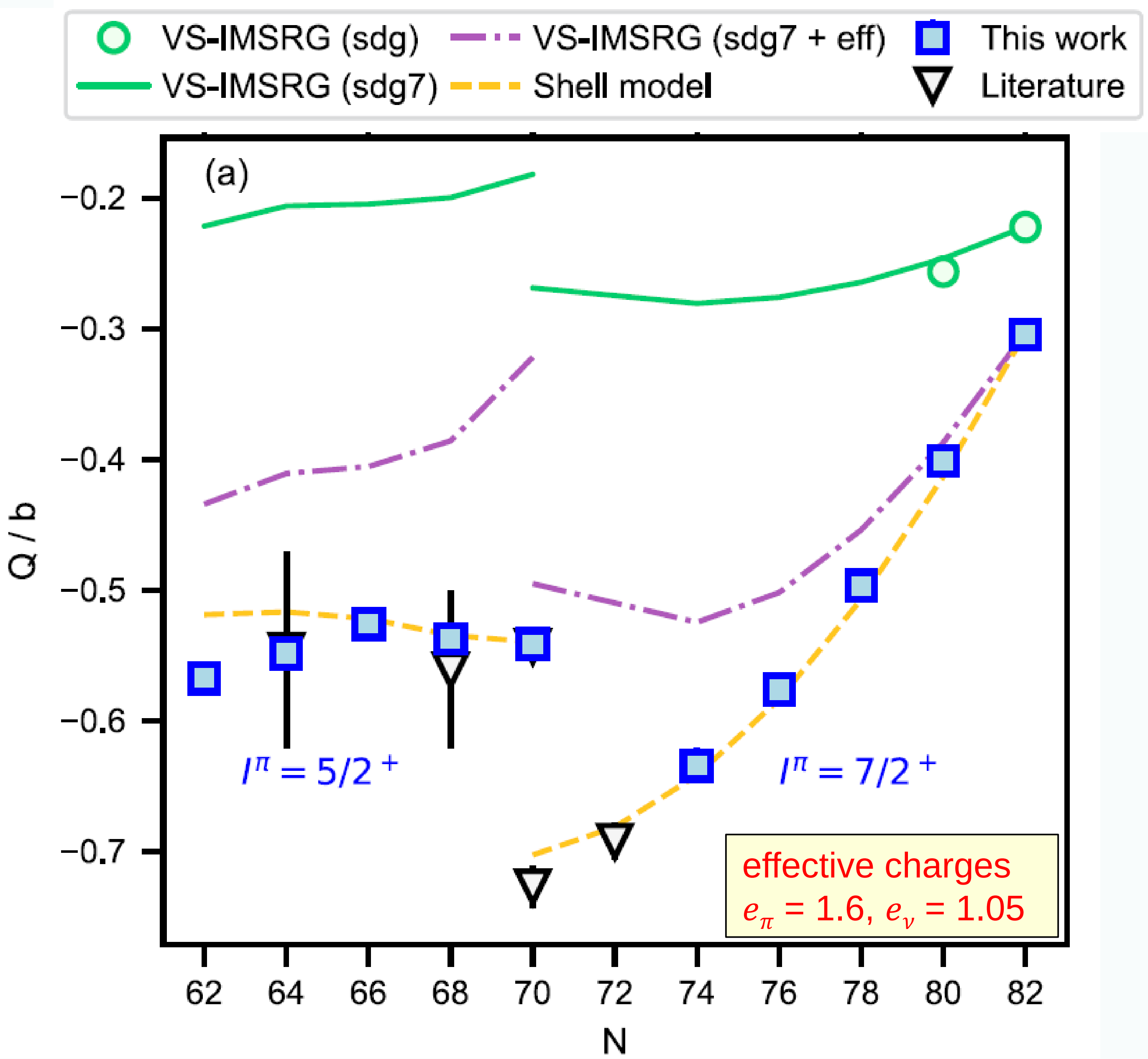
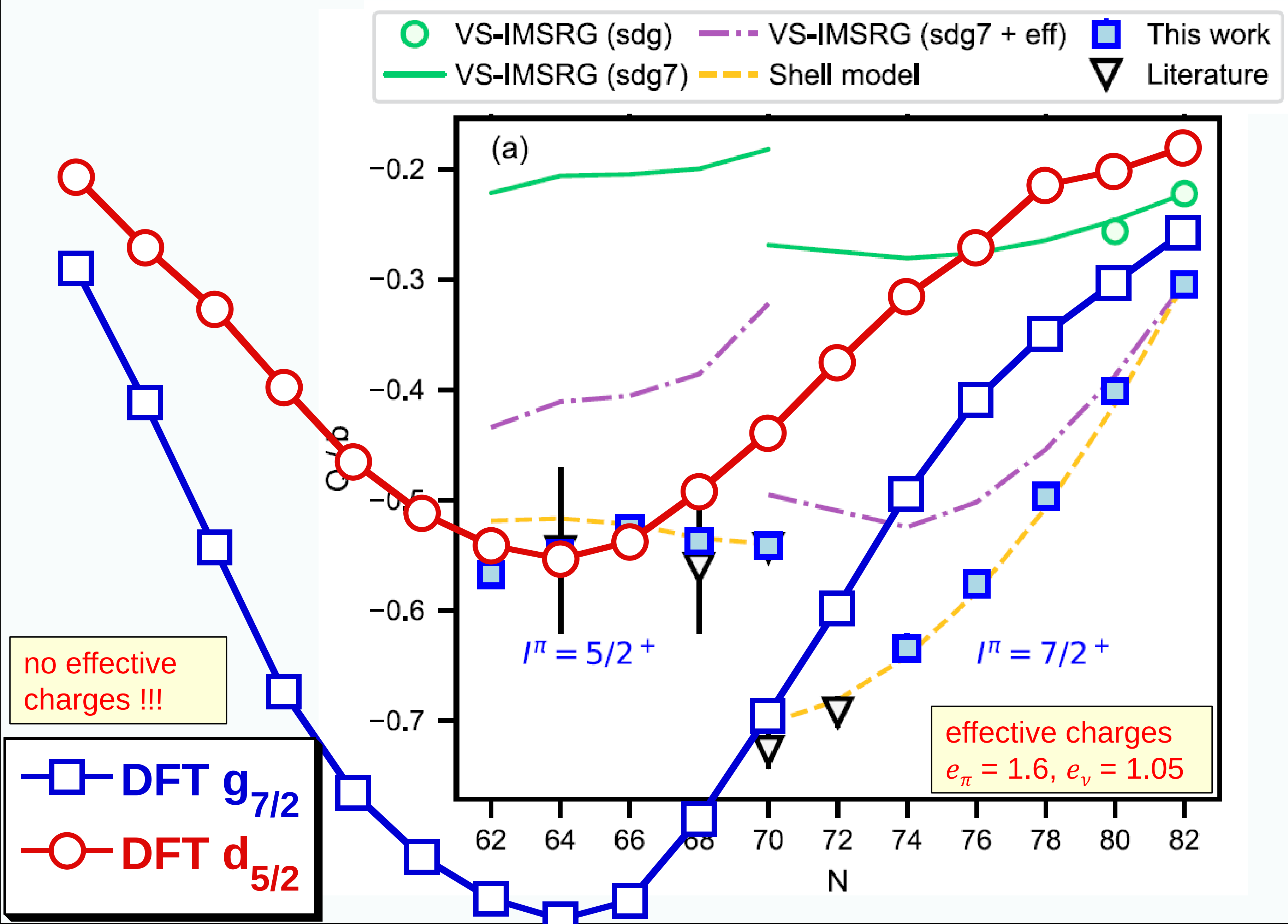
Quadrupole moments in Sb



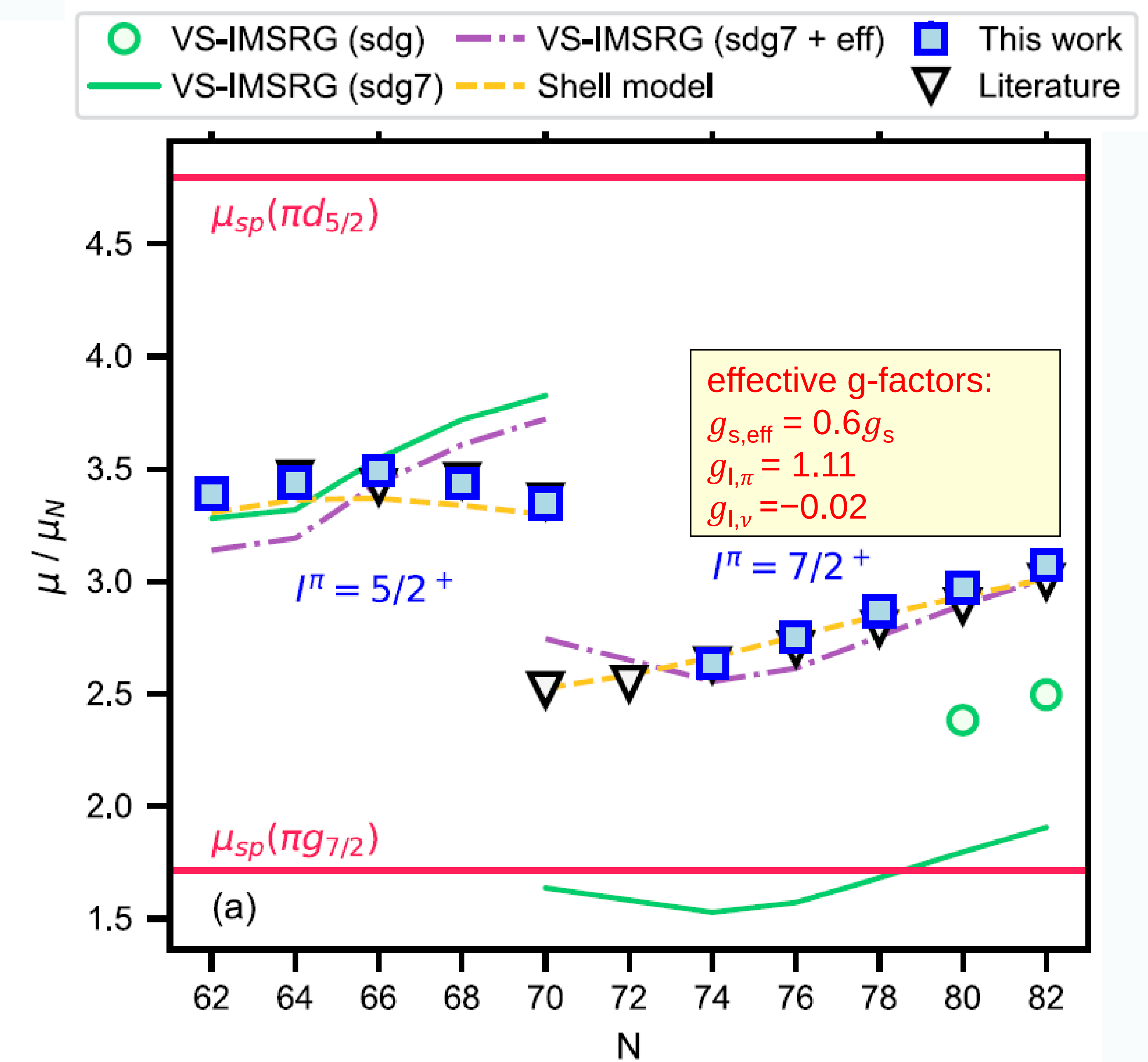
S. Lechner *et al.*, Phys. Lett. B 847 (2023) 138278

Quadrupole moments in Sb



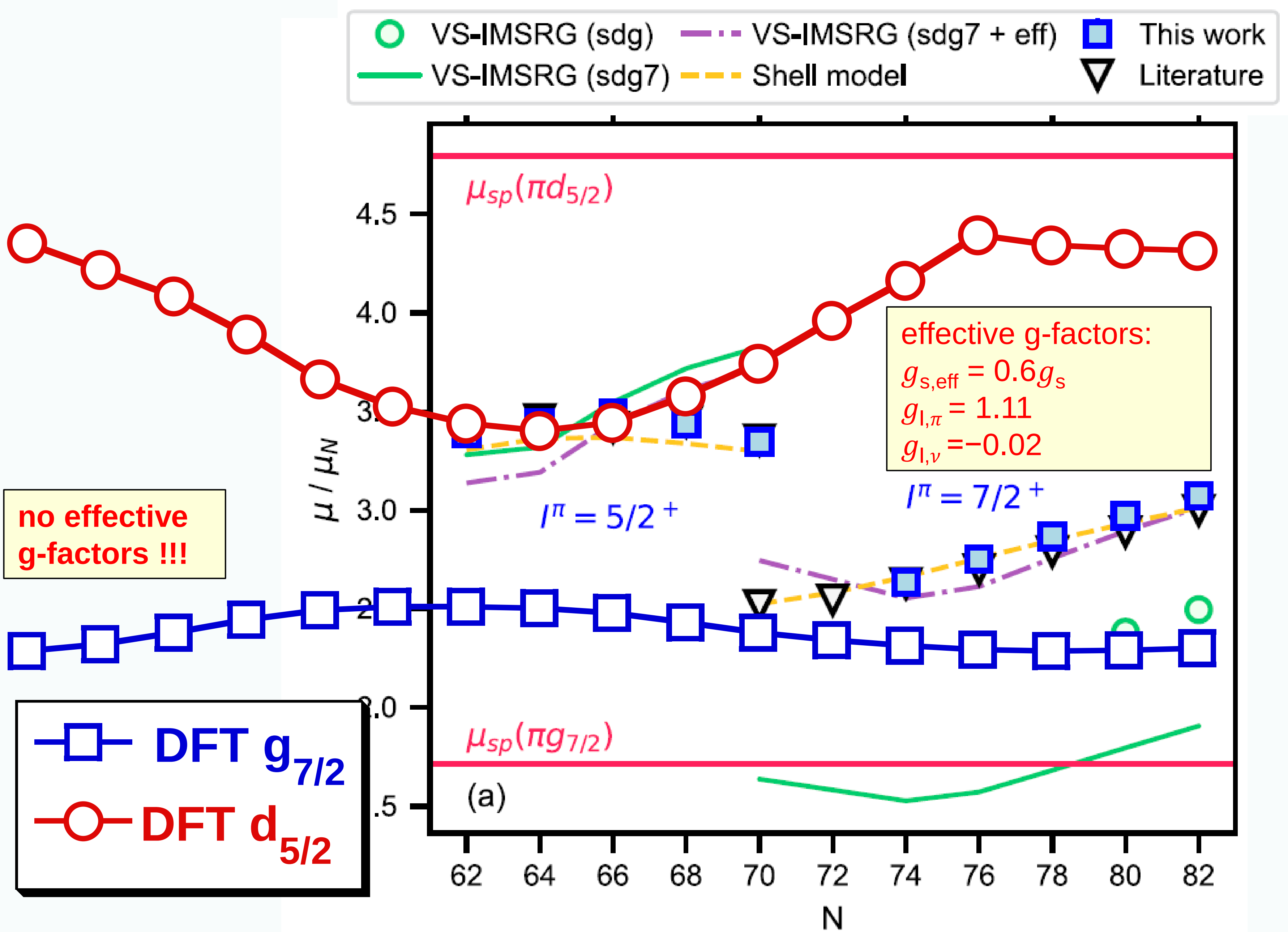
S. Lechner *et al.*, Phys. Lett. B 847 (2023) 138278

Magnetic dipole moments in Sb



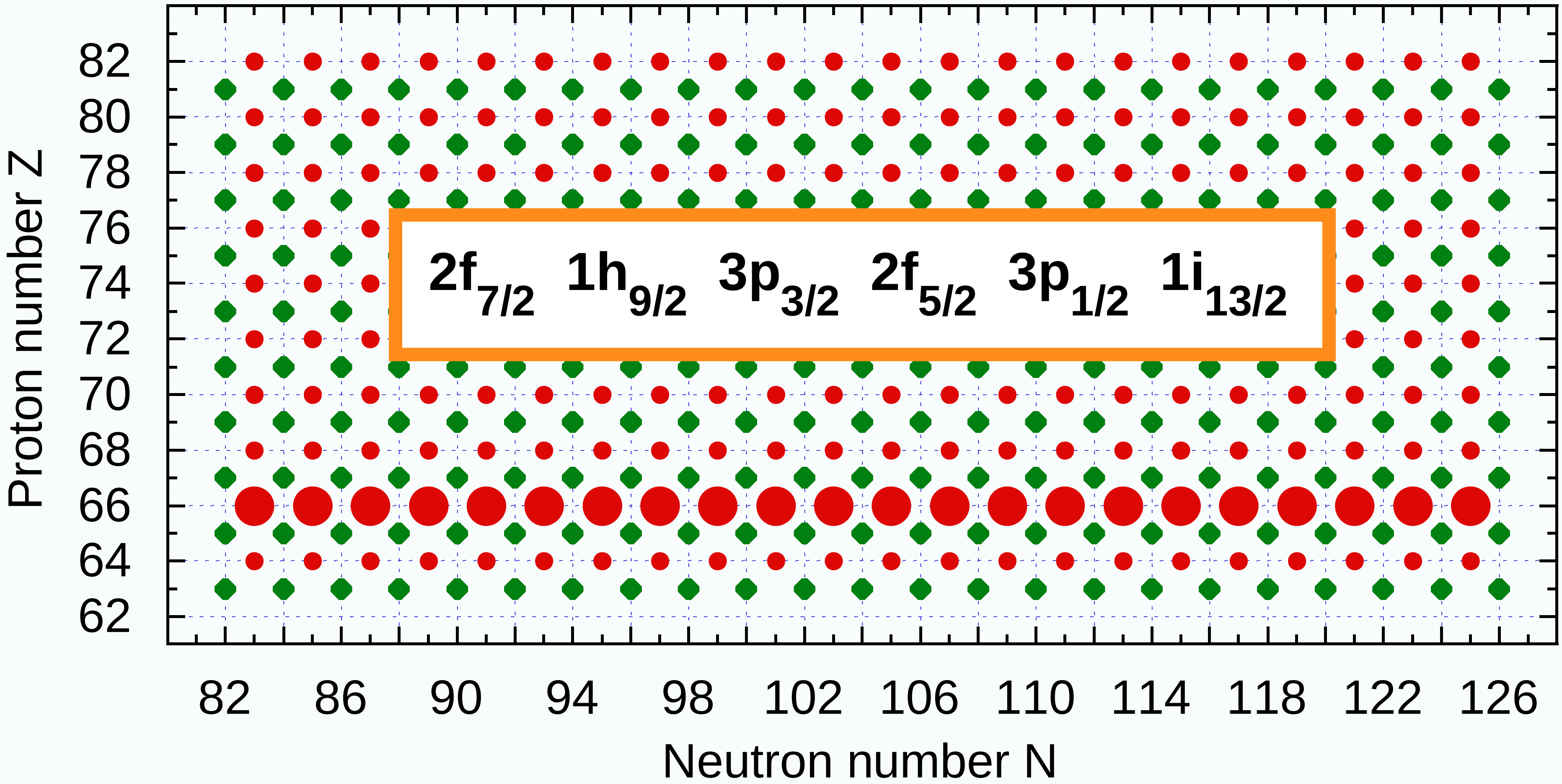
S. Lechner *et al.*, Phys. Lett. B 847 (2023) 138278

Magnetic dipole moments in Sb



S. Lechner *et al.*, Phys. Lett. B 847 (2023) 138278

The first systematic nuclear-DFT analysis of the electromagnetic moments in excited quasiparticle states



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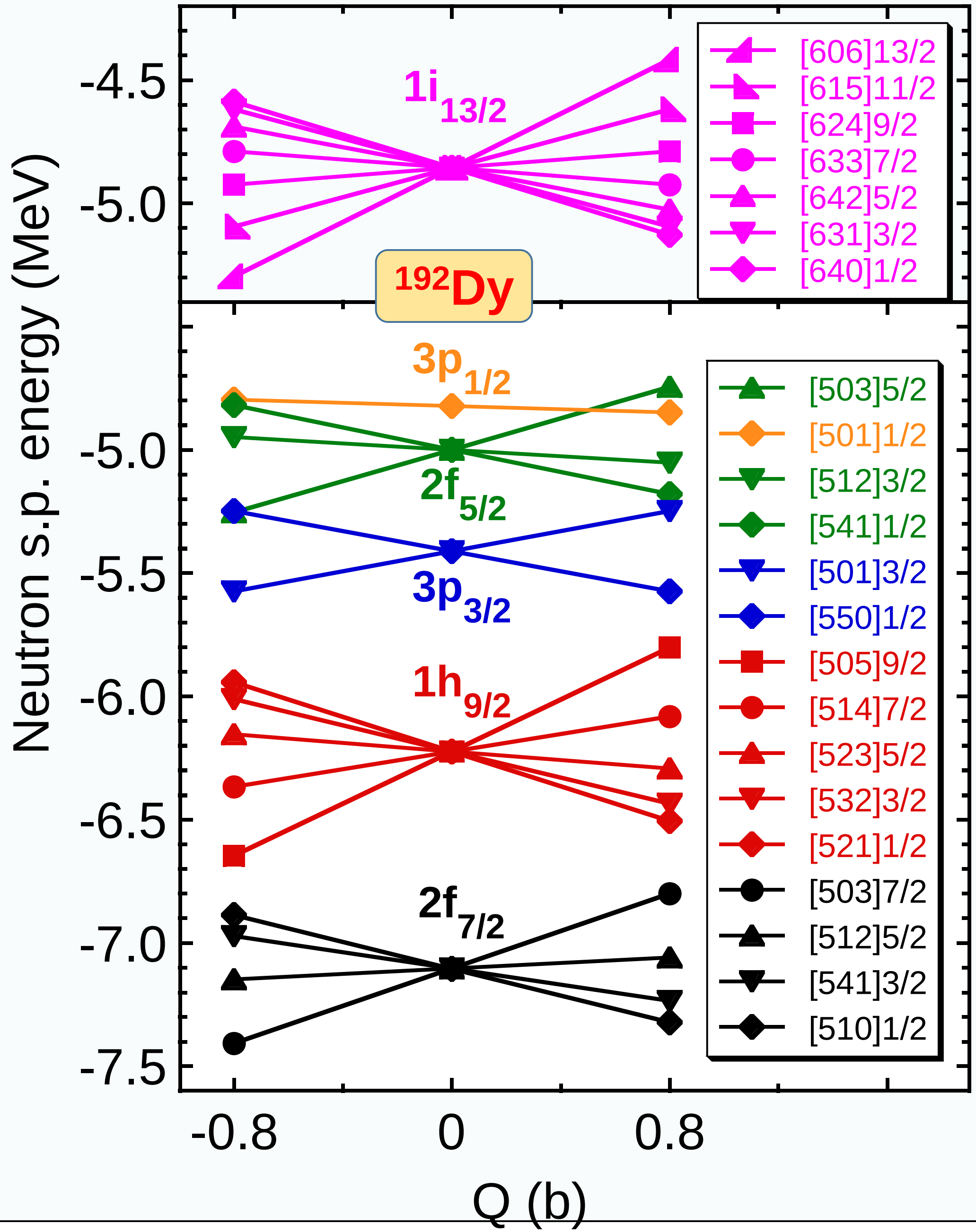
How to calculate odd nuclei in nuclear DFT?



without pairing

A even, $p > A$, $h \leq A$

$$|\Psi\rangle^{\text{even}}_{\text{HF}} = a^+_A \ldots a^+_2 a^+_1 |0\rangle$$

$$|\Psi\rangle^{\text{odd}}_{\text{HF}} = \begin{cases} a^+_p |\Psi\rangle^{\text{even}}_{\text{HF}} \\ a_h |\Psi\rangle^{\text{even}}_{\text{HF}} \end{cases}$$

with pairing

$$|\Psi\rangle^{\text{even}}_{\text{HFB}} = \prod_{\mu>0} \left(u_\mu + v_\mu a^+_{\bar{\mu}} a^+_\mu\right) |0\rangle$$

$$|\Psi\rangle^{\text{odd}}_{\text{HFB}} = \beta^+_\nu |\Psi\rangle^{\text{even}}_{\text{HFB}}$$

$$= a^+_\nu \prod_{\nu\neq\mu>0} \left(u_\mu + v_\mu a^+_{\bar{\mu}} a^+_\mu\right) |0\rangle$$

tagging quasiparticle states

$$\max_\mu \left\{ \langle \varphi_\nu | \phi^{\text{upper}}_\mu \rangle, \langle \varphi_\nu | \phi^{\text{lower}}_\mu \rangle \right\}$$

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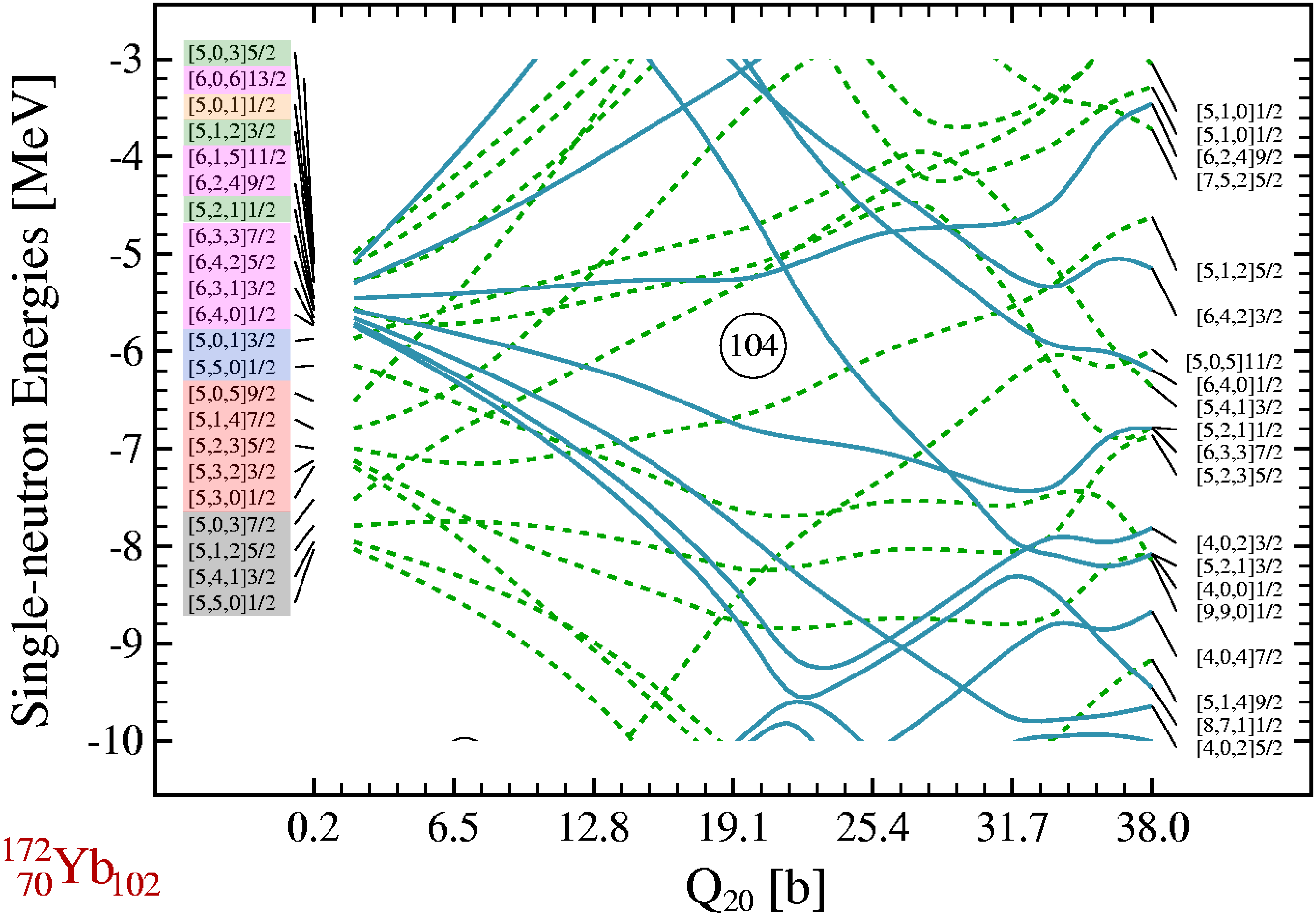

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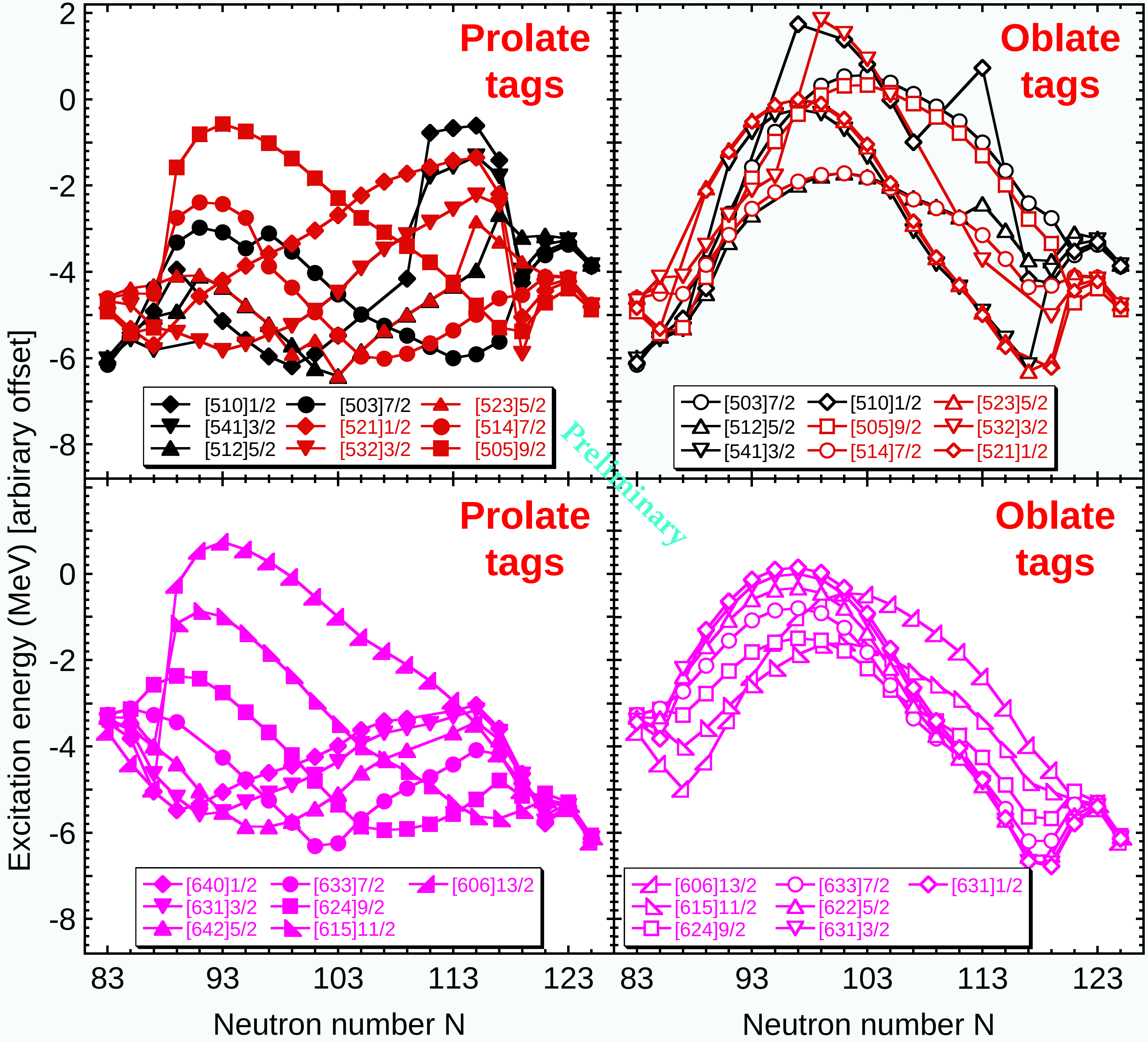
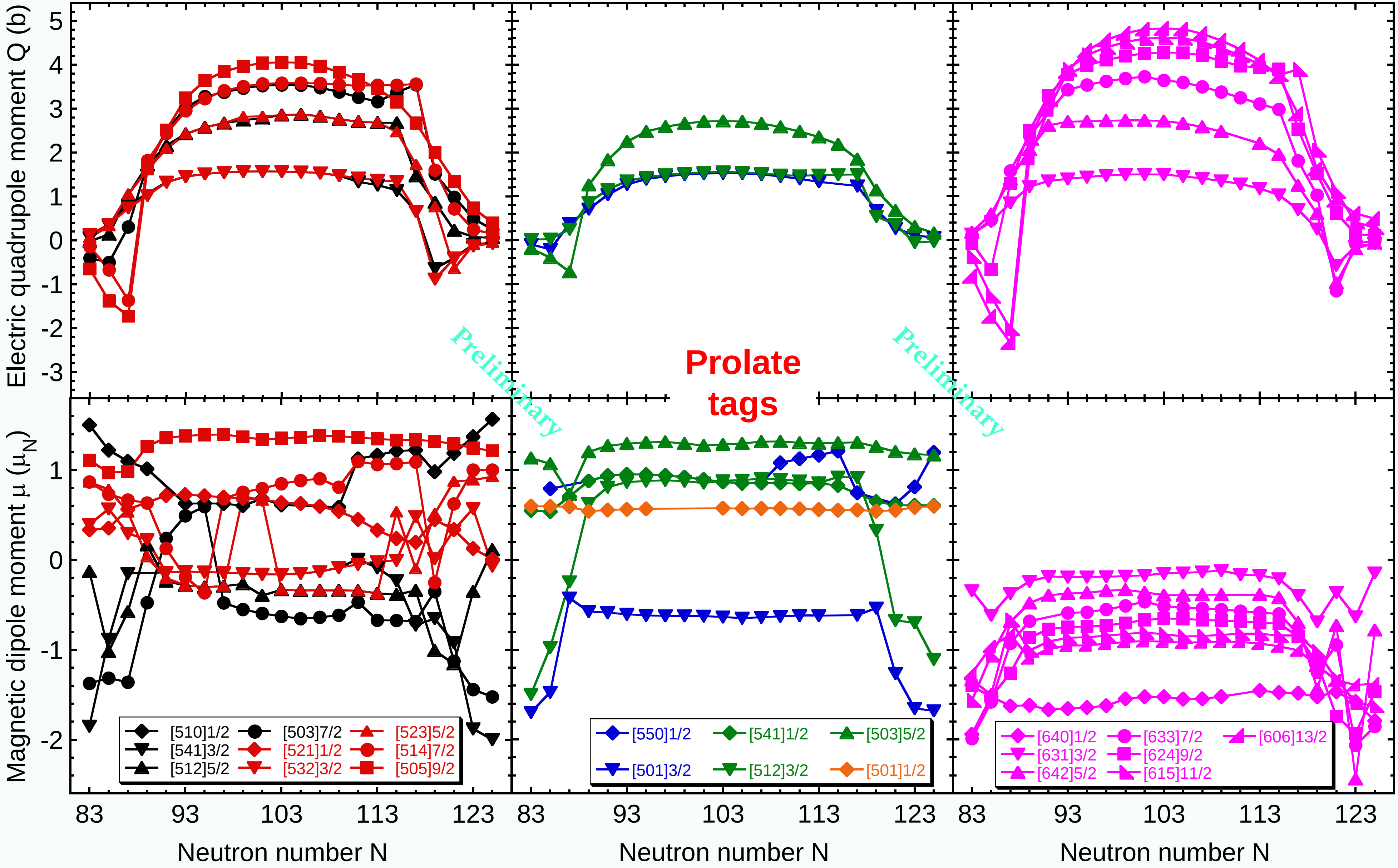
Excitation energies of odd dysprosium isotopes



Electromagnetic moments of odd dysprosium isotopes



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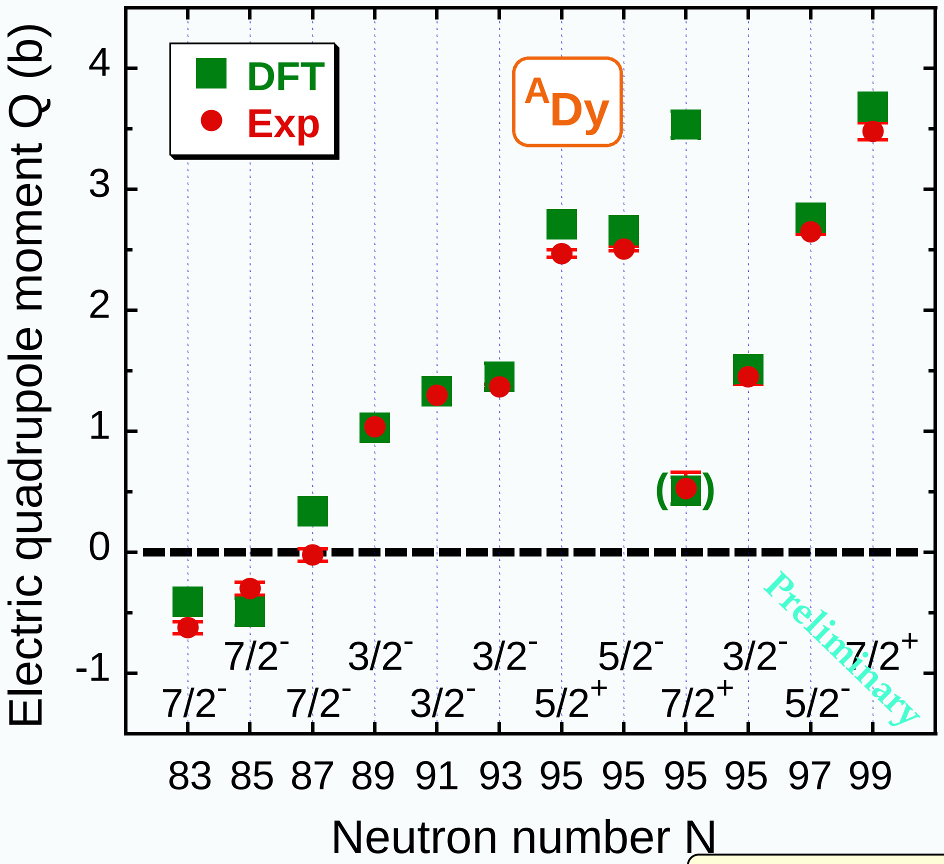
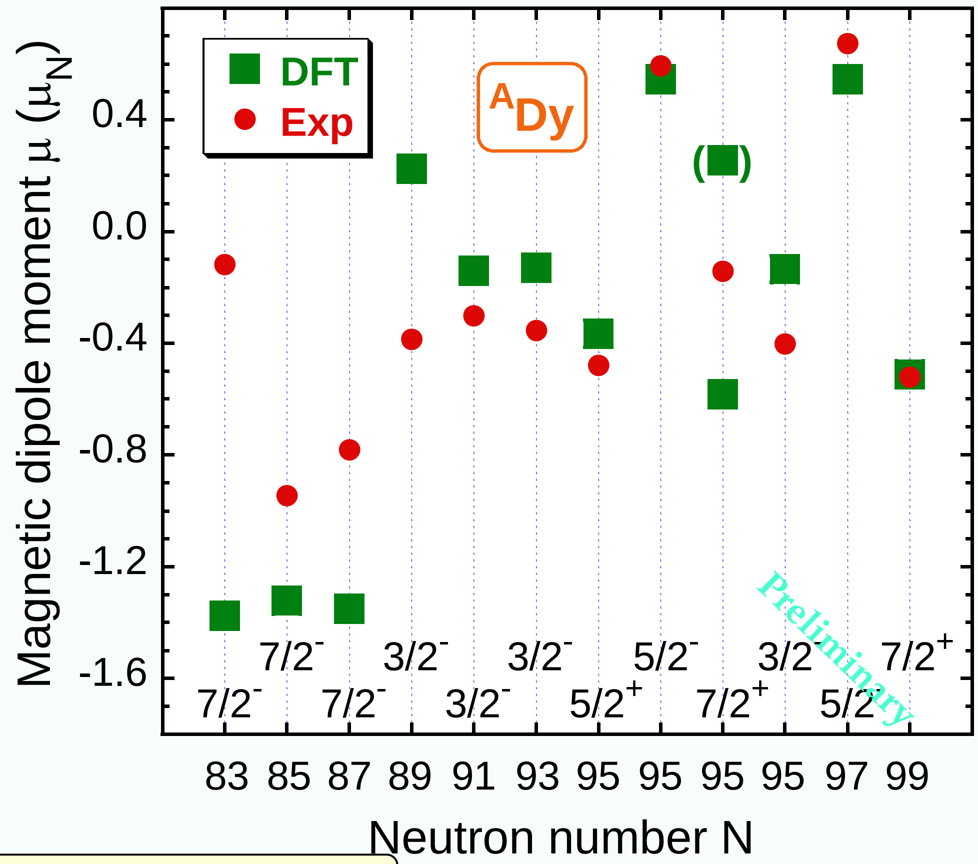
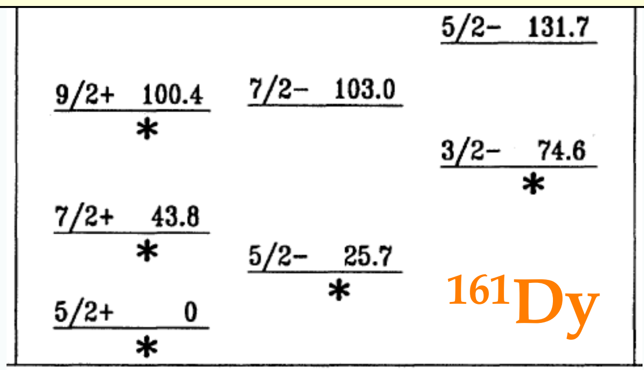
Electromagnetic moments of odd dysprosium isotopes





S. J. Margraf *et al.*, Phys. Rev. C52, 2429 (1995)



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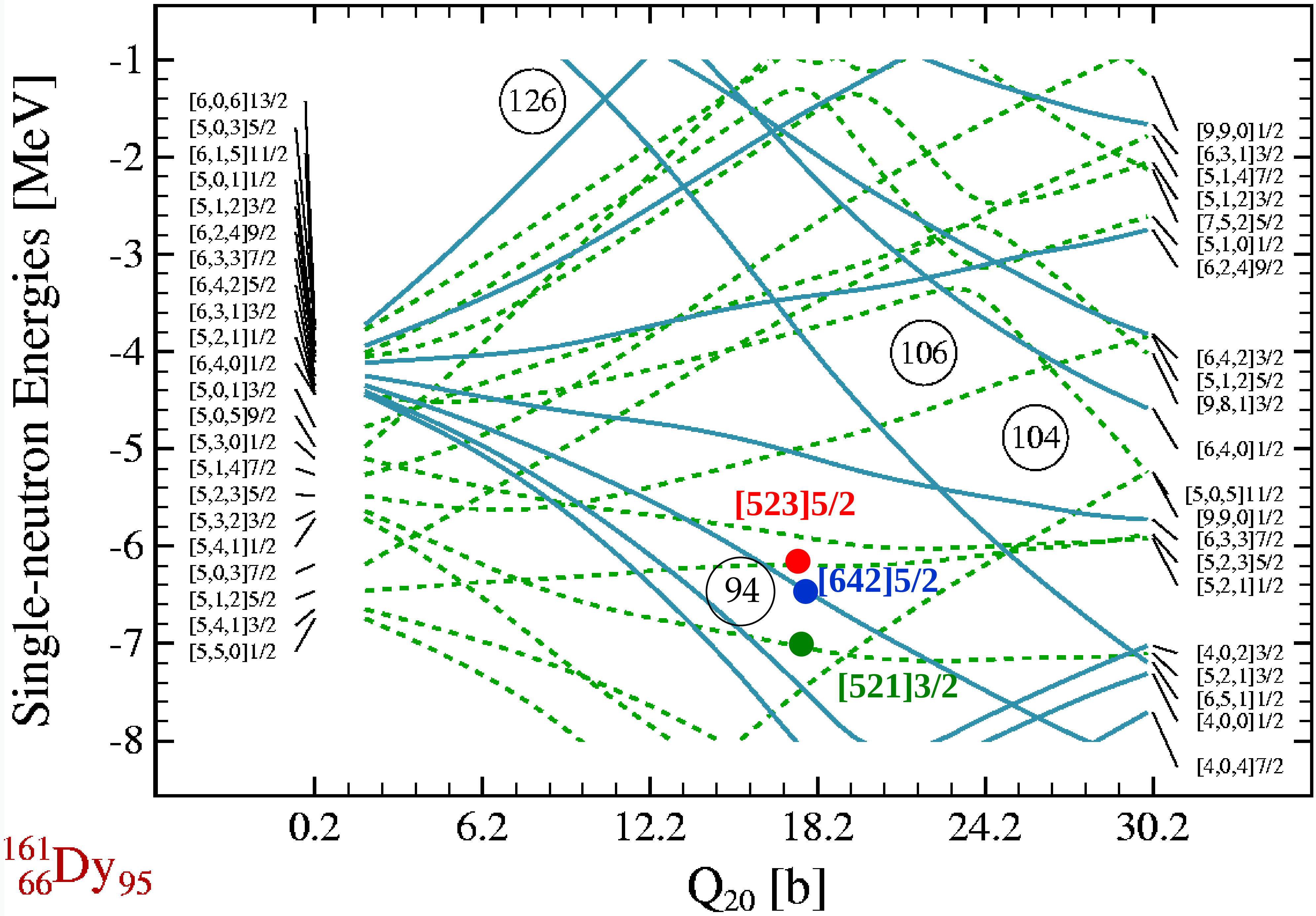

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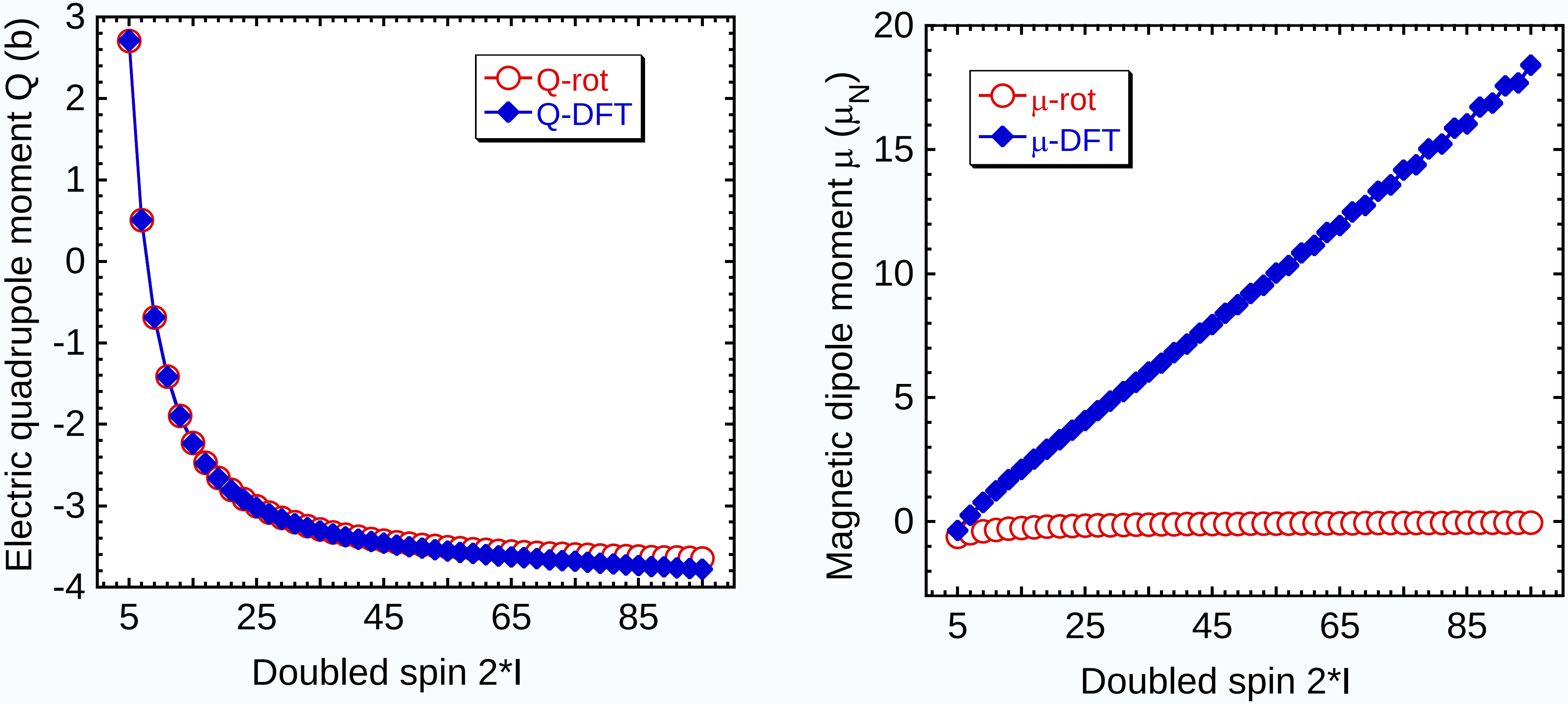
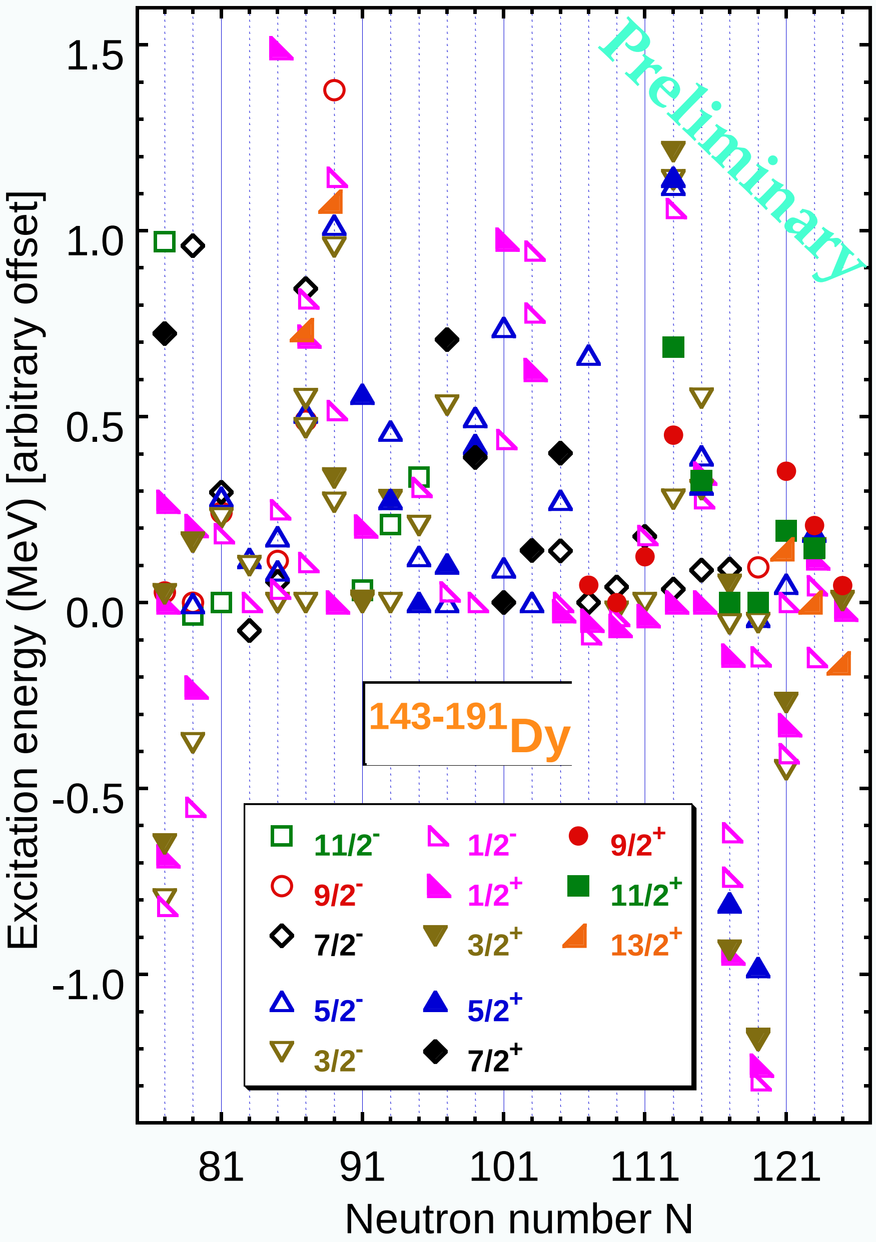
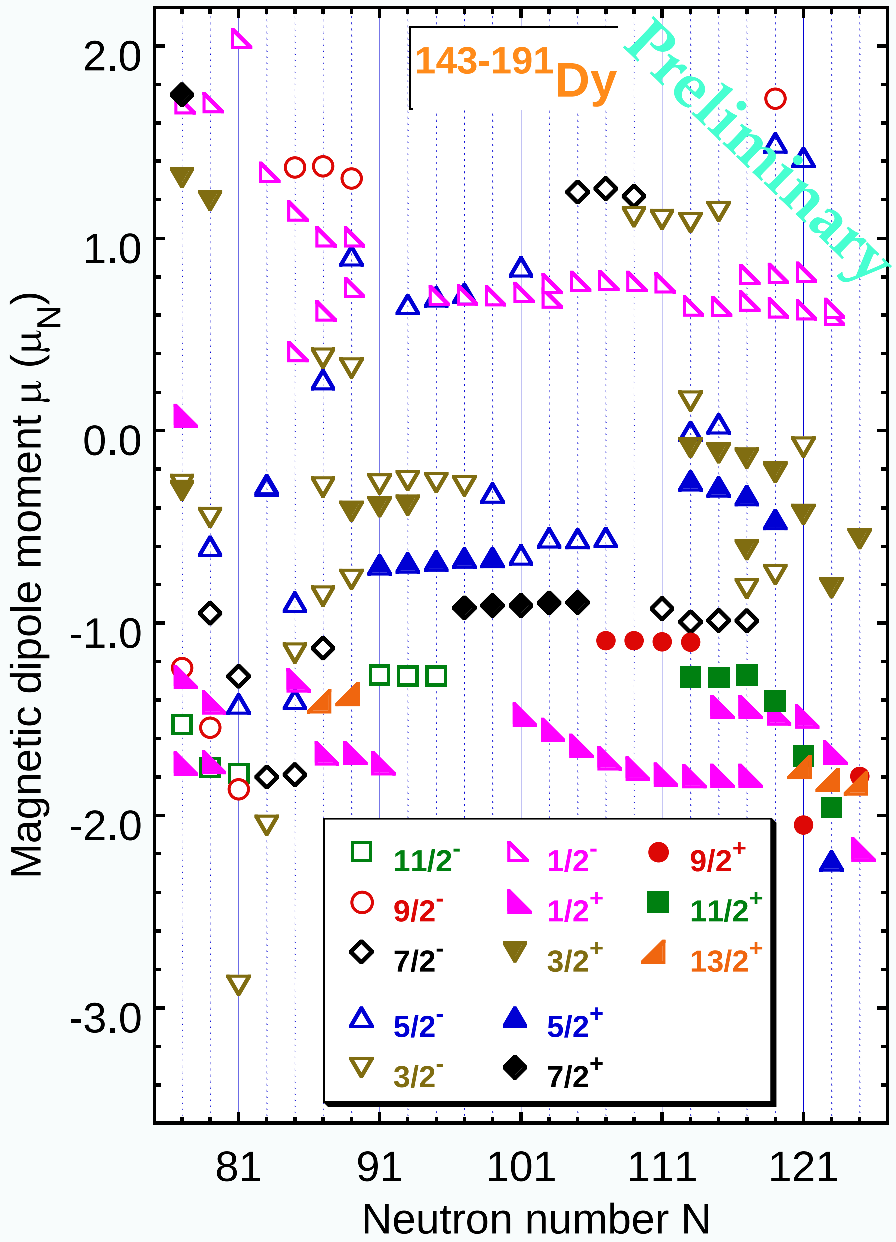
Electromagnetic moments – rigid-rotor approximation



Excitation energies & magnetic dipole moments of odd dysprosium isotopes





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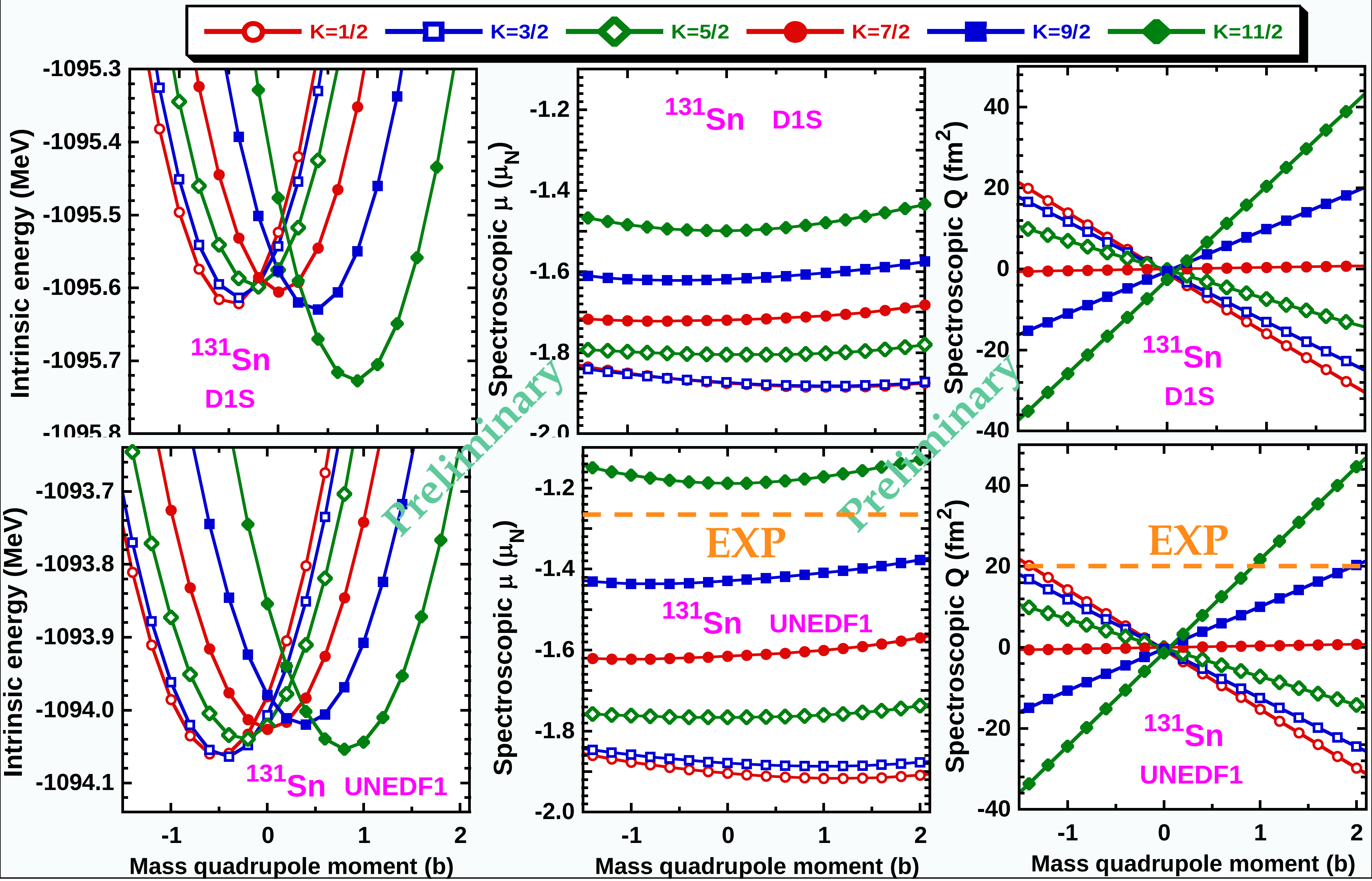
K-mixing



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Energies of the K-mixed states

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******************************************************************************
*                                                                            *
*                  RESULTS OF THE MULTI-REFERENCE CALCULATION                *
*                                                                            *
******************************************************************************
*   SPIN   N    EIG_OVERLAP    EIG_ENERGY   |                                *
*   ----   -    -----------    ----------   |                                *
*   11/2   1    5.979982E+00 -1092.439526 |                                  *
*   11/2   2    1.575148E-02 -1083.008302 |                                  *
*   11/2   3    2.225877E-03 -1080.289292 |                                  *
*   11/2   4    1.132094E-03 -1078.423819 |                                  *
*   11/2   5    6.412910E-04 -1069.869511 |                                  *
*   11/2   6    2.674966E-04 -1067.359363 |                                  *
******************************************************************************

E_intrinsic(11/2) = -1092.055162
E_projected(11/2) = -1092.310241
```

Preliminary

What’s next to consider	
Segré chart of electromagnetic moments	
Electromagnetic moments of odd-odd nuclei	★
More advanced functionals	★
Octupole deformation	
Triaxiality	★
Configuration interaction	
K-mixing	★★
Quadrupole/octupole collectivity	
Two-body meson-exchange currents	★★

Thank you