



Electromagnetic moments in heavy deformed open-shell odd nuclei

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Fundamental Physics with Radioactive Molecules
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The bottom line

**The nuclear electromagnetic moments
are all about:**

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



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Outline

1. Methodology*
2. Gd-Pb*
3. Dy-Os
4. Sn-Gd
5. In*
6. Ag*
7. Sn*
8. Sb
9. What next?
10. Two-body currents
11. K-mixing
12. Octupole vibration ^{171}Yb

***published**



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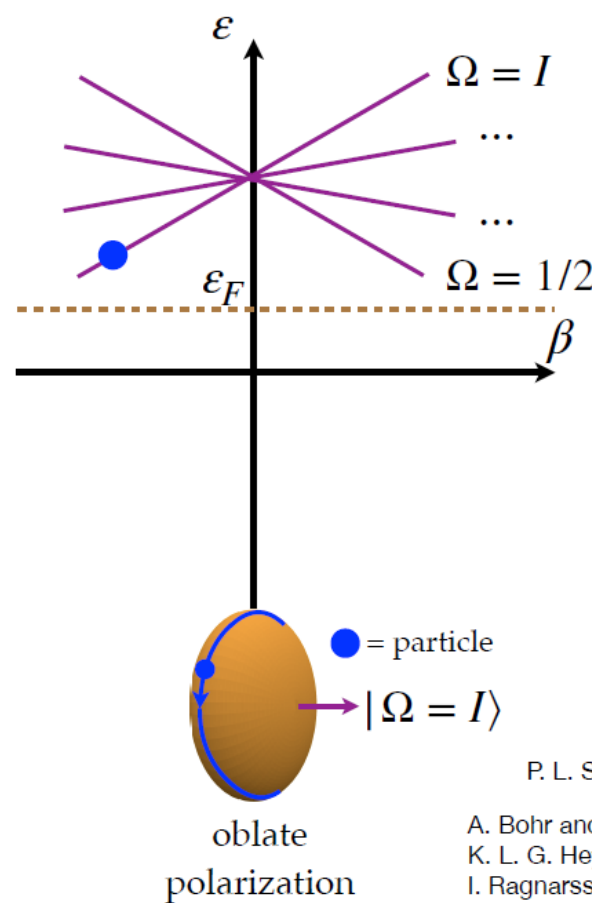
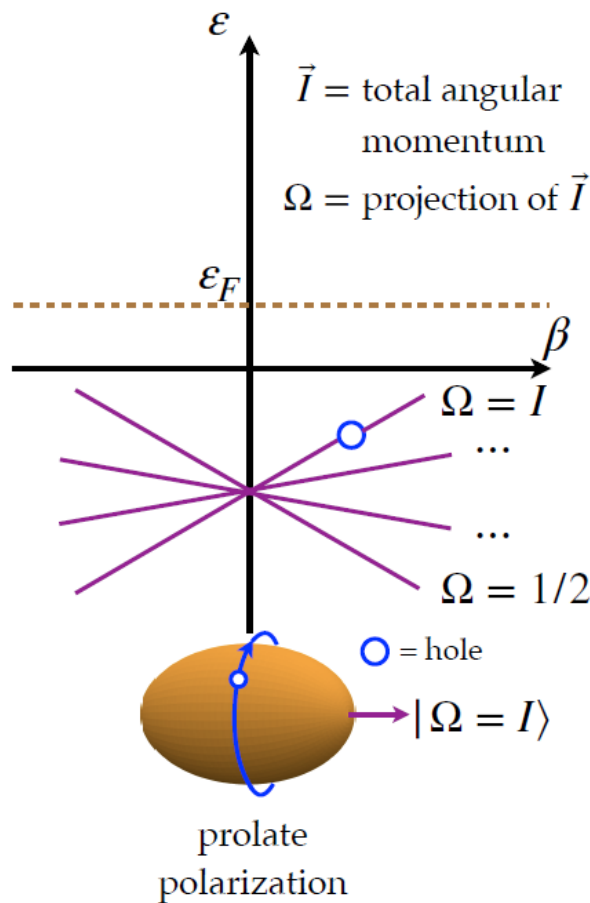


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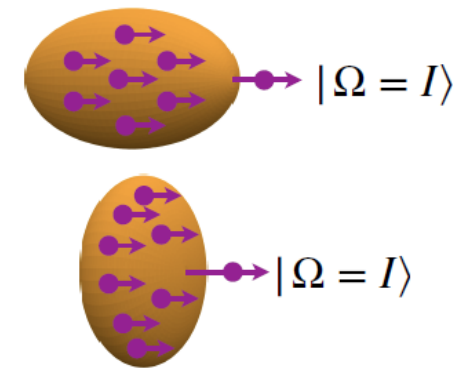


2

Shape and spin core polarizations



Spin polarization



Landau parameter g'_0 ($g'_0 = 1.7$)

$$g'_0 = N_0 (2C_1^S + 2C_1^T (3\pi^2 \rho_0 / 2)^{2/3})$$

$$\frac{1}{N_0} \approx 150 \frac{m}{m^*} \text{ MeV} \cdot \text{fm}^3$$

P. L. Sassarini et al., *J. Phys. G: Nucl. Part. Phys.* **49**, 11LT01 (2022)

A. Bohr and B. R. Mottelson, *Nuclear Structure* Vol. 1

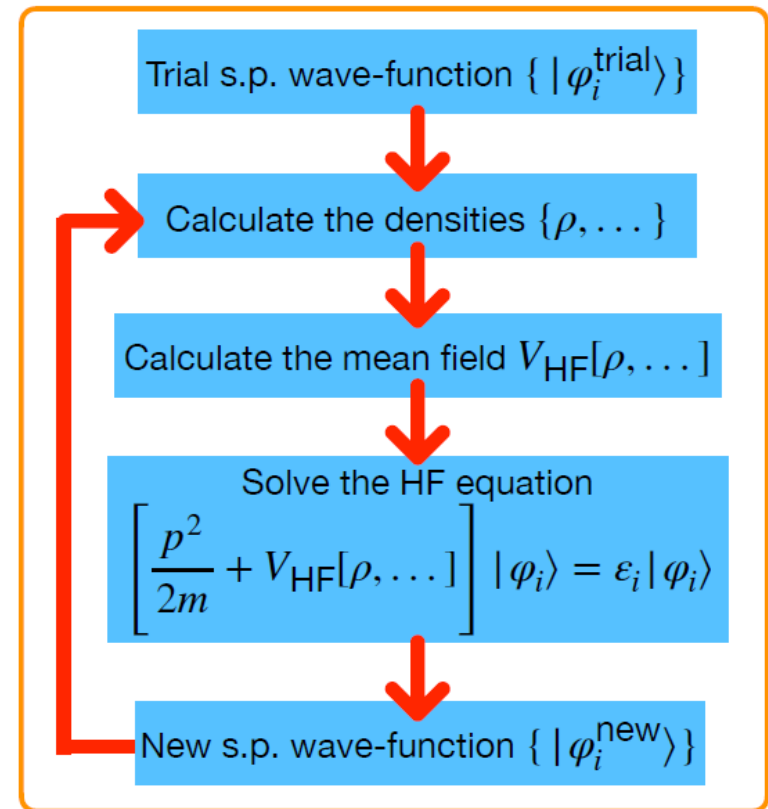
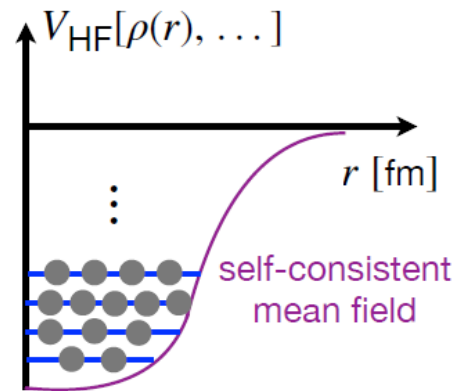
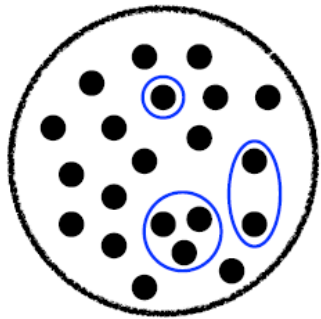
K. L. G. Heyde, *The Nuclear Shell Model*

I. Ragnarsson and S. G. Nilsson, *Shapes and Shells in Nuclear Structure*



1

Nuclear density functional theory



Energy density functional
 $\mathcal{E}[\rho(\mathbf{r}), \mathbf{s}(\mathbf{r}), \boldsymbol{\tau}(\mathbf{r}), \mathbf{T}(\mathbf{r}), \mathbf{j}(\mathbf{r}), \vec{J}(\mathbf{r})]$

Coupling constants

T-even : $C_t^\rho, C_t^{\Delta\rho}, C_t^\tau, C_t^J, C_t^{\nabla J}$

T-odd : $C_t^s, C_t^{\Delta s}, C_t^T, C_t^j, C_t^{\nabla j}$

Parametrization: UNEDF1

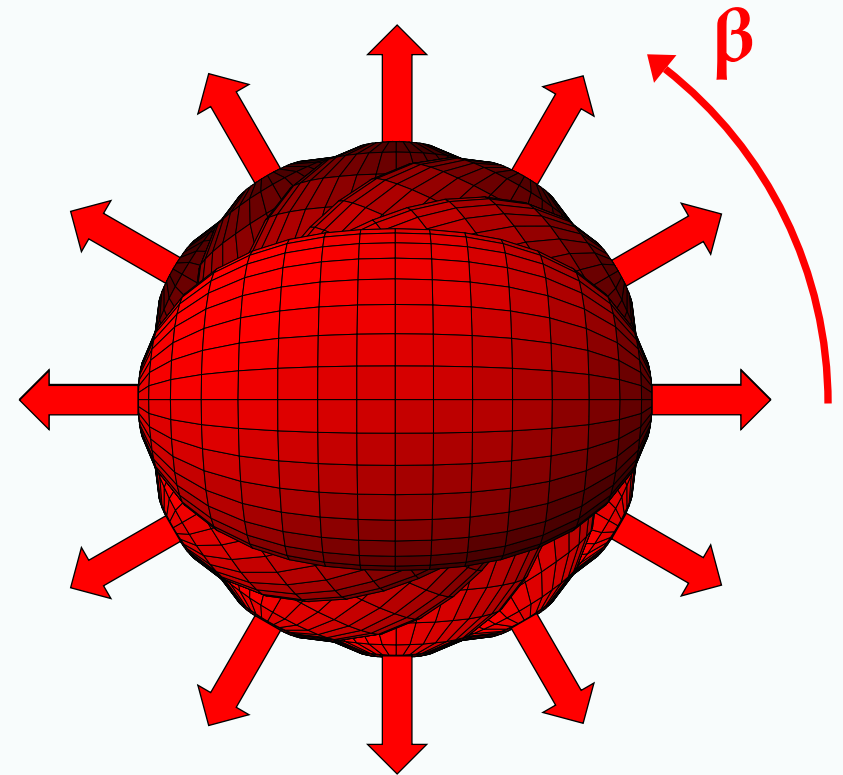
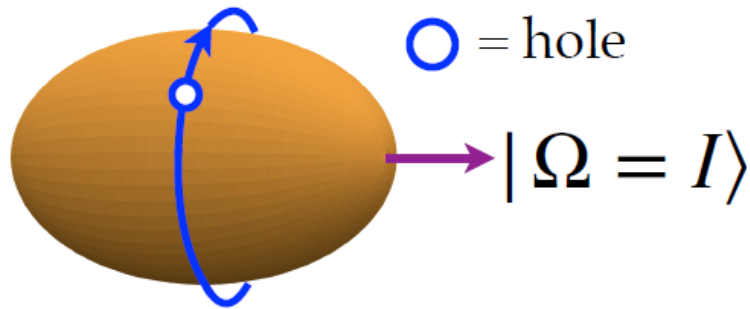
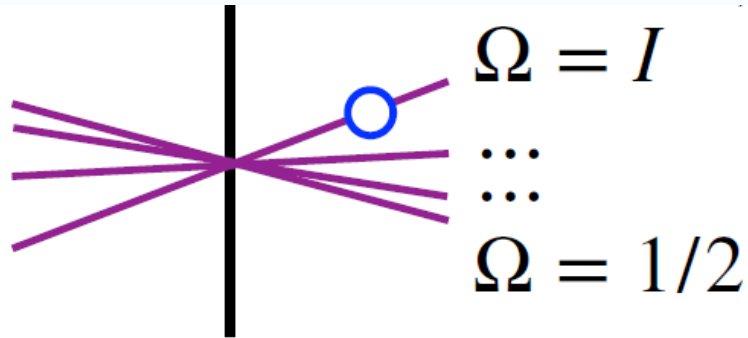
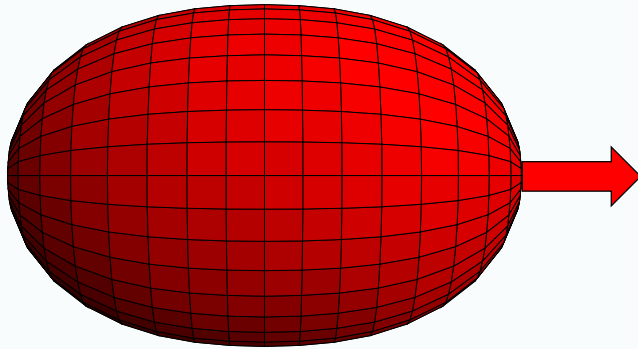
Hartree-Fock
(HF)
equation

M. Kortelainen et al., Phys. Rev. C 85, 024304 (2012)



Time-odd spin alignment & symmetry restoration

**“Intrinsic”
Symmetry broken**



**“Laboratory”
Symmetry restored**

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

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



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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*

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

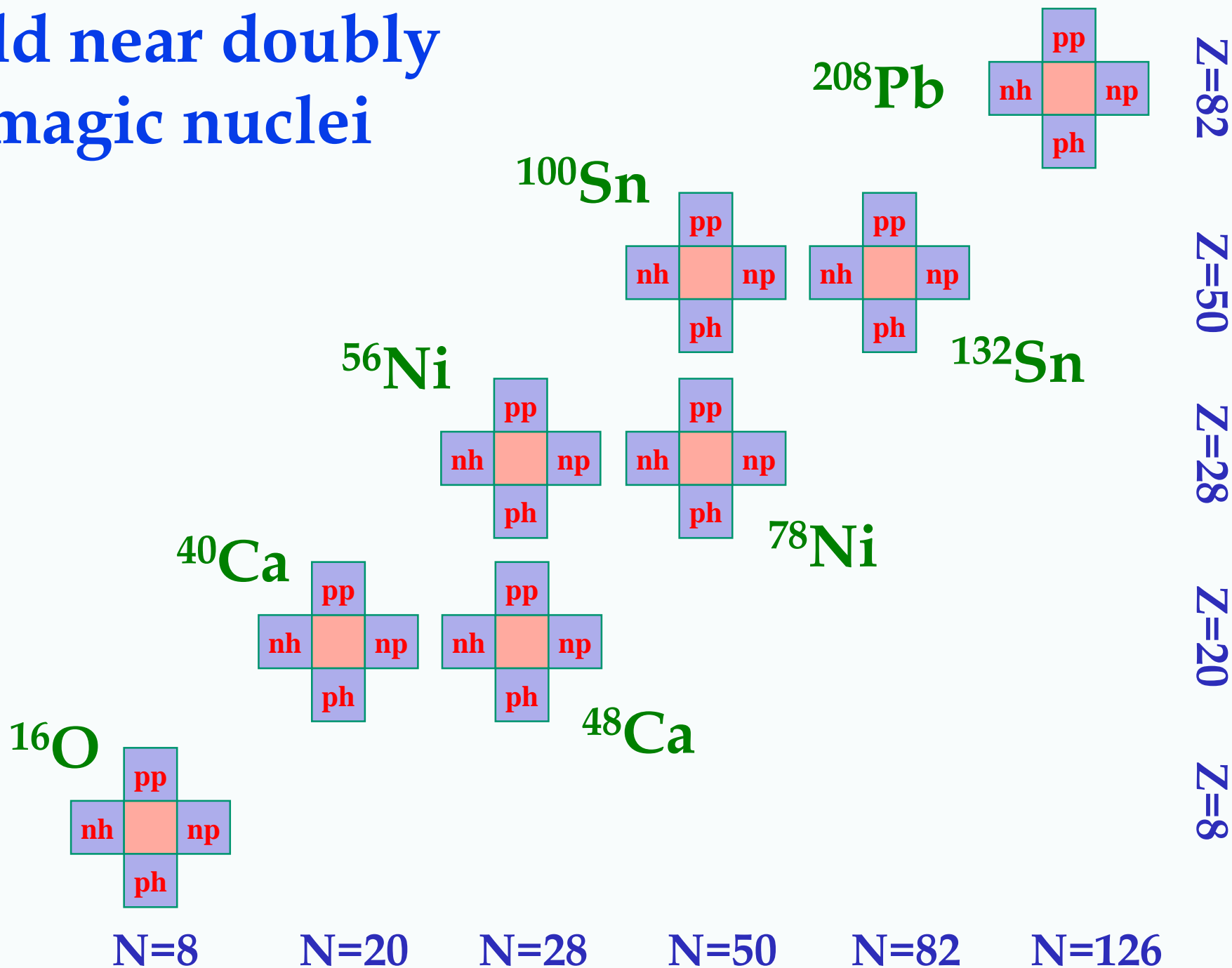
$$g_s^{(i)} = g_p(g_n) = 5.59(-3.83) \\ g_\ell^{(i)} = 1(0)$$

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

Spectroscopic moments = moments measured experimentally



Odd near doubly magic nuclei



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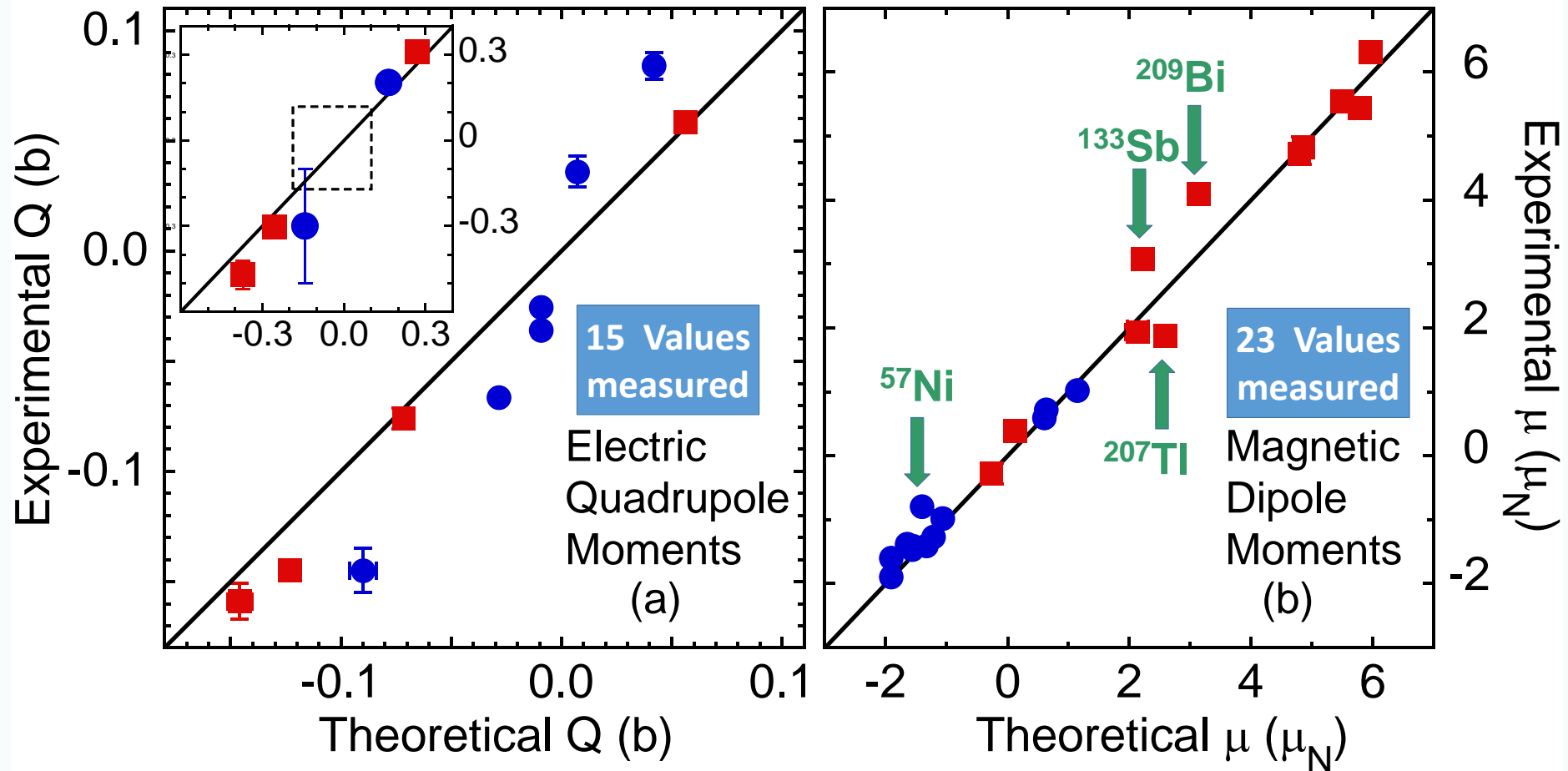


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Quadrupole & dipole moments

P. Sassarini *et al.*, J. Phys. G49 (2022) 11LT01



- Proton-odd (squares) & neutron-odd (circles) nuclei
- Average of UNEDF1, SLy4, SkO', D1S, N3LO functionals
- RMS deviations much smaller than the residuals



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Effective spin g-factor? Who ordered that?

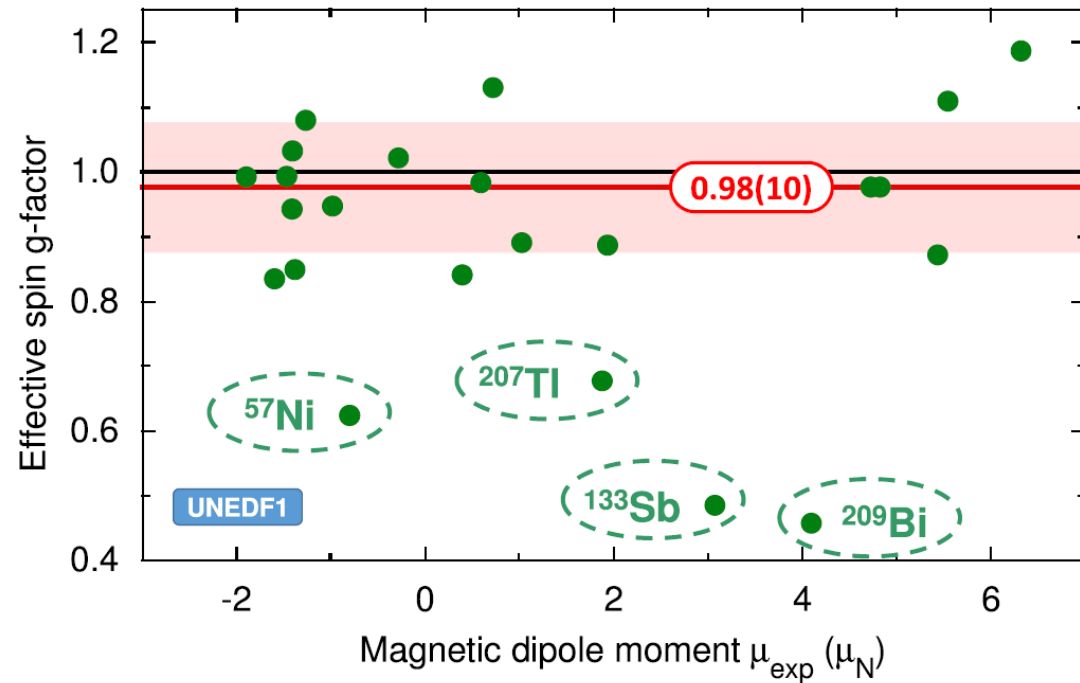
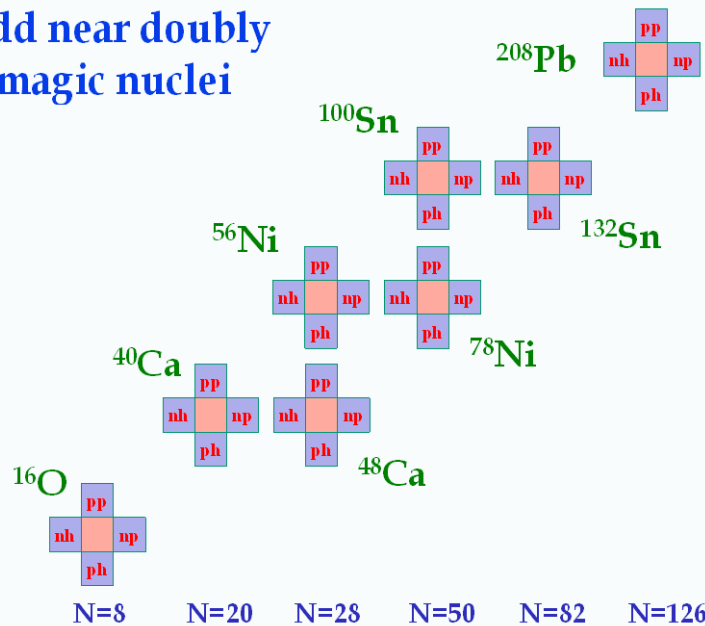
P. Sassarini et al., J. Phys. G49 (2022) 11LT01

$$g_s^{(i)} = g_p(g_n) = 5.59(-3.83) \times g^{\text{eff}} ???$$

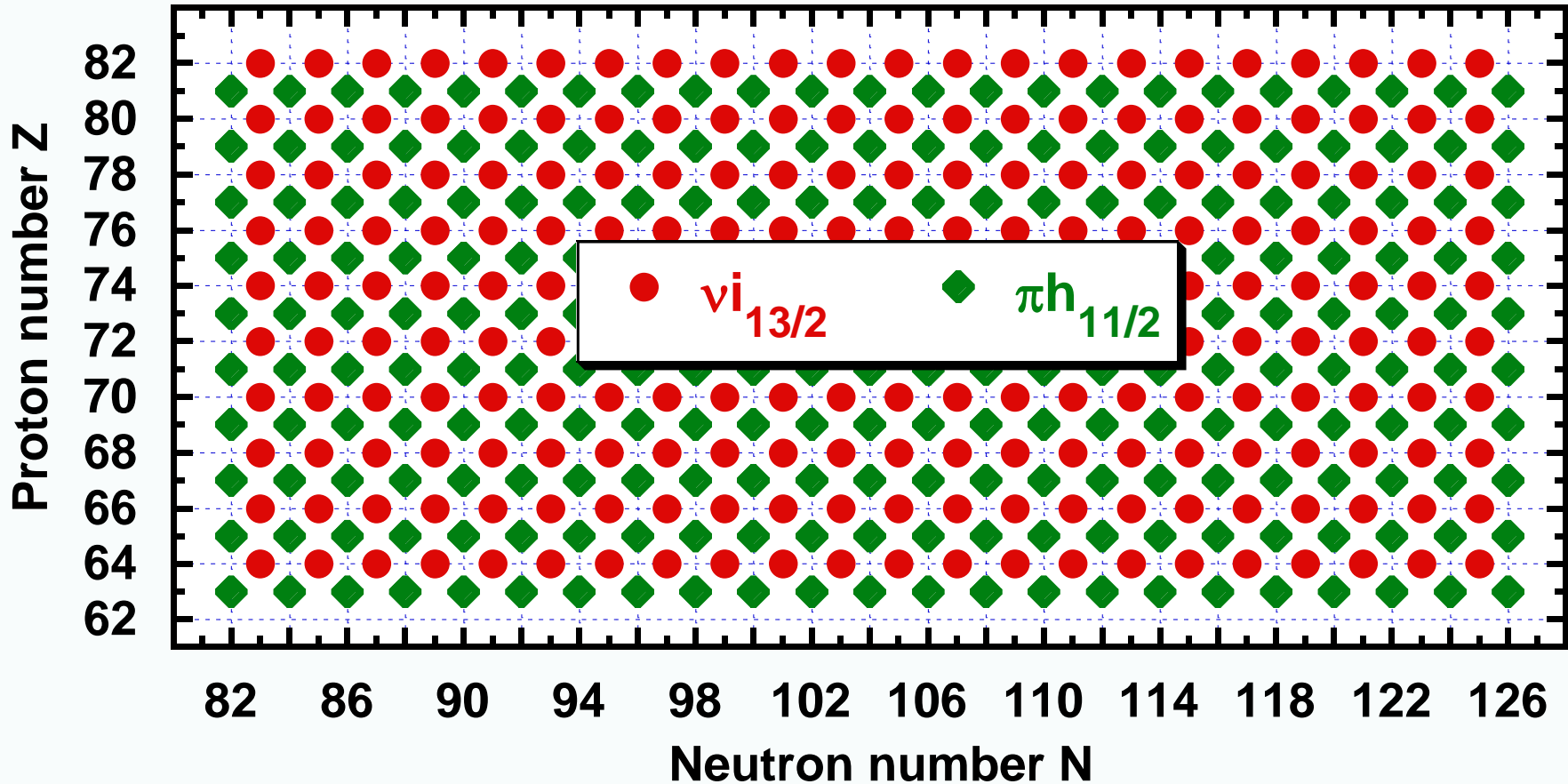
$$g_\ell^{(i)} = 1(0)$$

Landau parameter g'_0 ($g'_0 = 1.7$)
 $g'_0 = N_0 (2C_1^s + 2C_1^T (3\pi^2 \rho_0 / 2)^{2/3})$
 $\frac{1}{N_0} \approx 150 \frac{m}{m^*} \text{ MeV} \cdot \text{fm}^3$

Odd near doubly magic nuclei



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



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

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



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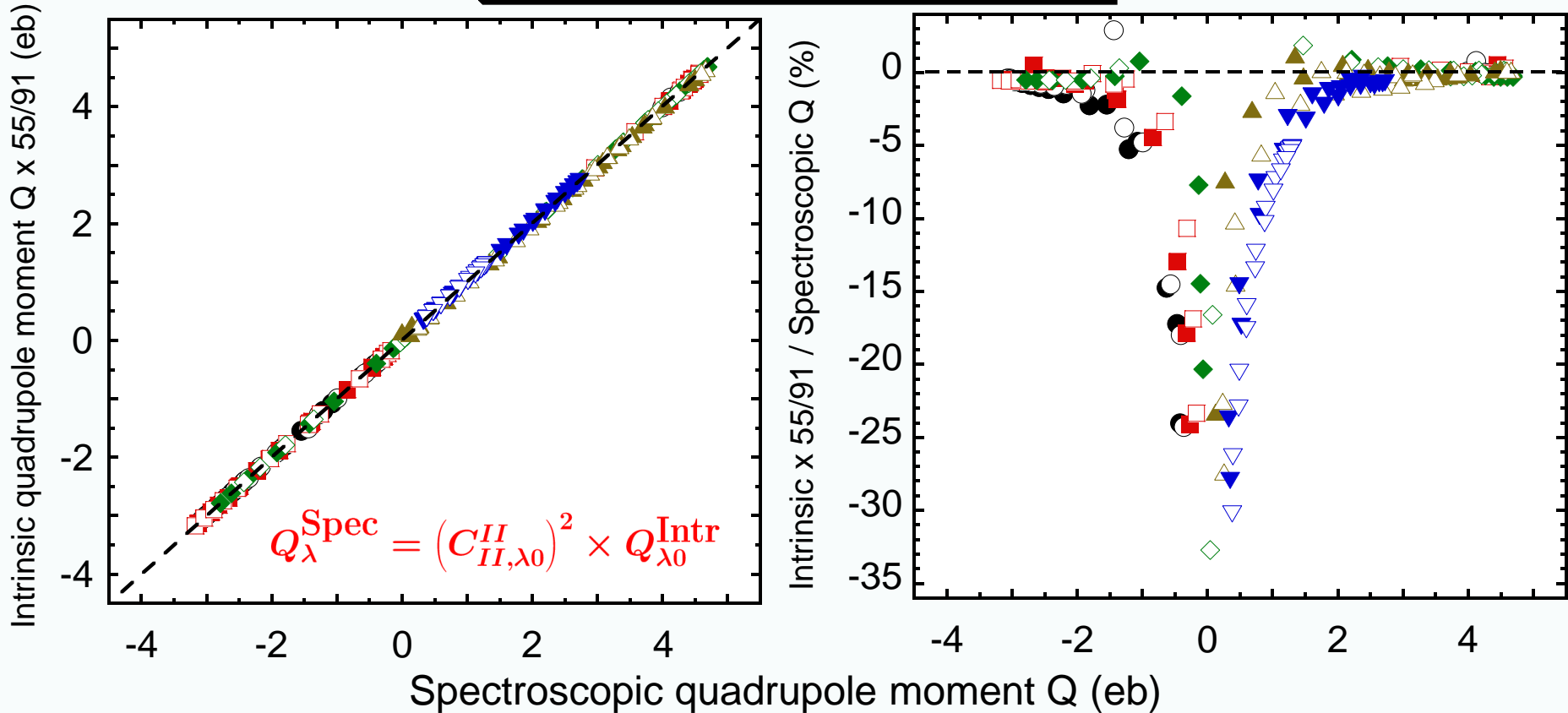
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Heavy deformed $\pi 11/2^-$ odd-Z nuclei



Conclusion:

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

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



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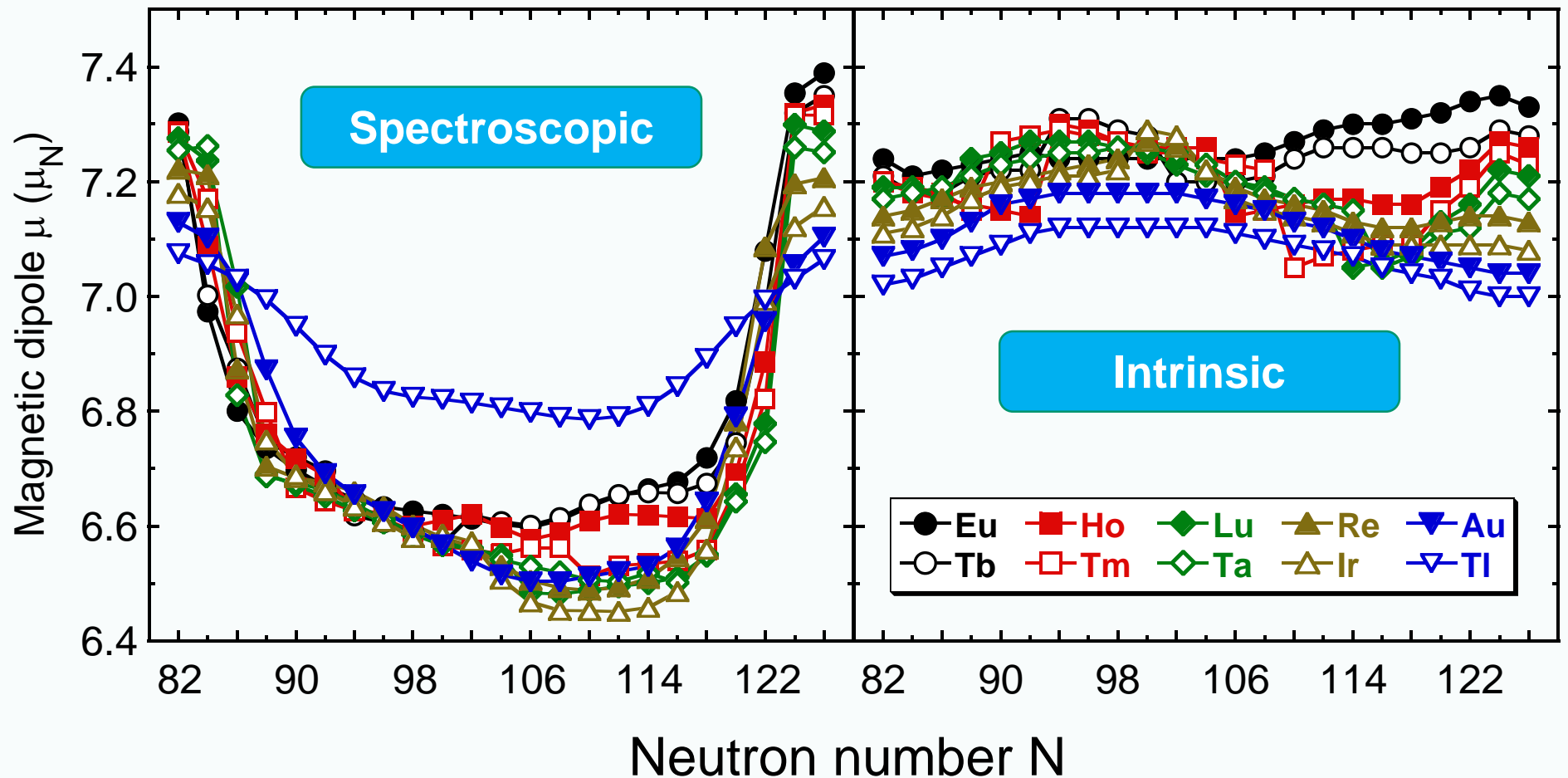
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Heavy deformed $\pi 11/2^-$ odd-Z nuclei



Conclusion:
Spectroscopic magnetic dipole moments
cannot be inferred from the intrinsic ones

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



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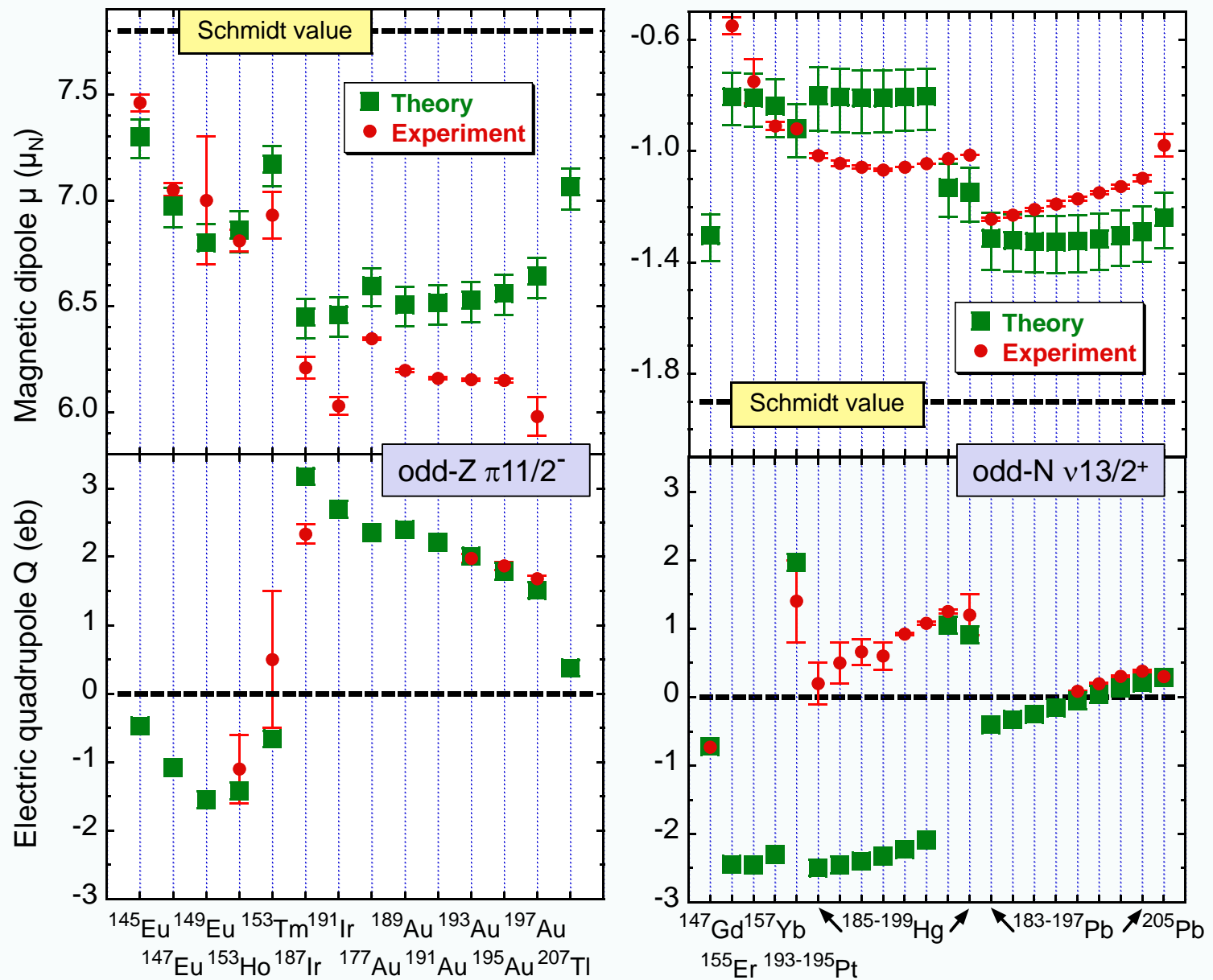
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Spectroscopic moments: theory vs. experiment



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



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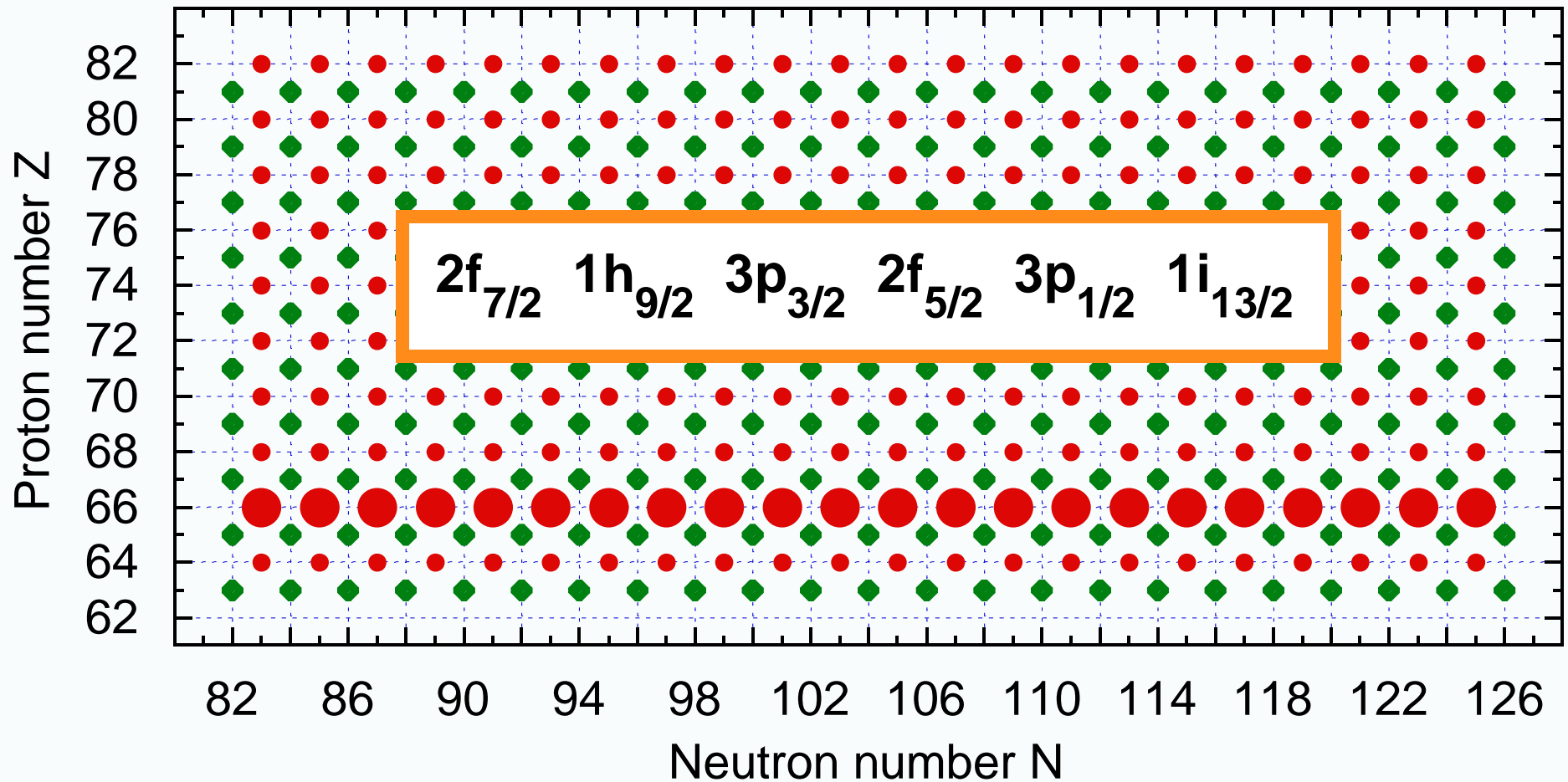


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The first systematic nuclear-DFT analysis of the electromagnetic moments in excited quasiparticle states

J. Dobaczewski *et al.*, to be published



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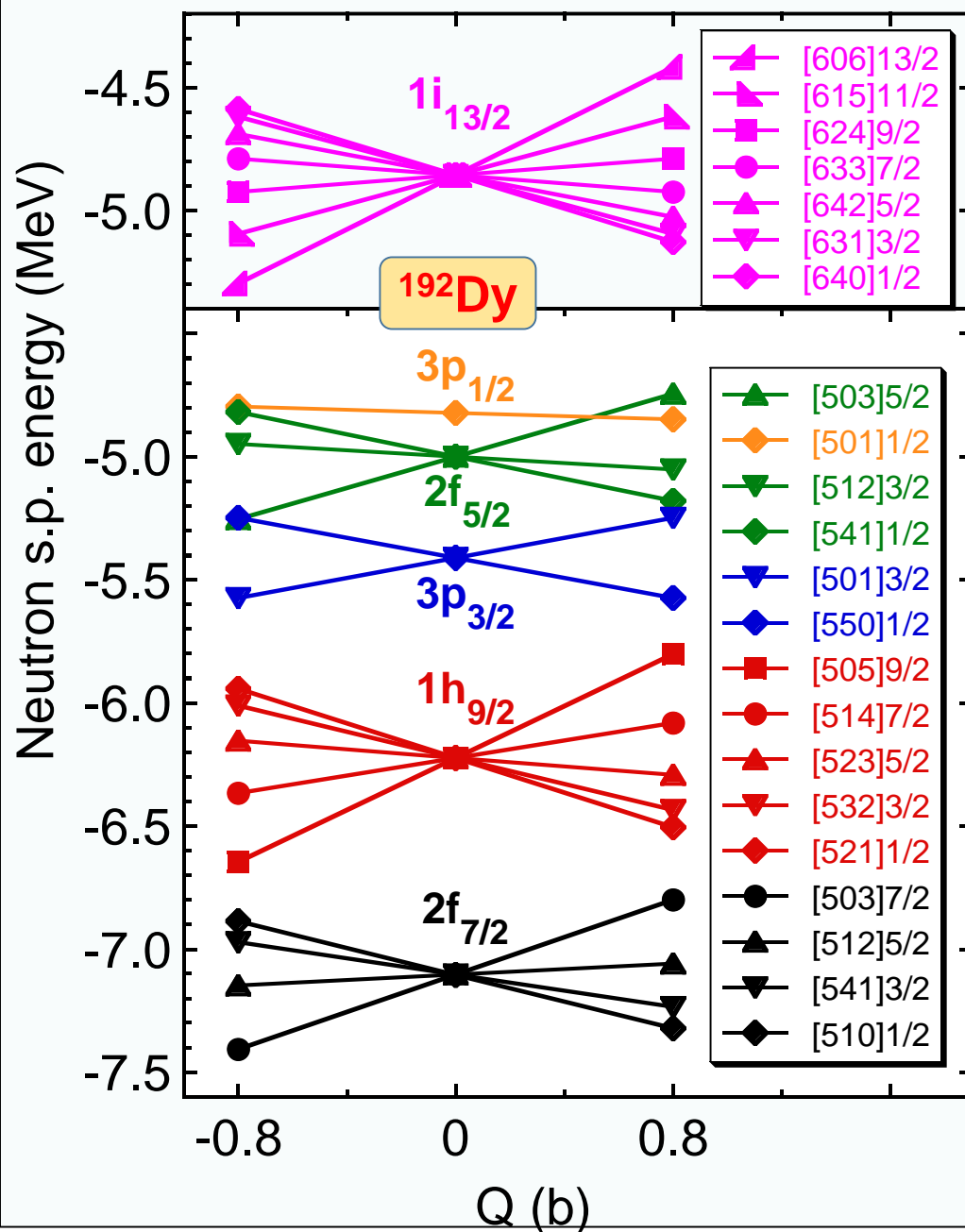
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How to calculate odd nuclei in nuclear DFT?



without pairing

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

$$|\Psi\rangle_{\text{HF}}^{\text{even}} = a_A^+ \dots a_2^+ a_1^+ |0\rangle$$

$$|\Psi\rangle_{\text{HF}}^{\text{odd}} = \begin{cases} a_p^+ |\Psi\rangle_{\text{HF}}^{\text{even}} \\ a_h |\Psi\rangle_{\text{HF}}^{\text{even}} \end{cases}$$

with pairing

$$|\Psi\rangle_{\text{HFB}}^{\text{even}} = \prod_{\mu>0} (u_\mu + v_\mu a_\mu^+ a_\mu^+) |0\rangle$$

$$|\Psi\rangle_{\text{HFB}}^{\text{odd}} = \beta_\nu^+ |\Psi\rangle_{\text{HFB}}^{\text{even}}$$

$$= a_\nu^+ \prod_{\nu \neq \mu > 0} (u_\mu + v_\mu a_\mu^+ a_\mu^+) |0\rangle$$

tagging quasiparticle states

$$\max_\mu \{ \langle \varphi_\nu | \phi_\mu^{\text{upper}} \rangle, \langle \varphi_\nu | \phi_\mu^{\text{lower}} \rangle \}$$



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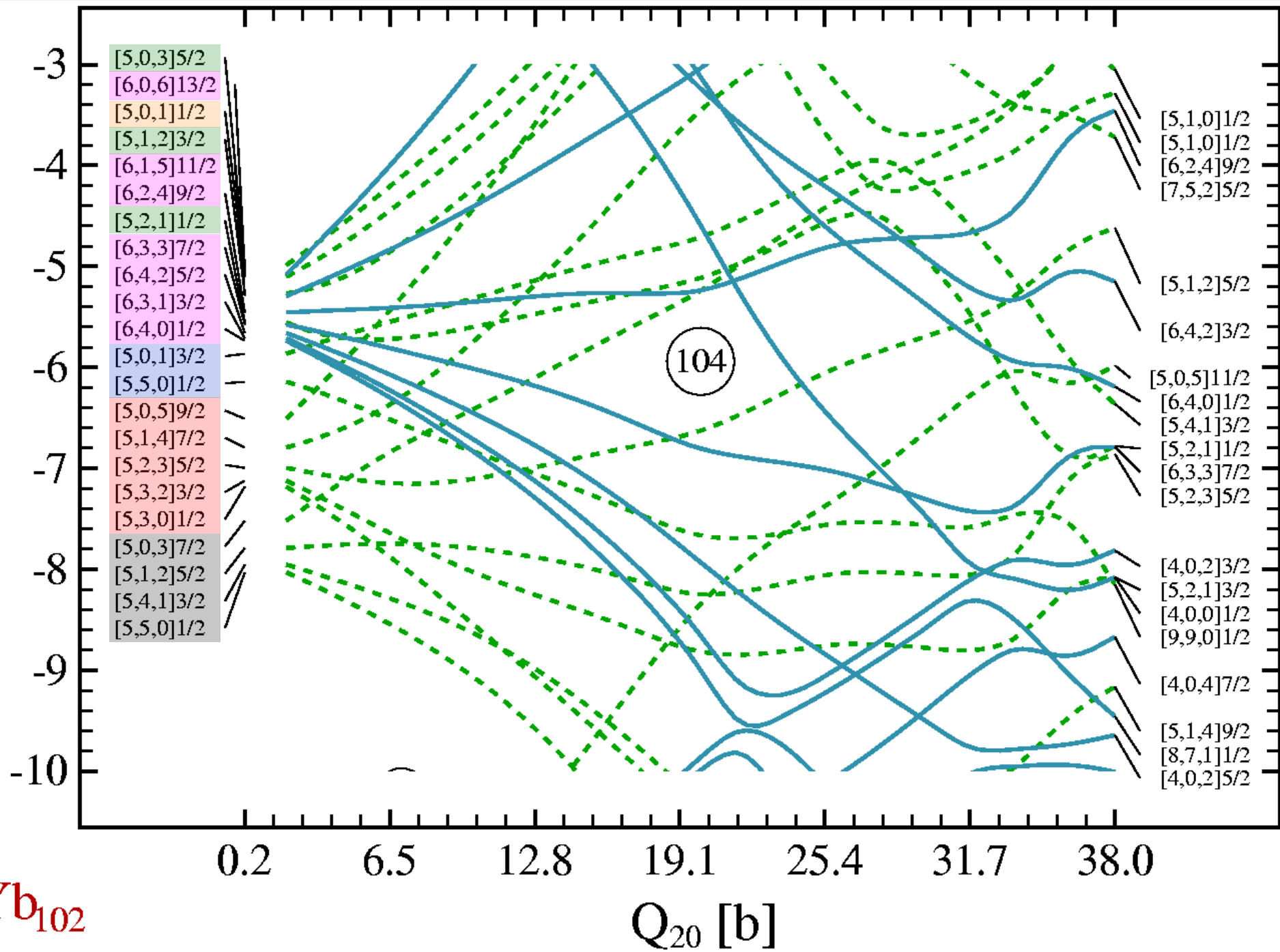
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Single-neutron Energies [MeV]



$^{172}_{70}\text{Yb}_{102}$



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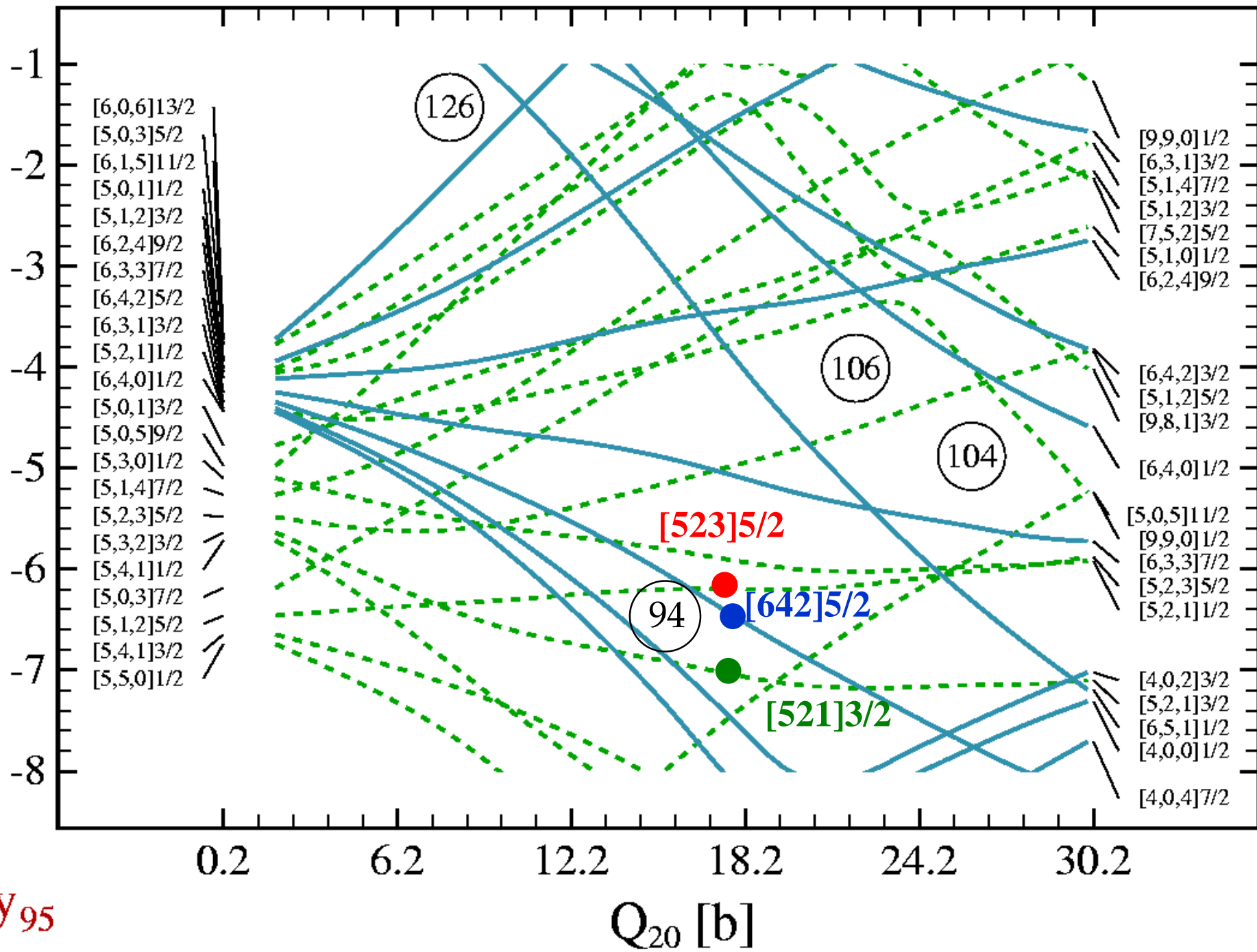
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Single-neutron Energies [MeV]



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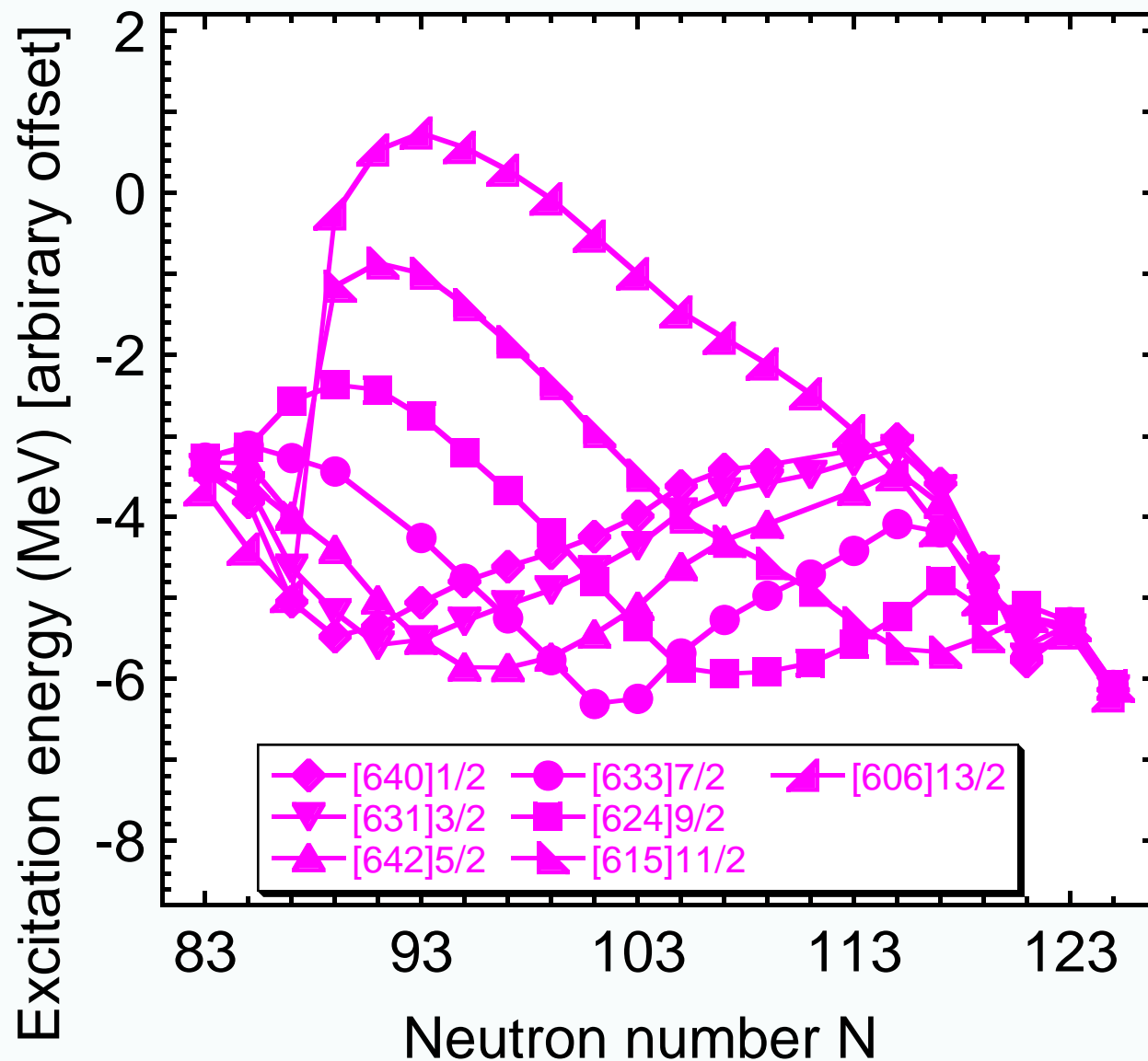
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Excitation energies of odd dysprosium isotopes



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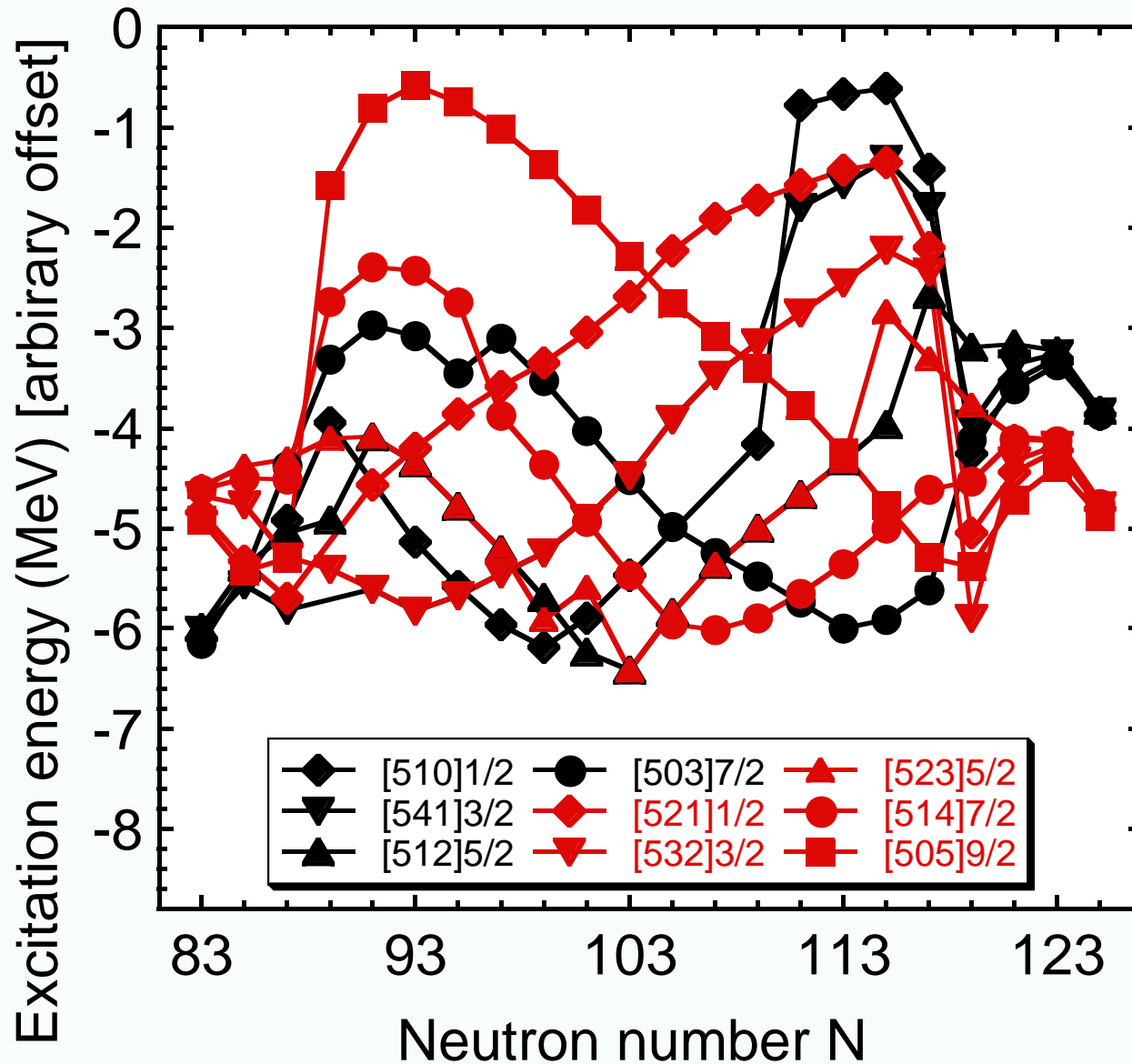
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Excitation energies of odd dysprosium isotopes



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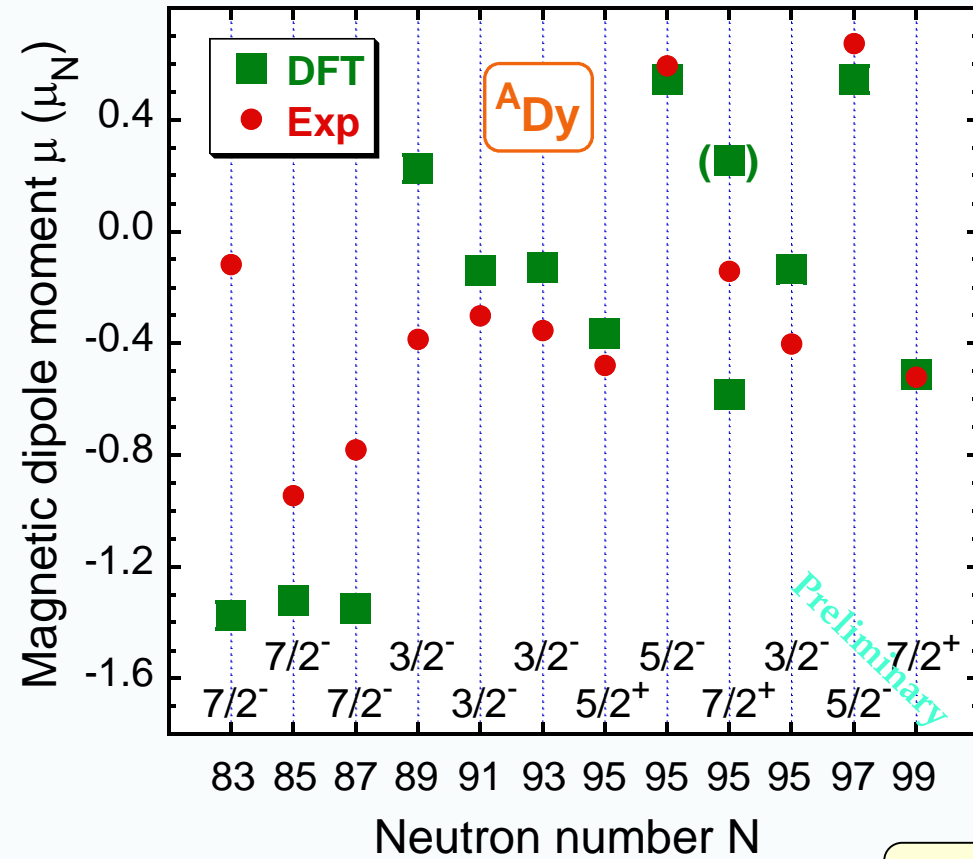
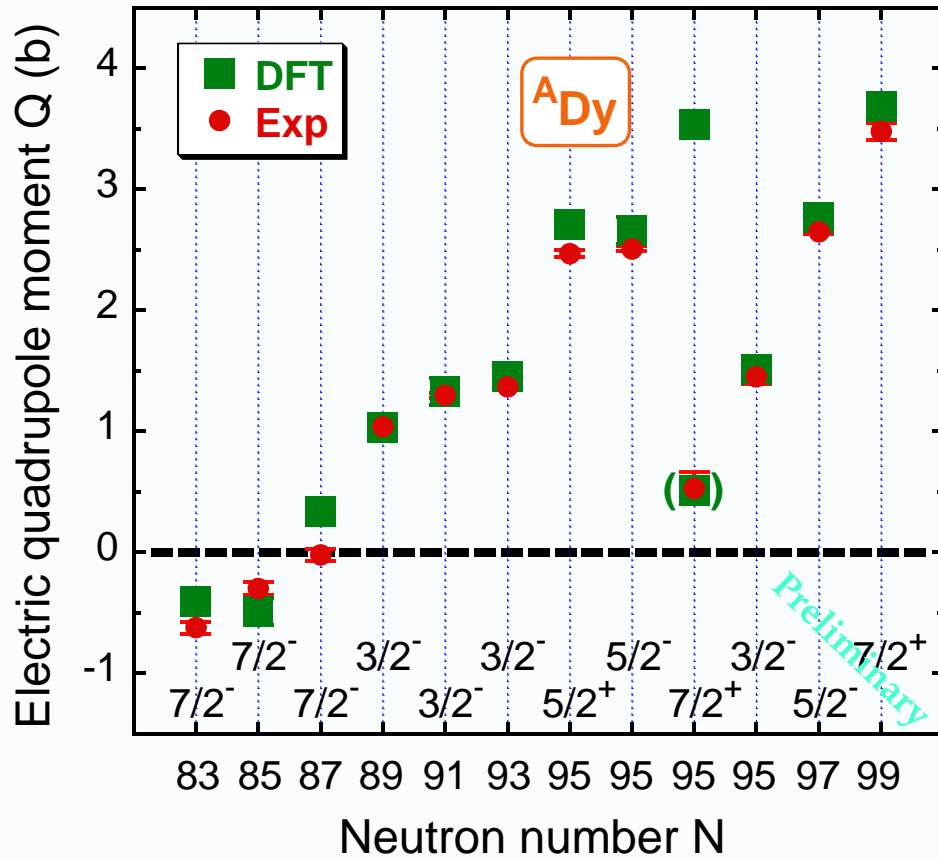
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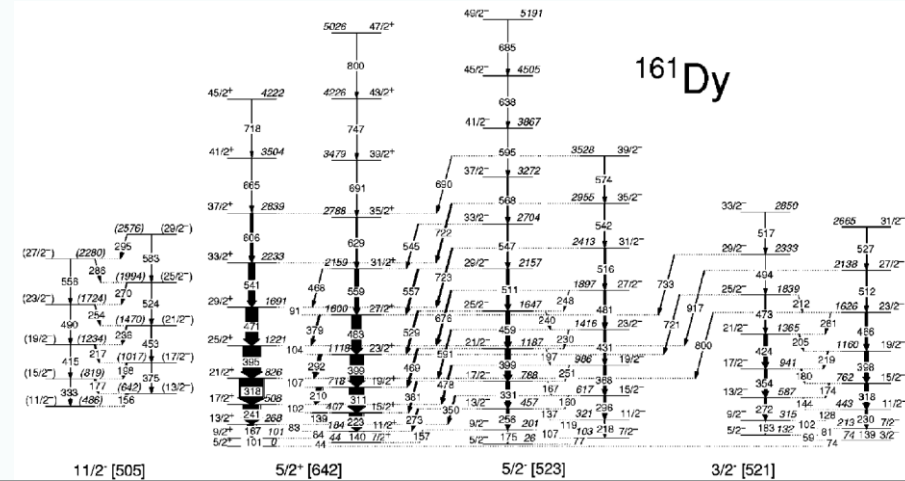
Electromagnetic moments of odd dysprosium isotopes



$9/2^+$	100.4	$7/2^-$	103.0	$5/2^-$	131.7
	*			$3/2^-$	74.6
$7/2^+$	43.8				*
	*	$5/2^-$	25.7		
$5/2^+$	0		*		
	*				

^{161}Dy

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



A. Jungclauss *et al.*,
Phys. Rev. C67, 034302 (2003)



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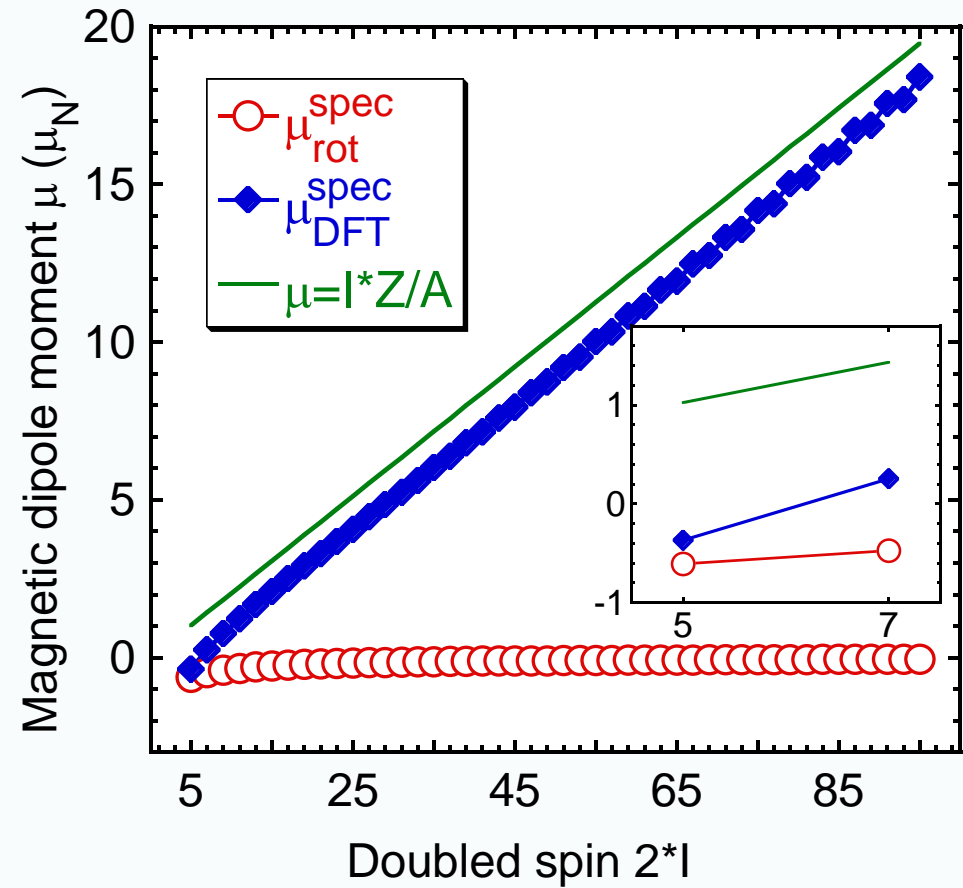
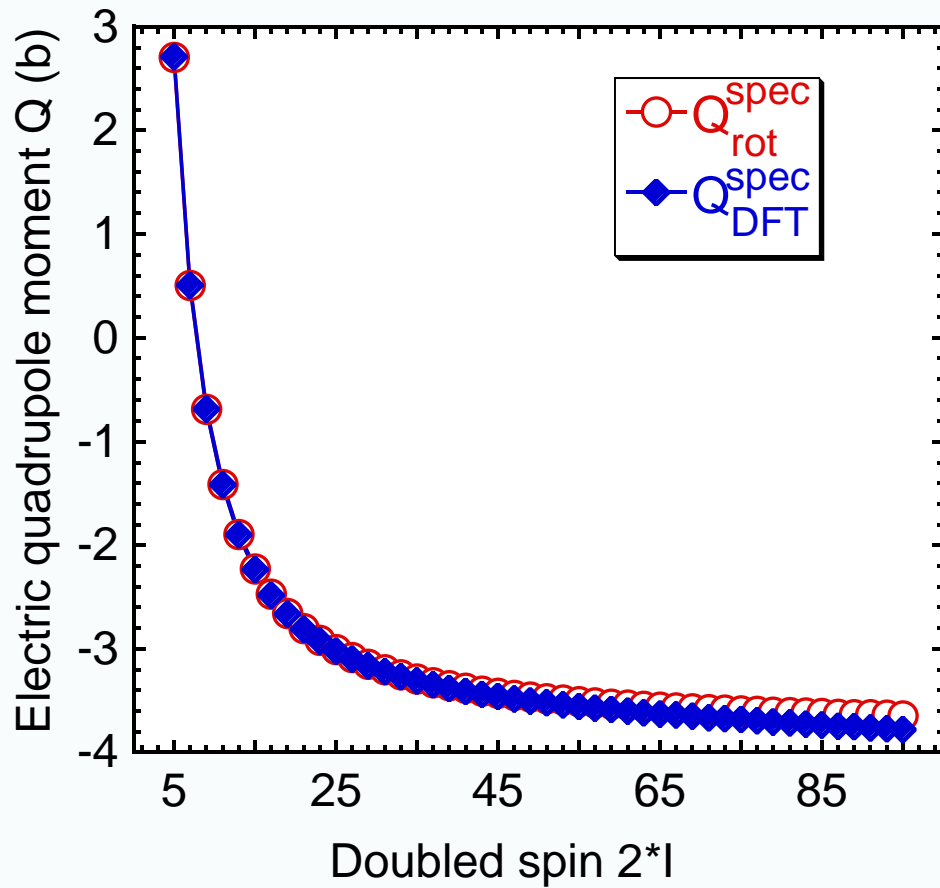


Electromagnetic moments – the rigid-rotor approximation

$^{161}\text{Dy } 5/2^+ \text{ UNEDF1, } g'_0=1.7$

$$Q_{\text{rot}}^{\text{spec}} = Q_{20}^{\text{intr}} \times C_{\text{II},20}^{\text{II}} \times C_{\text{IK},20}^{\text{IK}}$$

$$\mu_{\text{rot}}^{\text{spec}} = \mu_z^{\text{intr}} \times C_{\text{II},10}^{\text{II}} \times C_{\text{IK},10}^{\text{IK}}$$



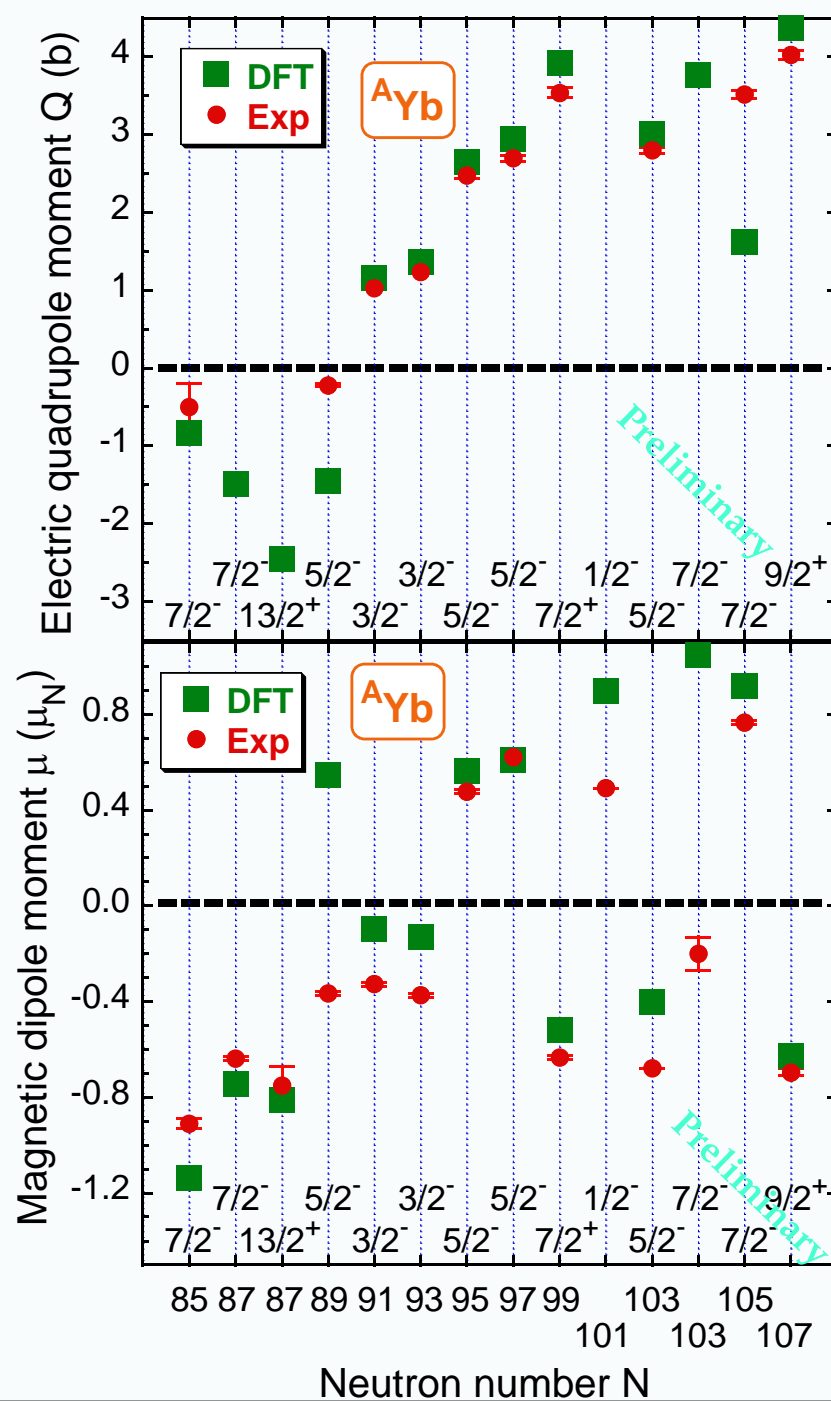
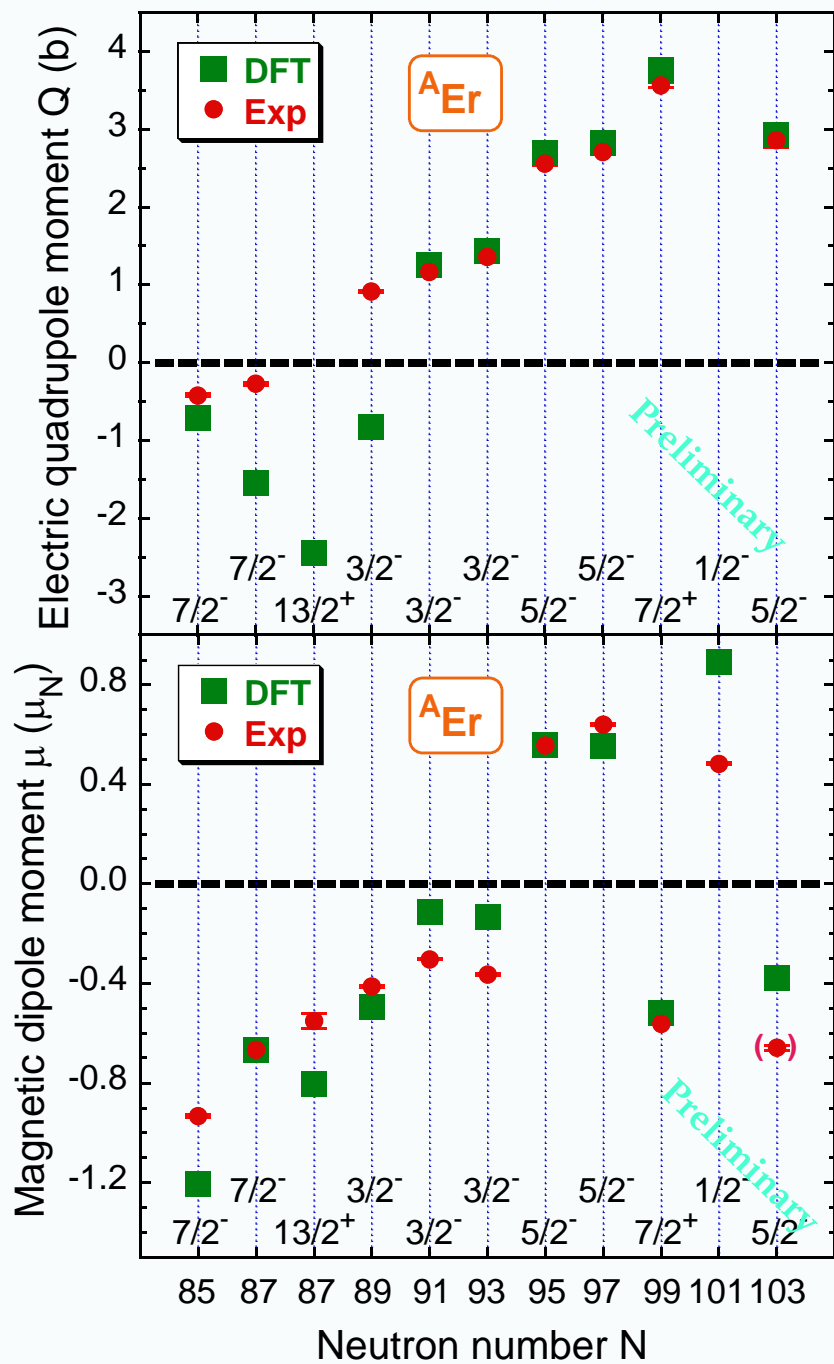
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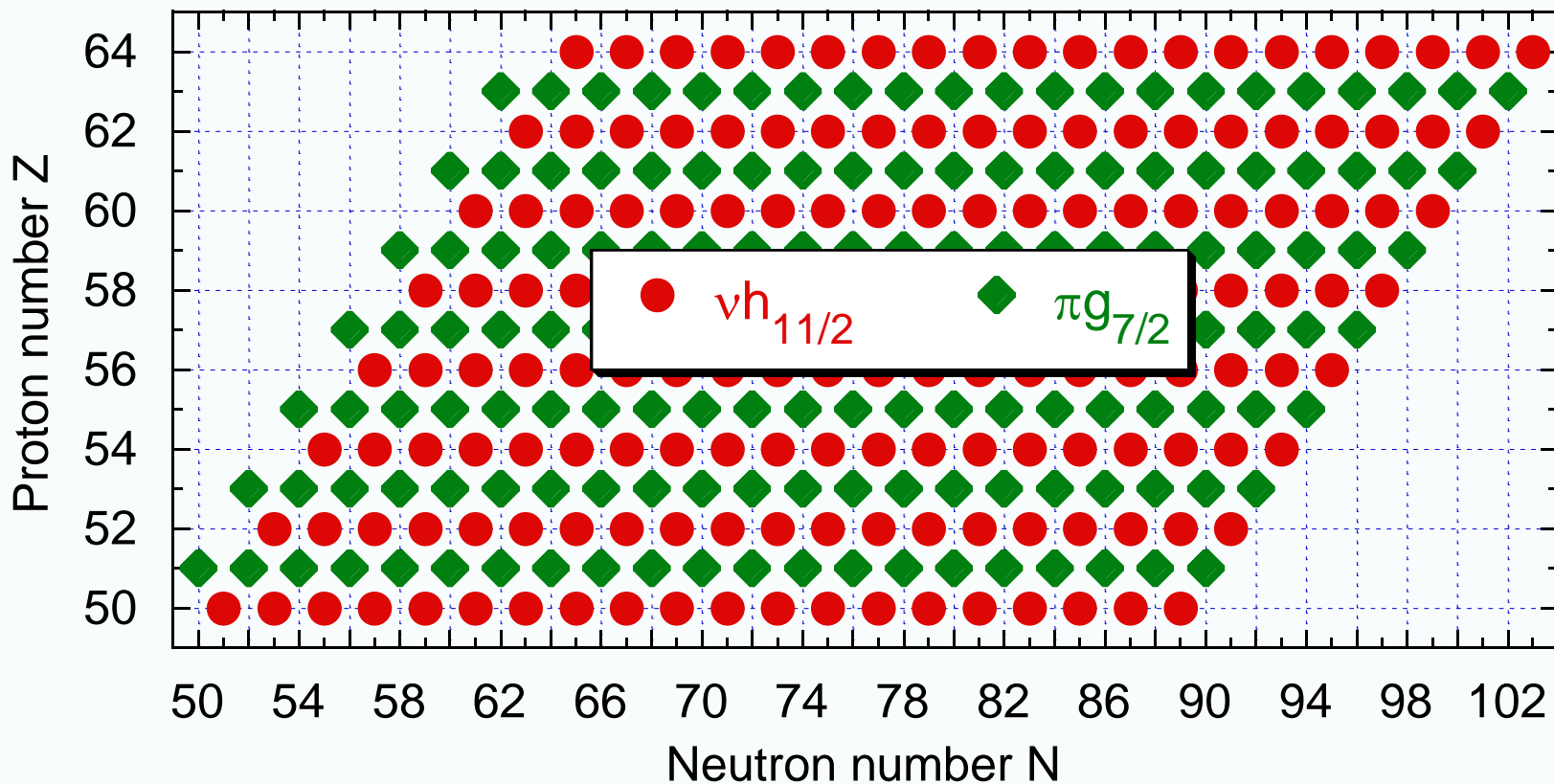


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Nuclear-DFT analysis of electromagnetic moments between the Sn and Gd isotopes



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



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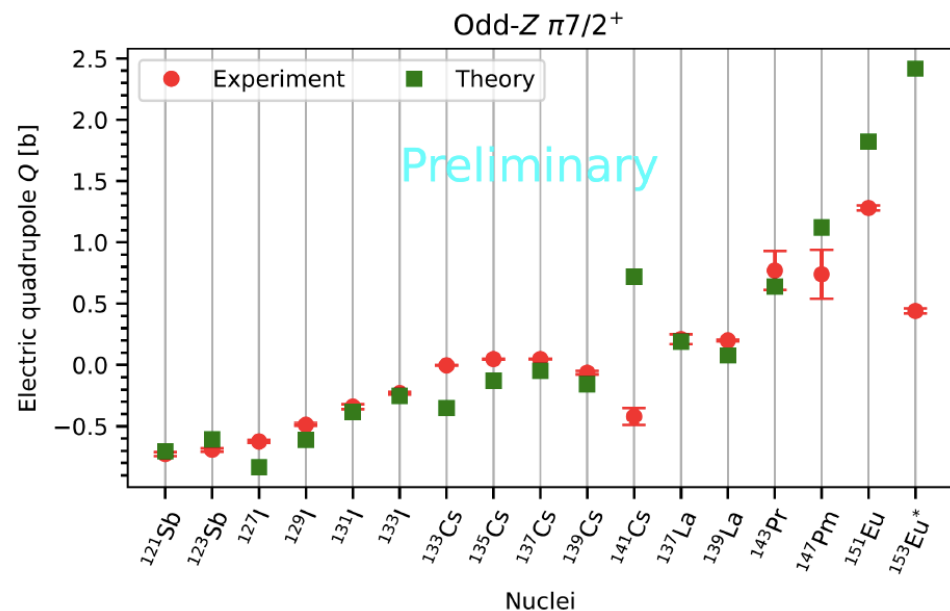
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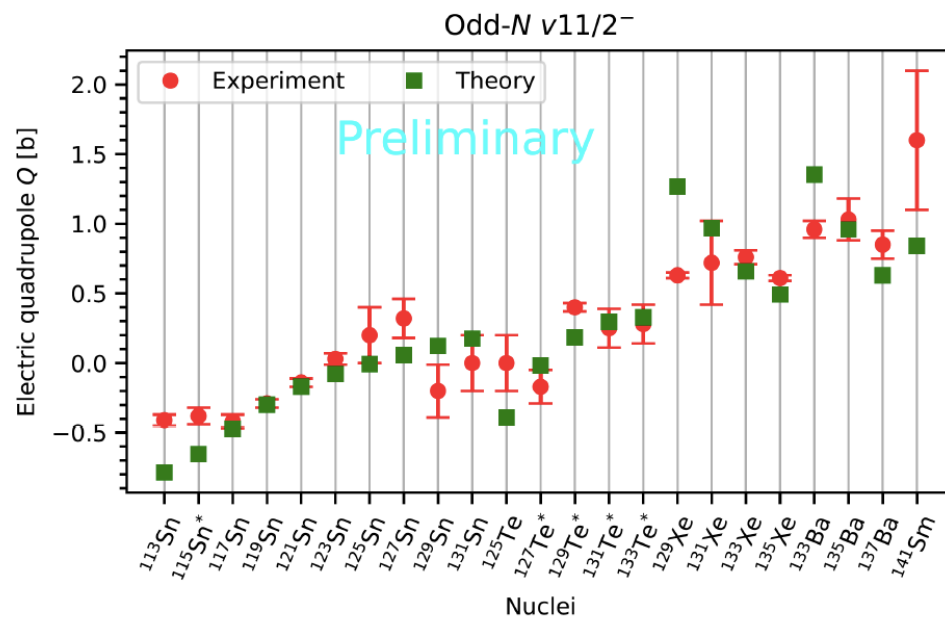


Quadrupole moments: theory vs. experiment



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



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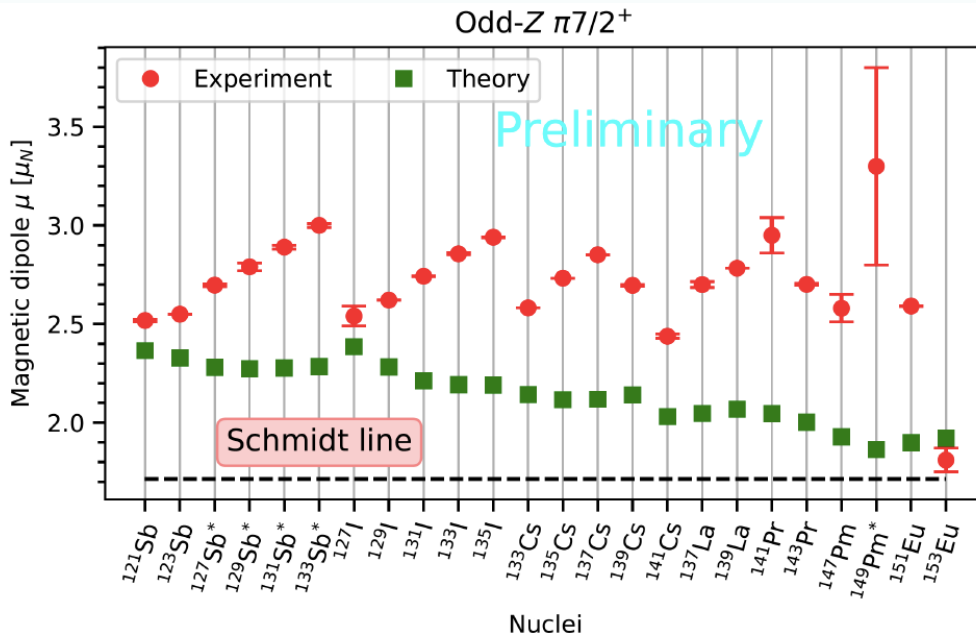
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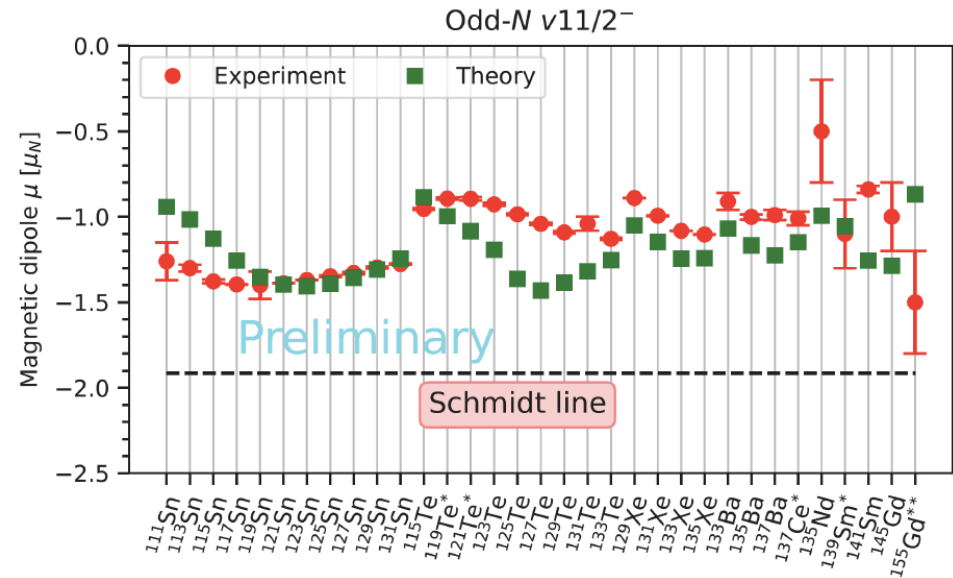


Magnetic dipole moments: theory vs. experiment



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



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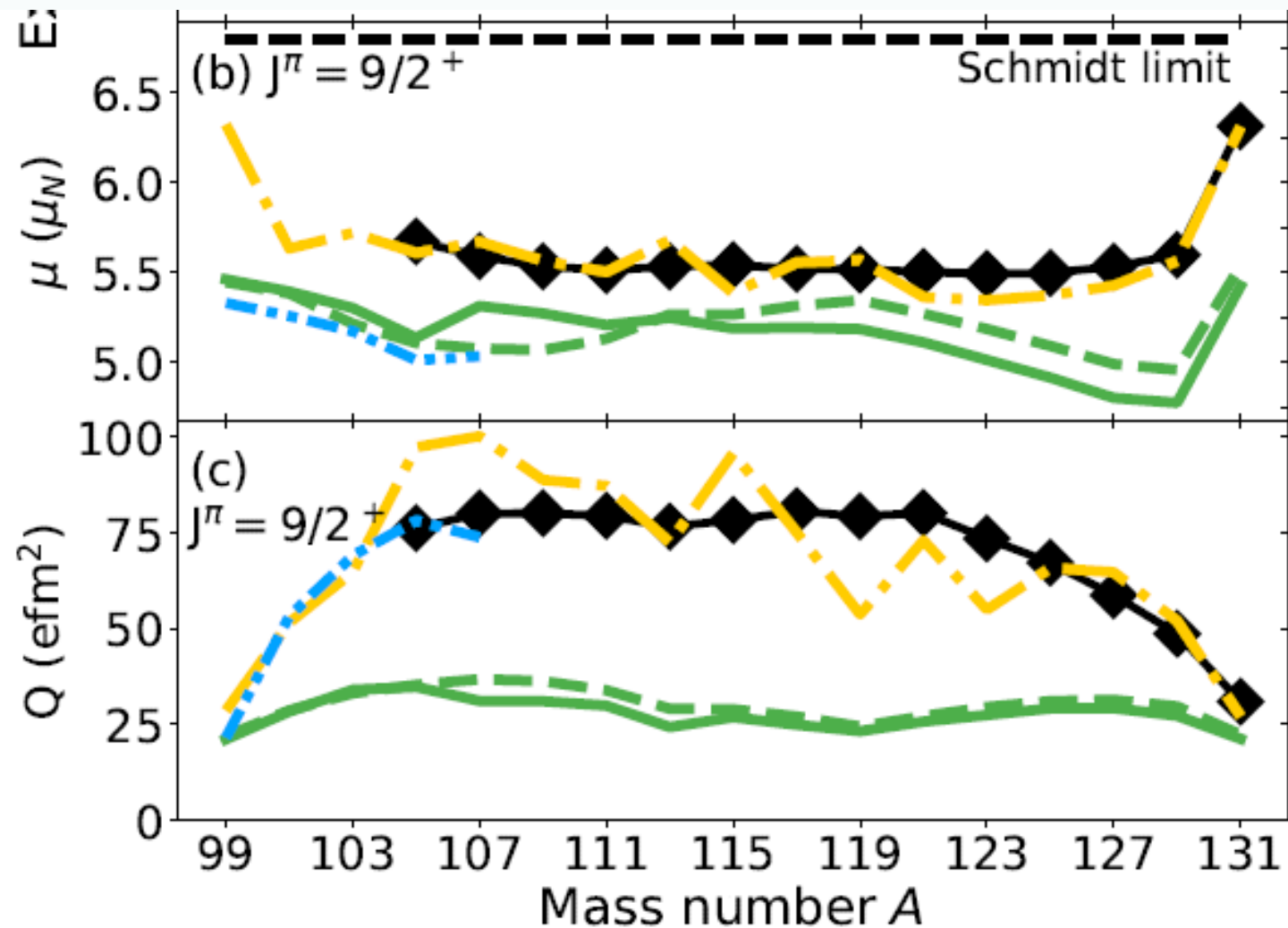
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Moments of the 9/2 states in In



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

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



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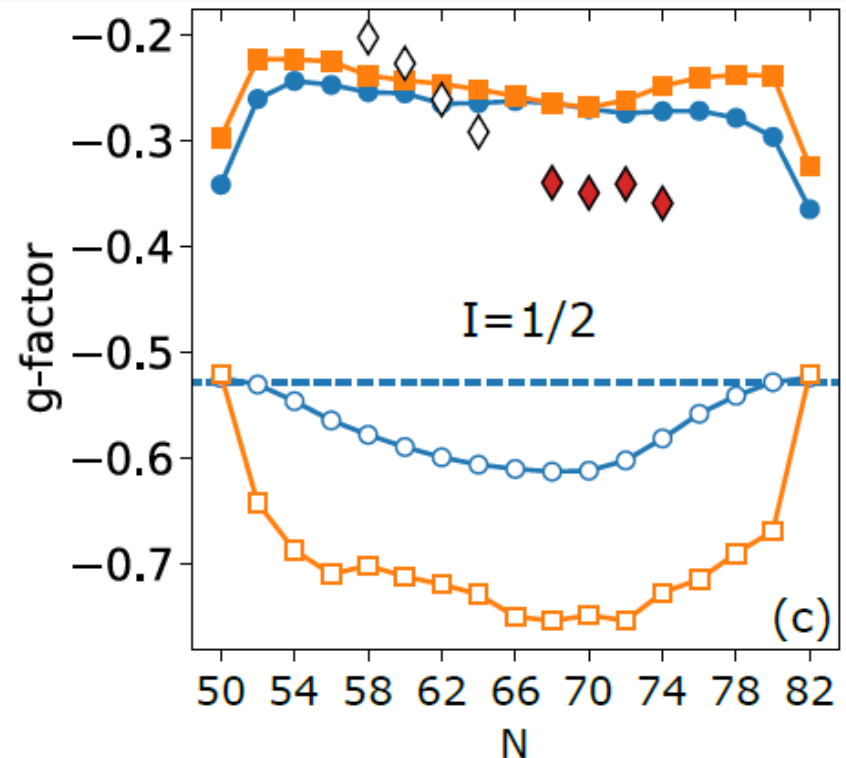
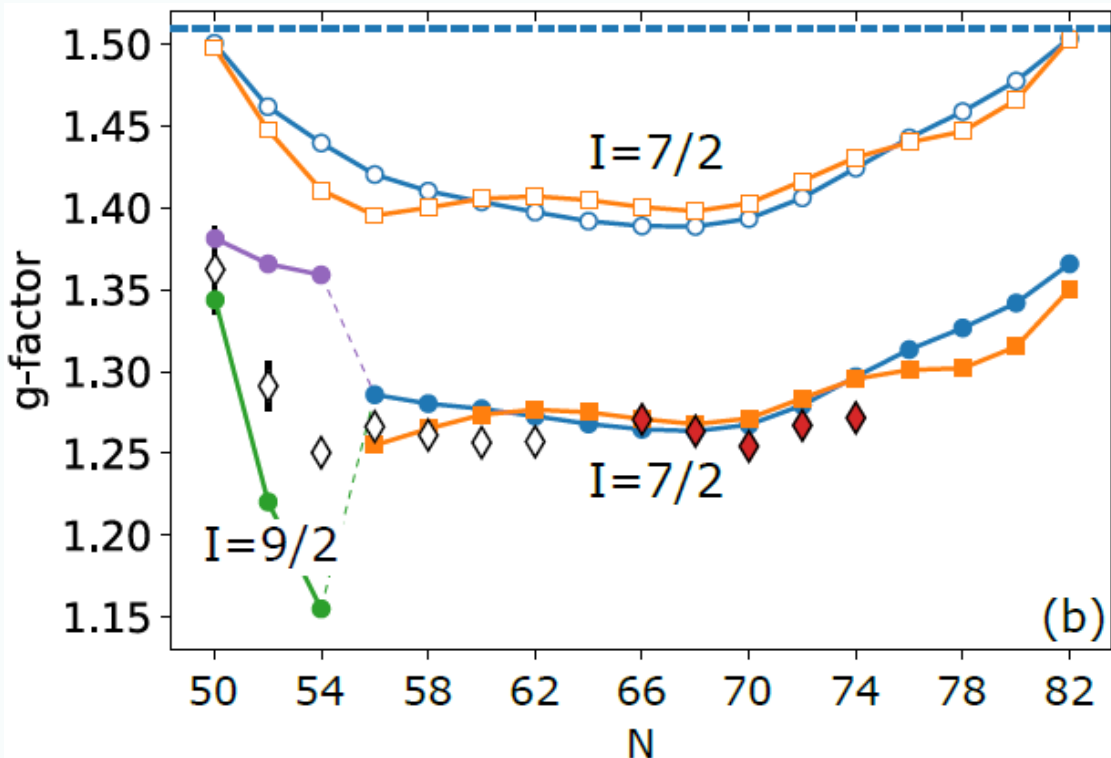
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Moments of the 1/2, 7/2 & 9/2 states in Ag



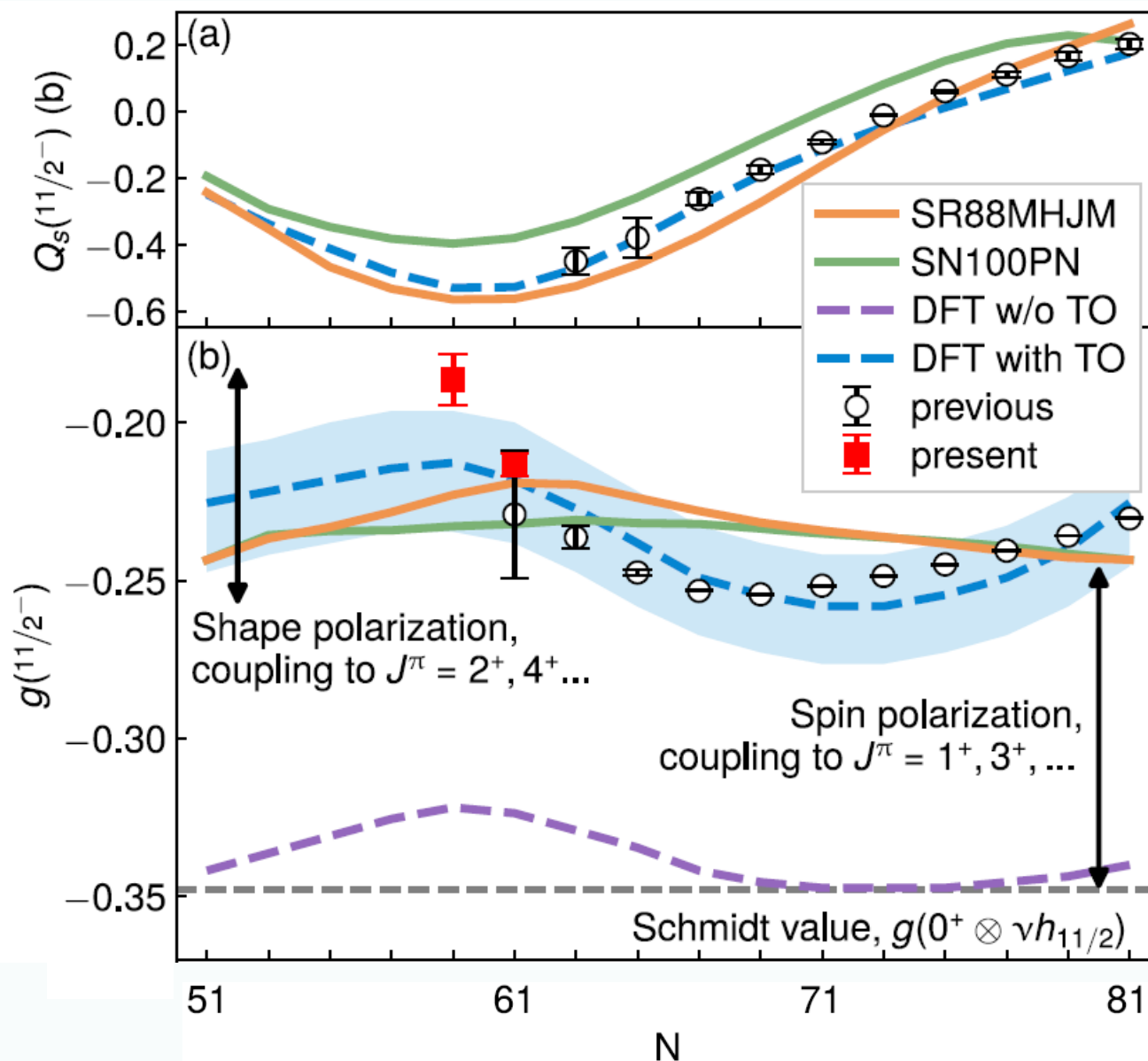
Experiment ◆ This work
◆ Literature

UNEDF1 □ $g'_0 = 0$ UNEDF1_{so} ○ $g'_0 = 0$ ● $g'_0 = 1.7$ $I = 9/2$ (7/2)
■ $g'_0 = 1.7$ ● $g'_0 = 1.7$ ● $g'_0 = 1.7$ $I = 9/2$

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



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

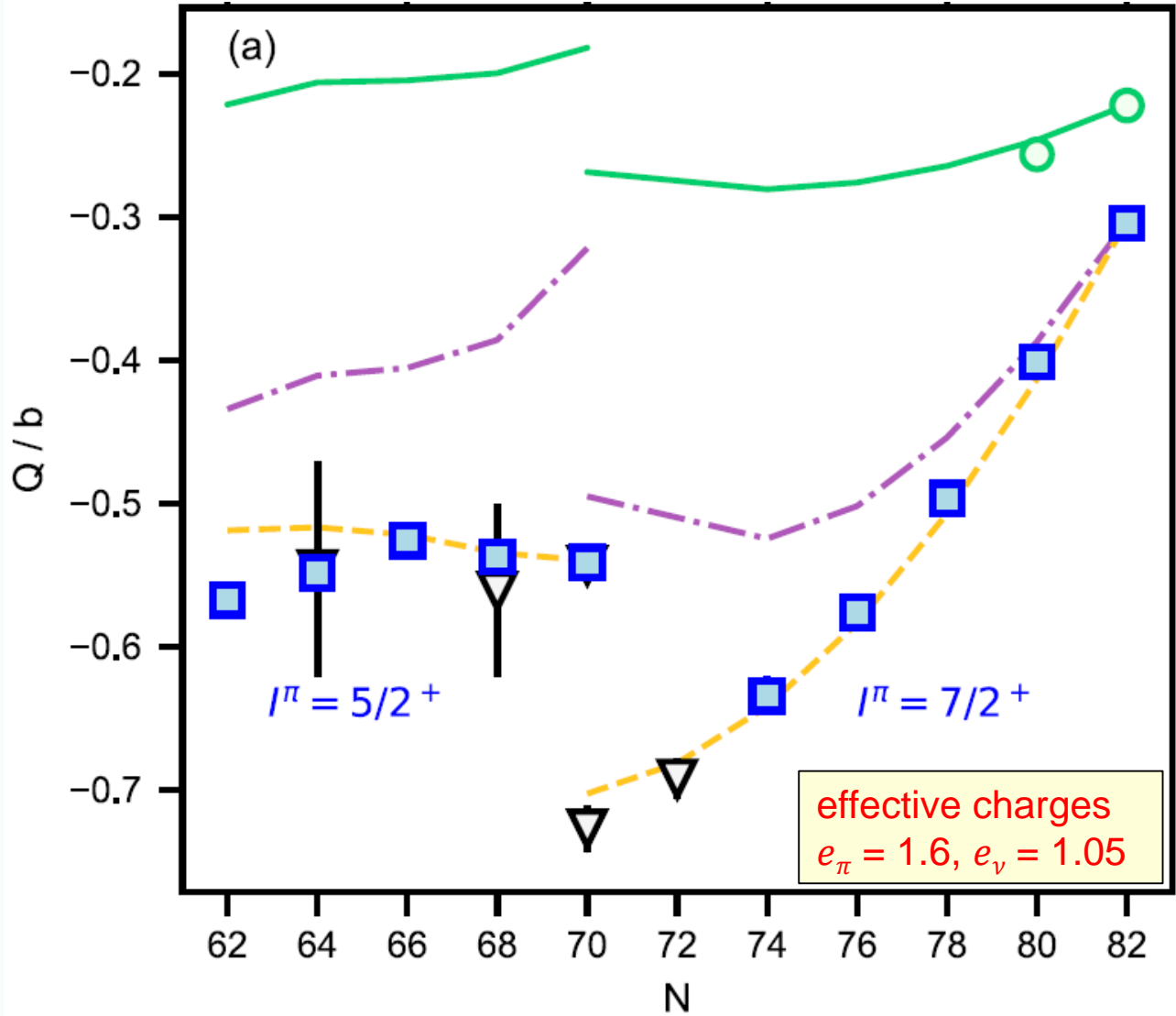
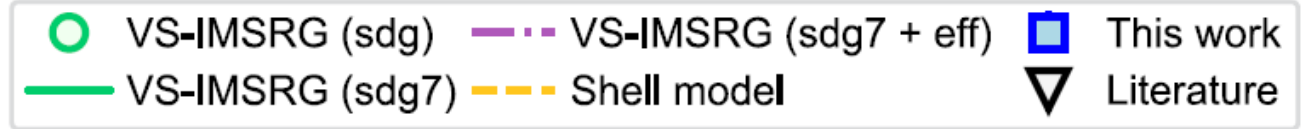


$g = \mu/I$

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



Quadrupole moments in Sb



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



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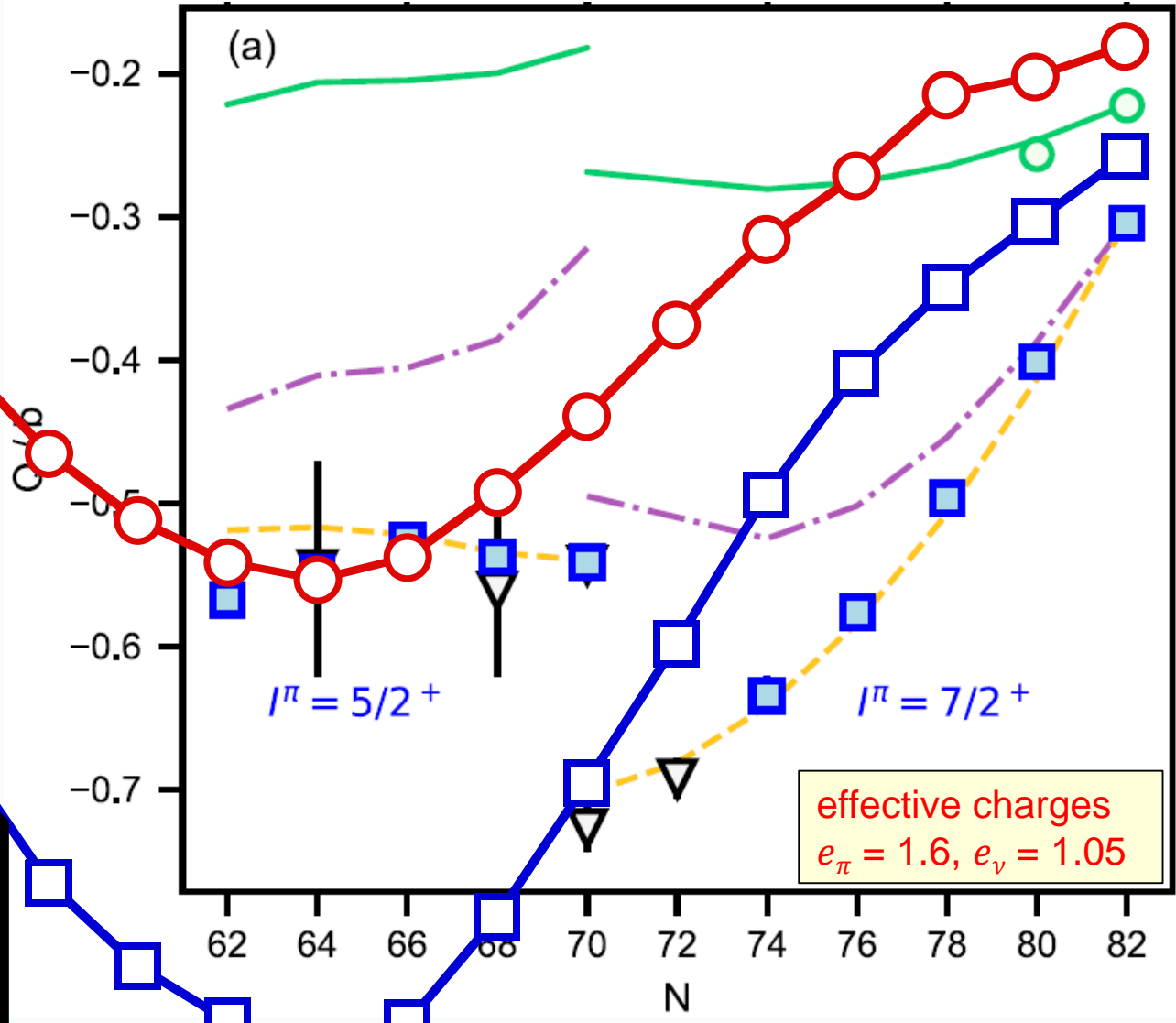
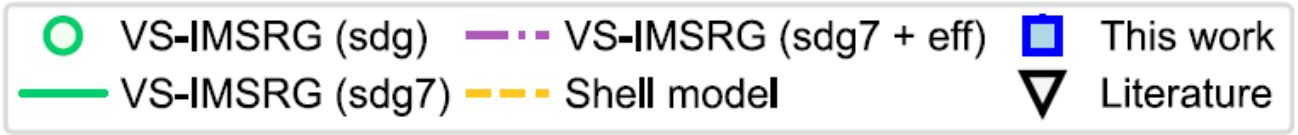
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Quadrupole moments in Sb



no effective charges !!!

—□— DFT $g_{7/2}$
—○— DFT $d_{5/2}$

effective charges
 $e_\pi = 1.6, e_\nu = 1.05$

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



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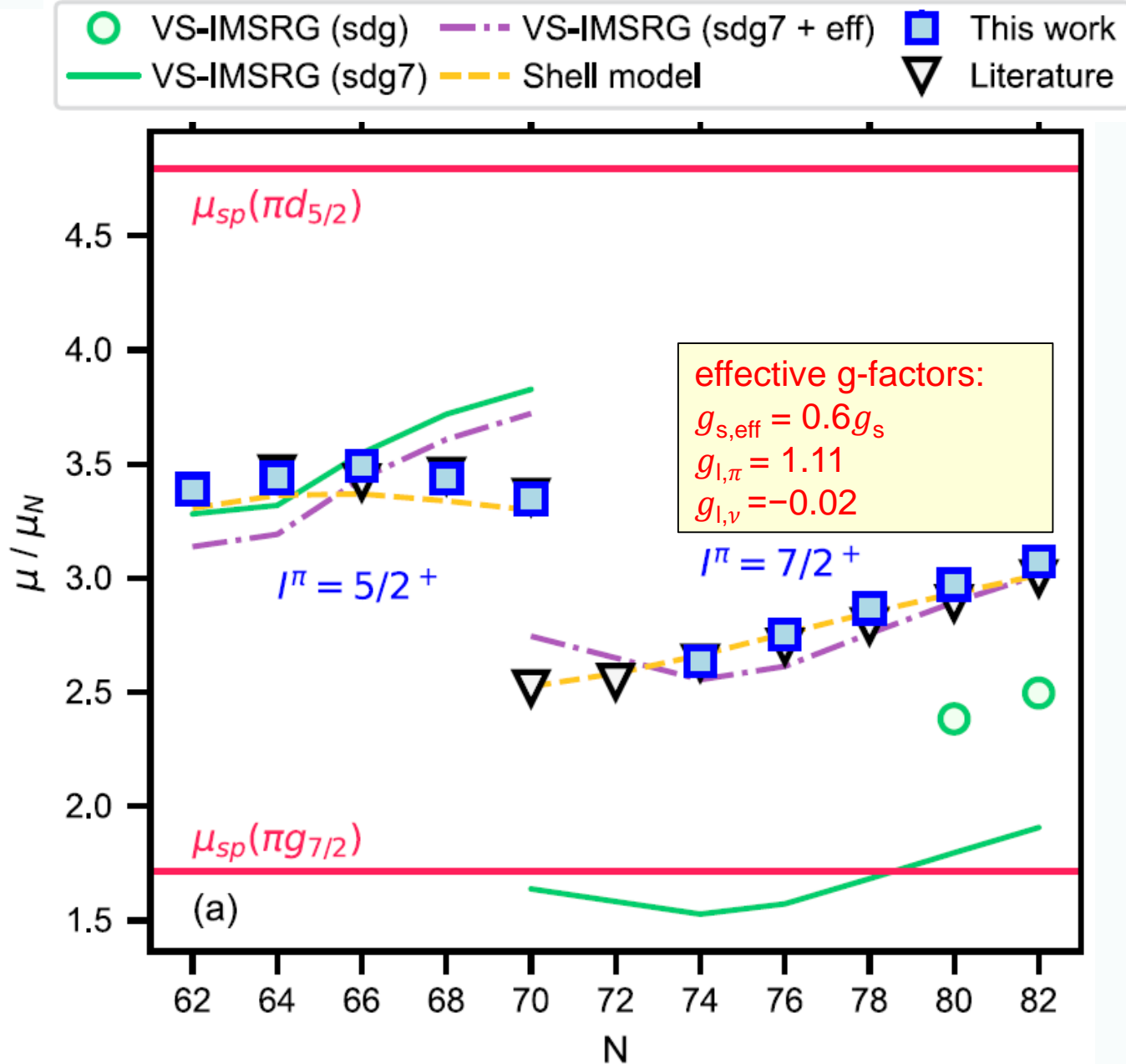
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Magnetic dipole moments in Sb



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



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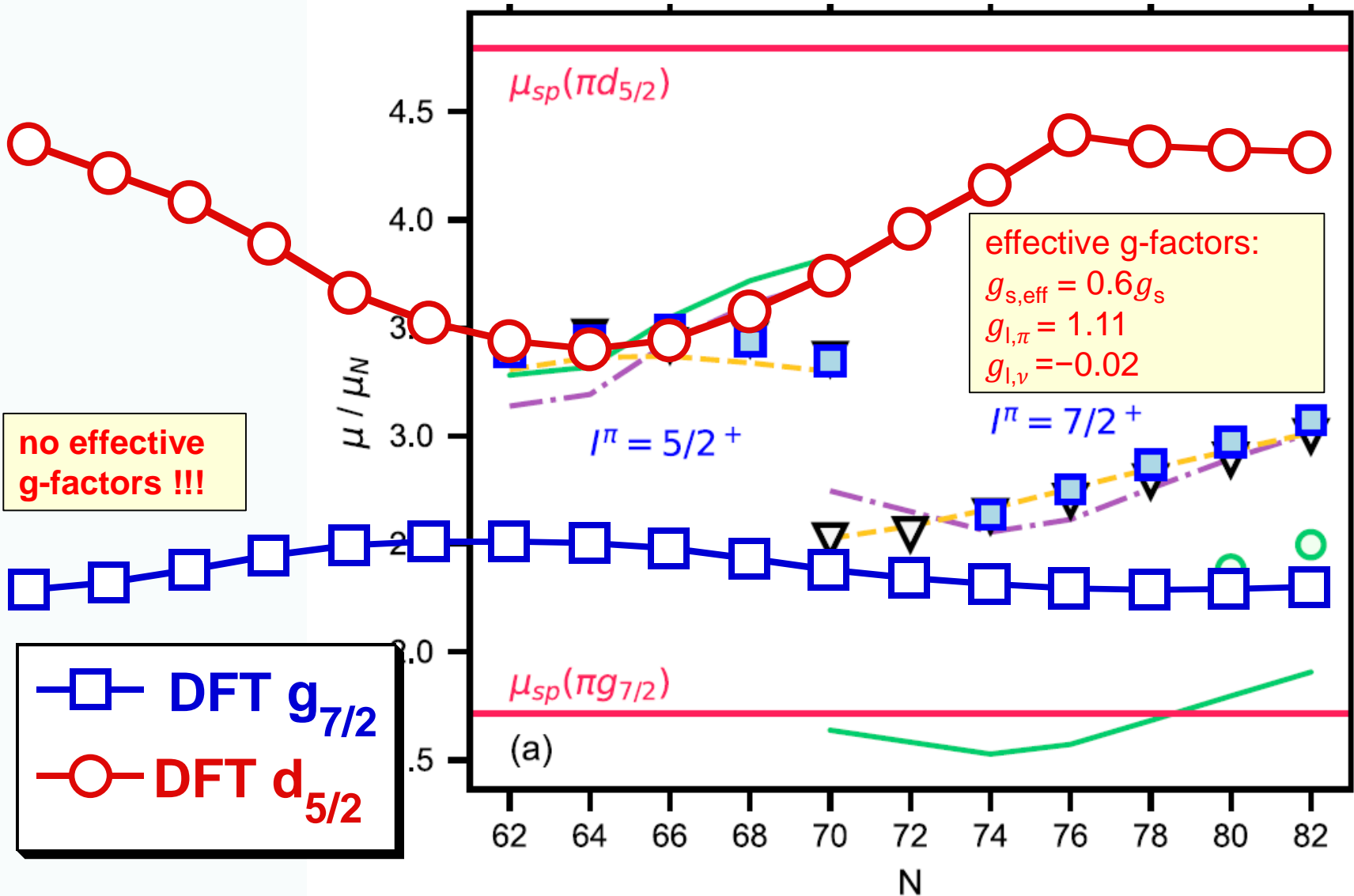
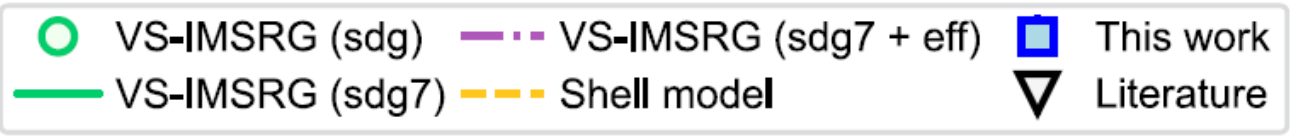
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Magnetic dipole moments in Sb



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



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



Two-body-current corrections to magnetic moments

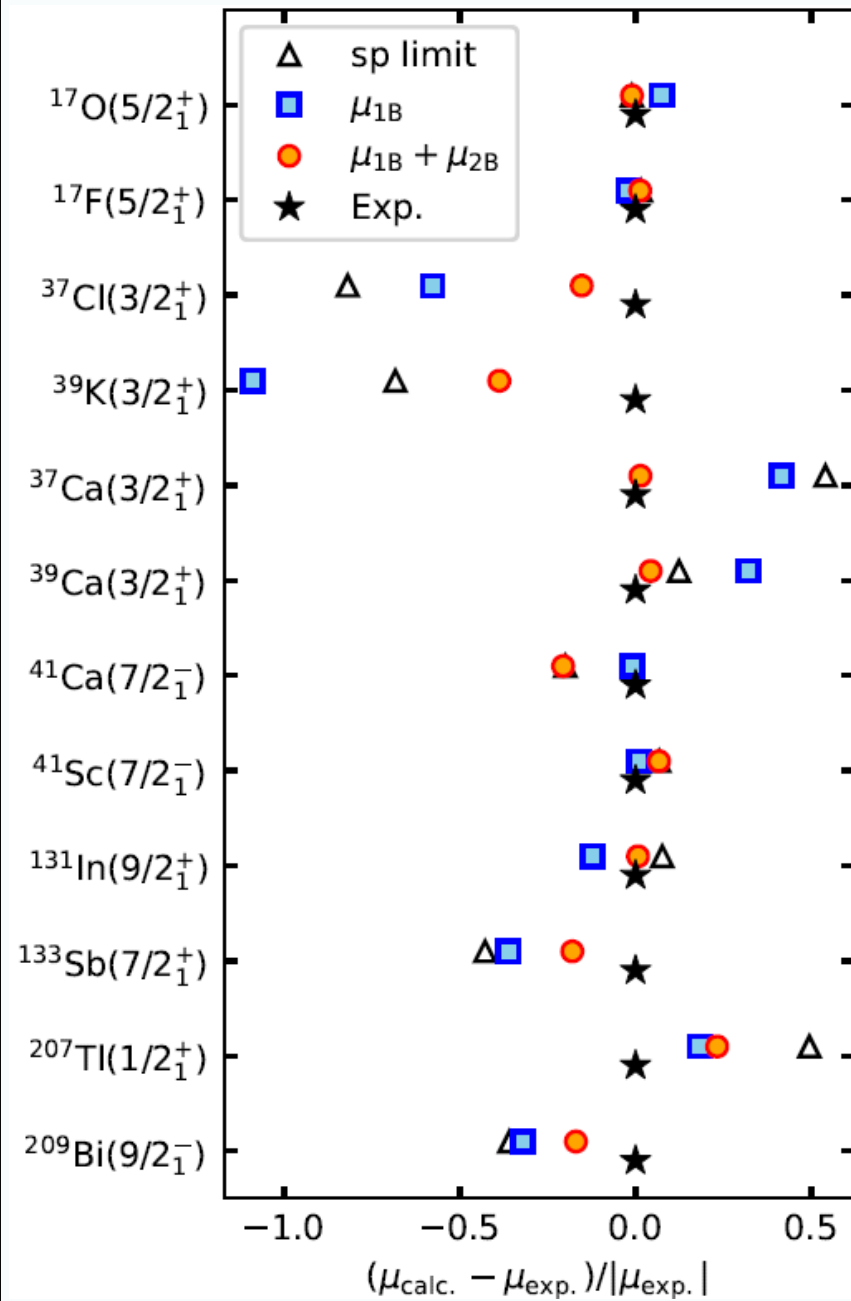


FIG. 1. Magnetic dipole moments of near doubly magic nuclei from $A = 17 - 209$ computed with the VS-IMSRG(2) relative to the experimental values. Results are shown at the one-body level, μ_{1B} (blue squares), and including 2BC, $\mu_{1B} + \mu_{2B}$ (red circles) based on the 1.8/2.0 (EM) NN+3N interactions. The experimental dipole moments (stars) are taken from Ref. [21, 35]. In addition, we show the simple single-particle (sp) limit (without many-body correlations and without 2BC).

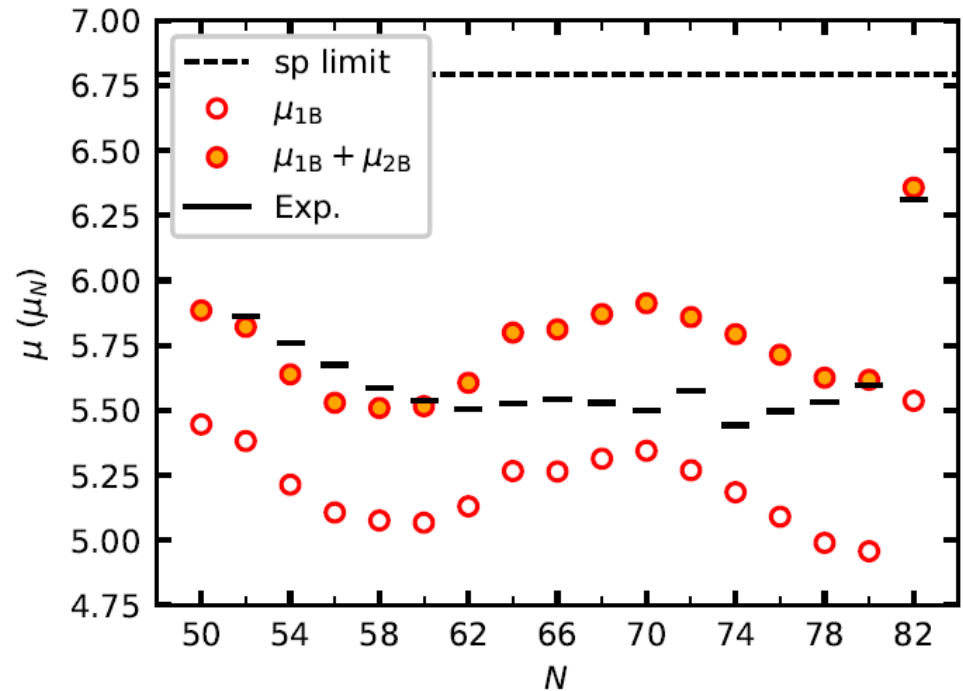


FIG. 4. Magnetic dipole moments of the $9/2^+$ ground state for the odd-mass indium isotopes computed with the VS-IMSRG(2) including 2BC, in comparison to experiment [21, 52].

T. Miyagi et al., arXiv:2311.14383



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NLO magnetic moment operators

(slide by Herlik Wigowo)

The NLO intrinsic and Sachs contributions to the magnetic moment operator are given by

$$\hat{\boldsymbol{\mu}}_{2b}^{\text{NLO, int}}(\mathbf{r}) = -\frac{g_A^2 m_\pi}{8\pi F_\pi^2} (\hat{\boldsymbol{\tau}}_1 \times \hat{\boldsymbol{\tau}}_2)_z \left\{ \left(1 + \frac{1}{m_\pi r}\right) [(\hat{\boldsymbol{\sigma}}_1 \times \hat{\boldsymbol{\sigma}}_2) \cdot \hat{\mathbf{r}}] \hat{\mathbf{r}} - (\hat{\boldsymbol{\sigma}}_1 \times \hat{\boldsymbol{\sigma}}_2) \right\} e^{-m_\pi r}$$

and

$$\hat{\boldsymbol{\mu}}_{2b}^{\text{NLO, Sachs}}(\mathbf{r}) = -\frac{1}{2} (\hat{\boldsymbol{\tau}}_1 \times \hat{\boldsymbol{\tau}}_2)_z V_{1\pi}(r) \mathbf{R}_{\text{NN}} \times \mathbf{r},$$

relative coordinate

COM

respectively, where

$$V_{1\pi}(r) = \frac{m_\pi^2 g_A^2}{12\pi F_\pi^2} (\hat{\boldsymbol{\tau}}_1 \cdot \hat{\boldsymbol{\tau}}_2) \left[\hat{S}_{12} \left(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}\right) + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 \right] \frac{e^{-m_\pi r}}{r}$$

Tensor operator:

$$\hat{S}_{12} = 3 (\hat{\mathbf{r}} \cdot \hat{\boldsymbol{\sigma}}_1) (\hat{\mathbf{r}} \cdot \hat{\boldsymbol{\sigma}}_2) - \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2.$$

R. Seutin, et.al, PRC 108, 054005 (2023)



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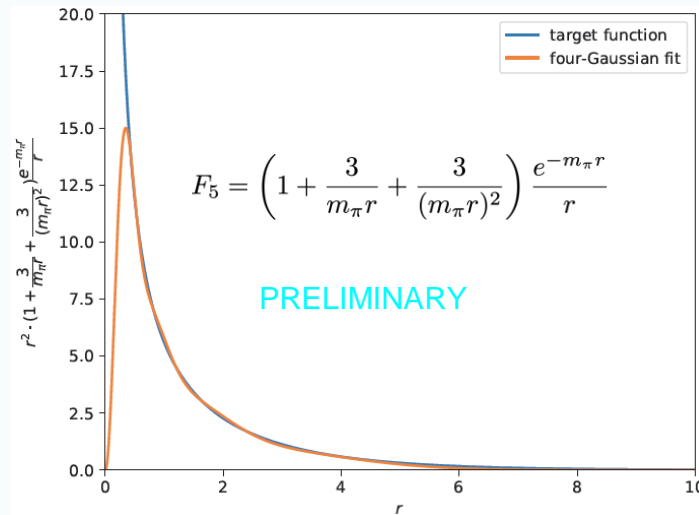
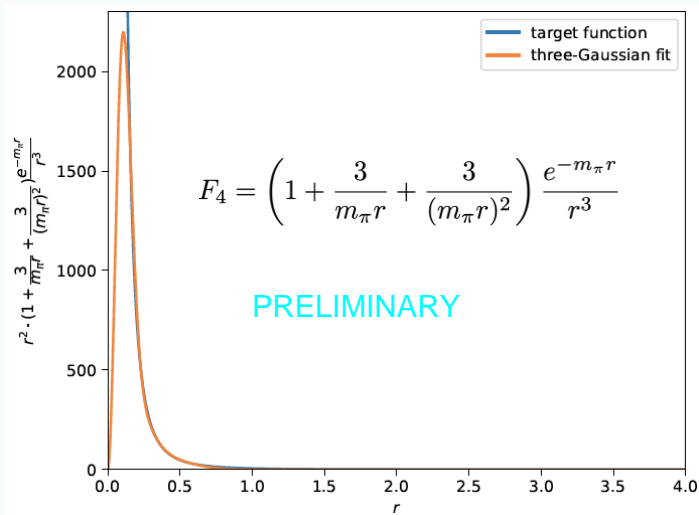
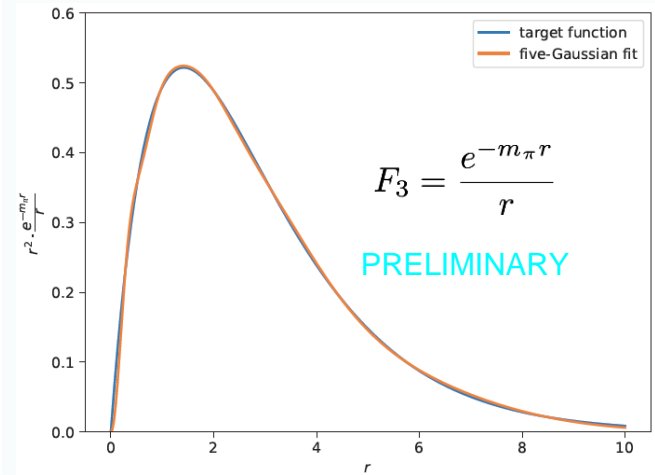
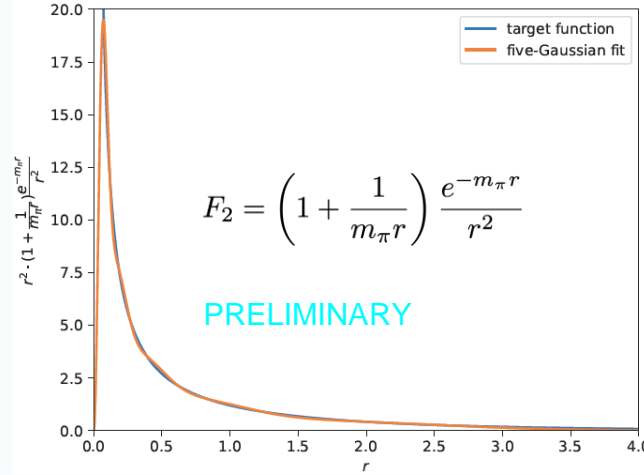
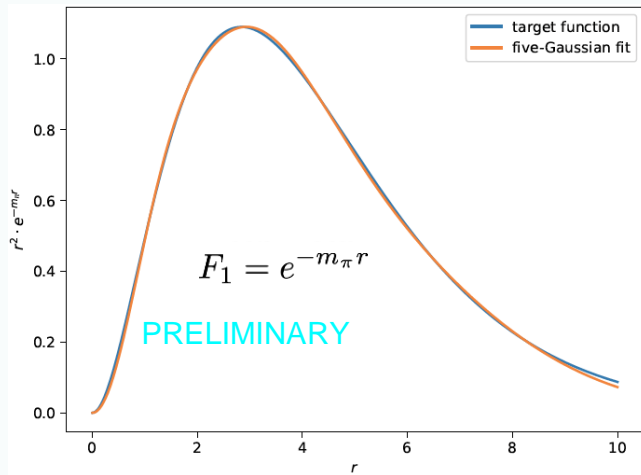


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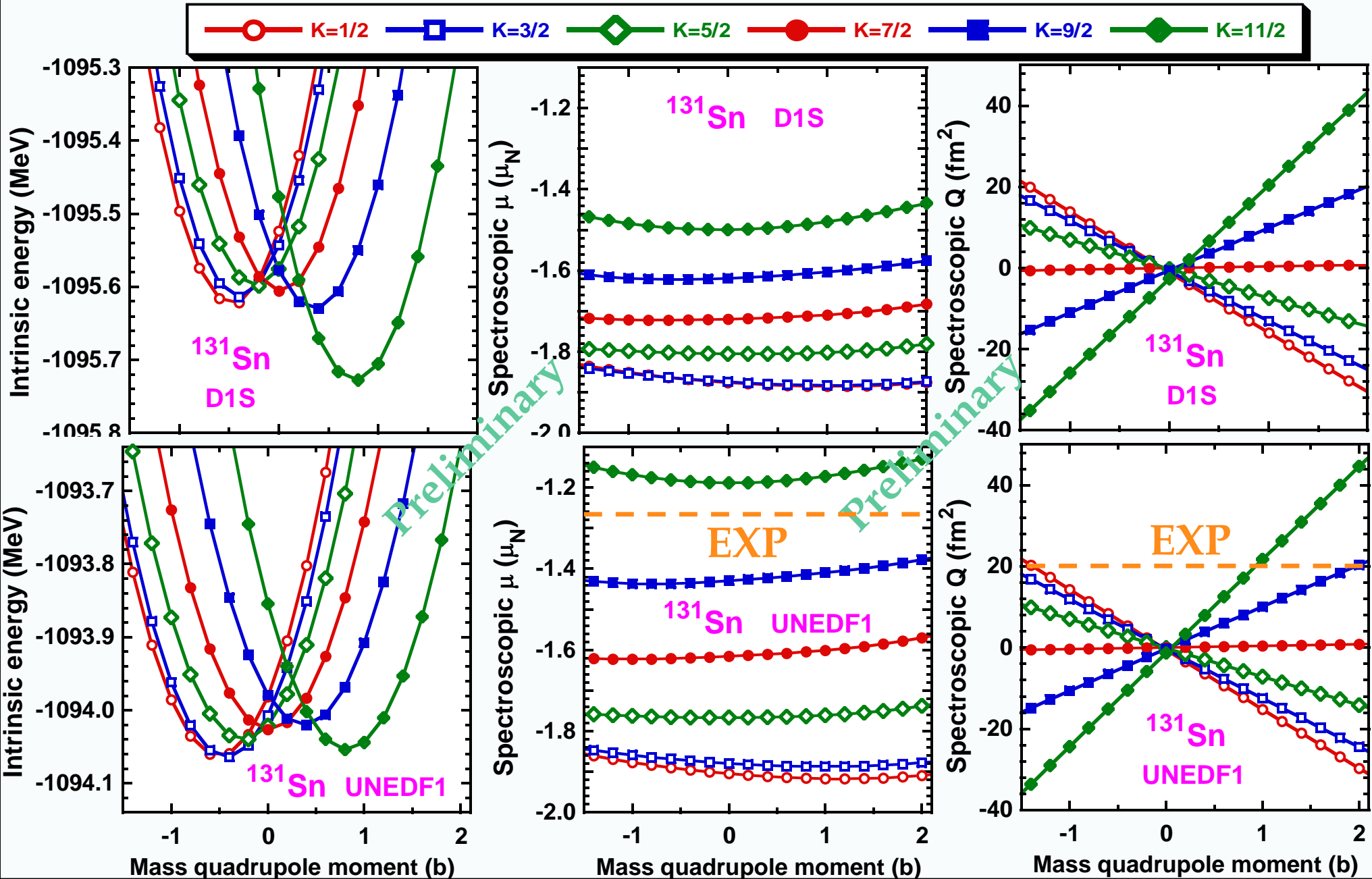


NLO magnetic moment operators

(slide by Herlik Wigowo)



K-mixing



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Energies of the K-mixed states

```
*****  
*  
*          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  |  
*****
```

Preliminary

$E_{\text{intrinsic}}(11/2) = -1092.055162$

$E_{\text{projected}}(11/2) = -1092.310241$



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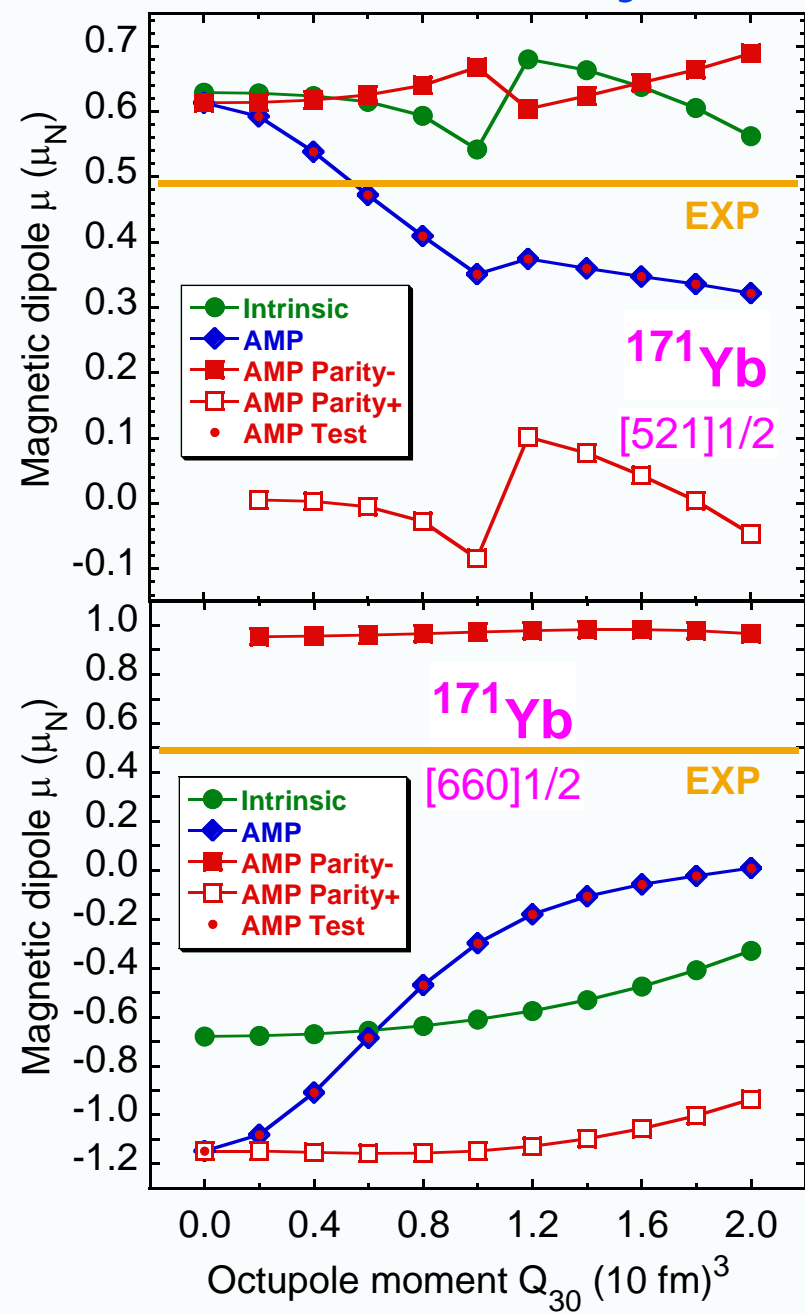
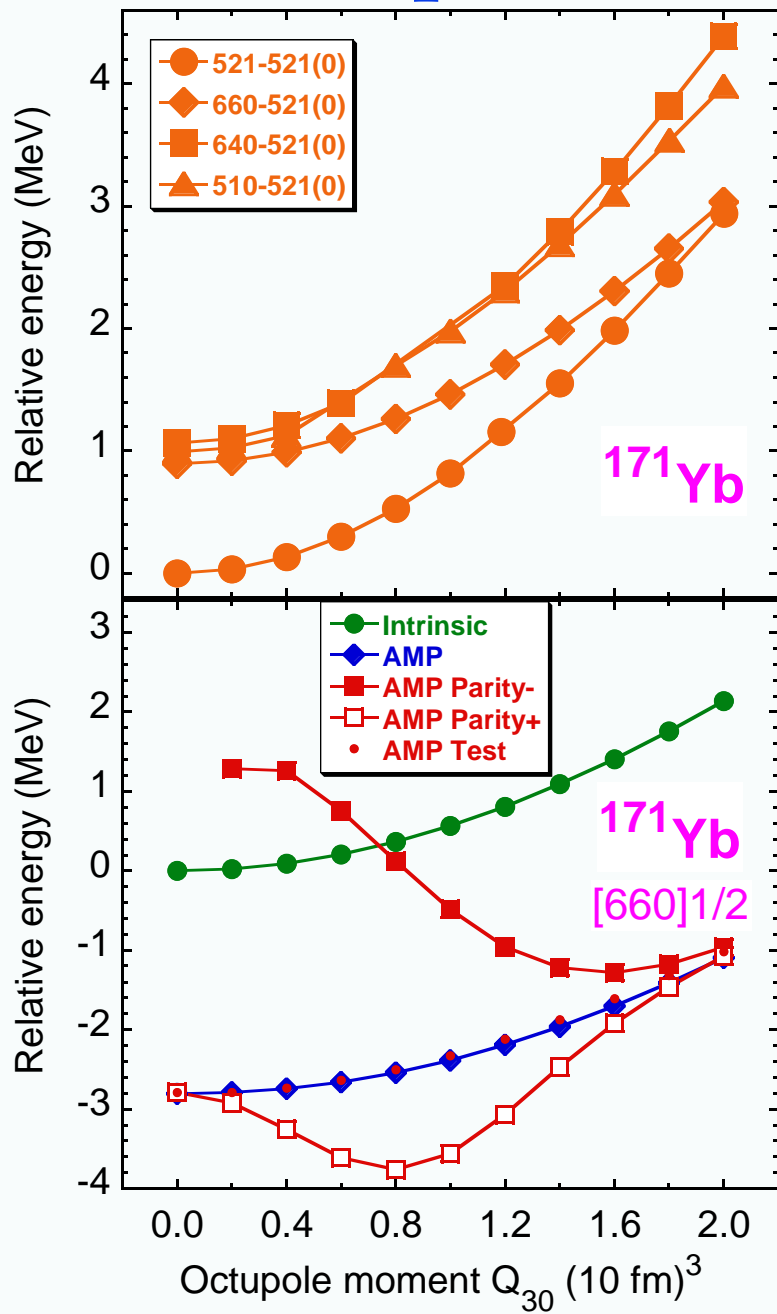
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Octupole deformation - a case study



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Thank you



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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:

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

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

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 $|Im\rangle$ 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 :

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

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

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]:

$$\text{for an odd proton: } \left\{ \begin{array}{ll} \mu = j - \frac{1}{2} + \mu_p & \text{for } j = l + \frac{1}{2} \\ \mu = \frac{j}{j+1} \left(j + \frac{3}{2} - \mu_p \right) & \text{for } j = l - \frac{1}{2} \end{array} \right. \quad (2.2)$$

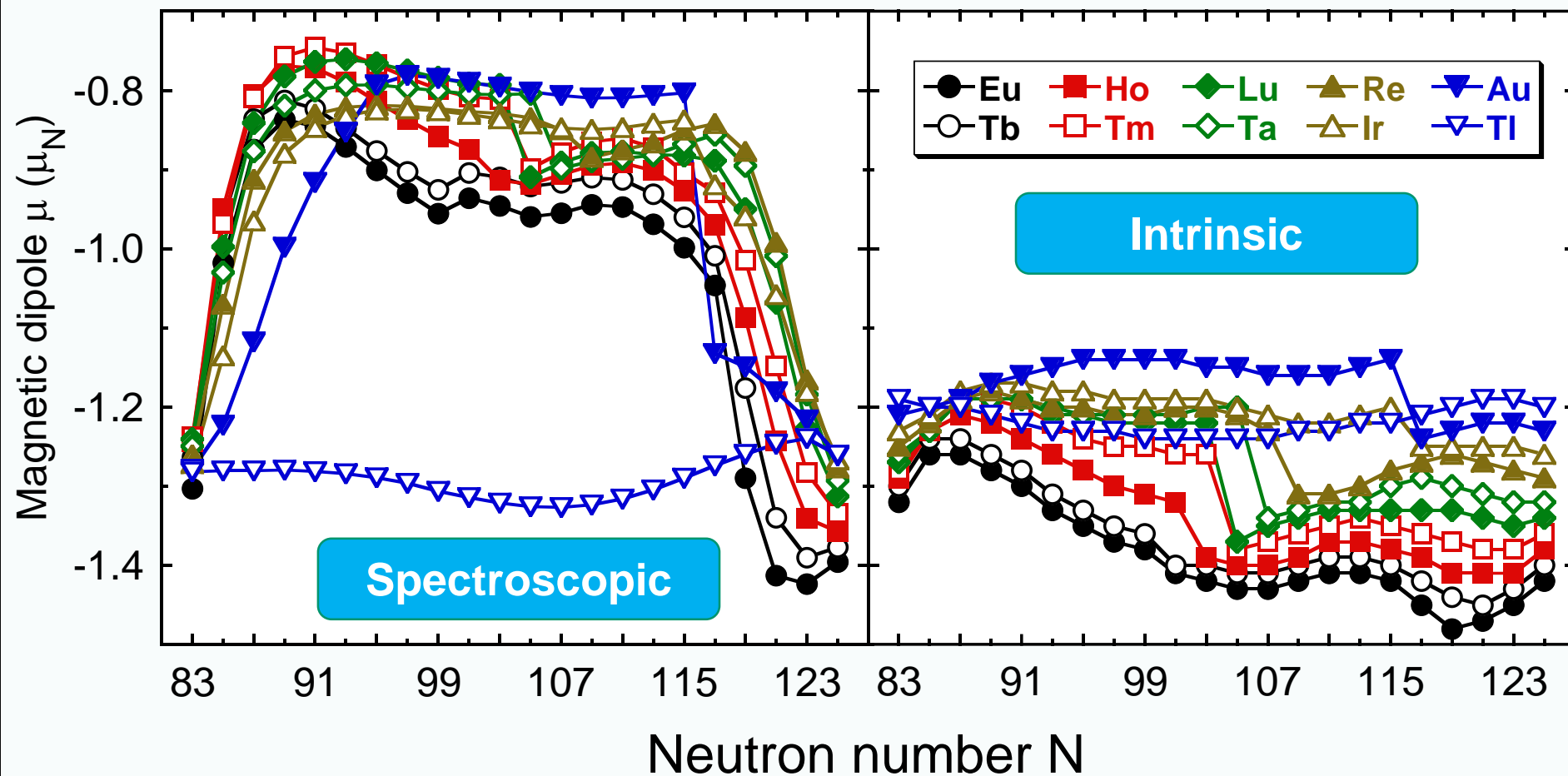
$$\text{for an odd neutron: } \left\{ \begin{array}{ll} \mu = \mu_n & \text{for } j = l + \frac{1}{2} \\ \mu = -\frac{j}{j+1} \mu_n & \text{for } j = l - \frac{1}{2} \end{array} \right. \quad (2.3)$$

**Schmidt
limits**

These single particle moments calculated using the free proton and free neutron moments ($\mu_p = +2.793$, $\mu_n = -1.913$) are called the Schmidt moments. In a nucleus, the magnetic



Heavy deformed $v13/2^+$ odd-N nuclei



Conclusion:
Spectroscopic magnetic dipole moments
cannot be inferred from the intrinsic ones

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



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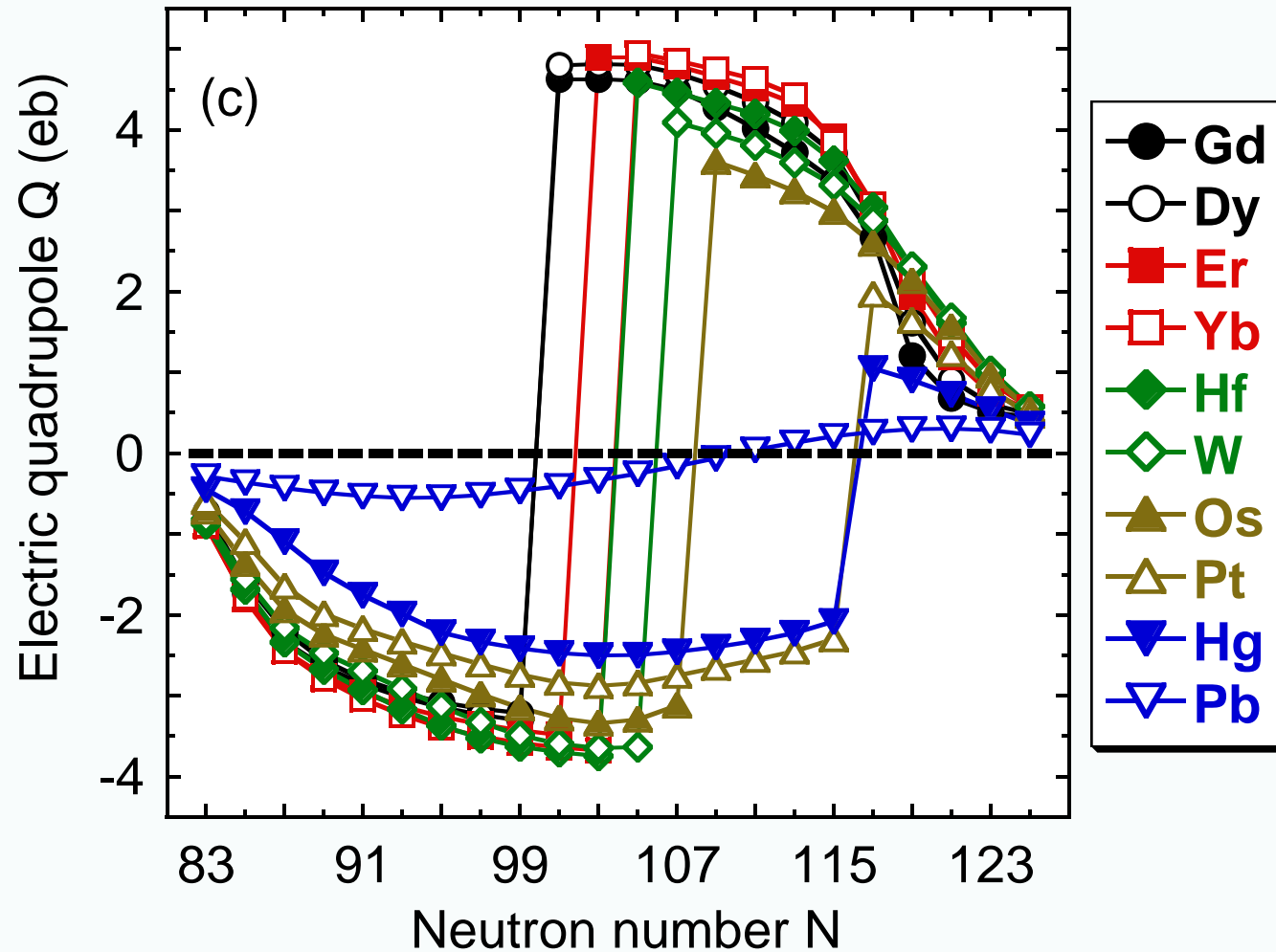
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Heavy deformed $v13/2^+$ odd-N nuclei



Conclusion:

Rules of oblate and prolate polarizations do extend from the magicity towards the open shell systems.

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



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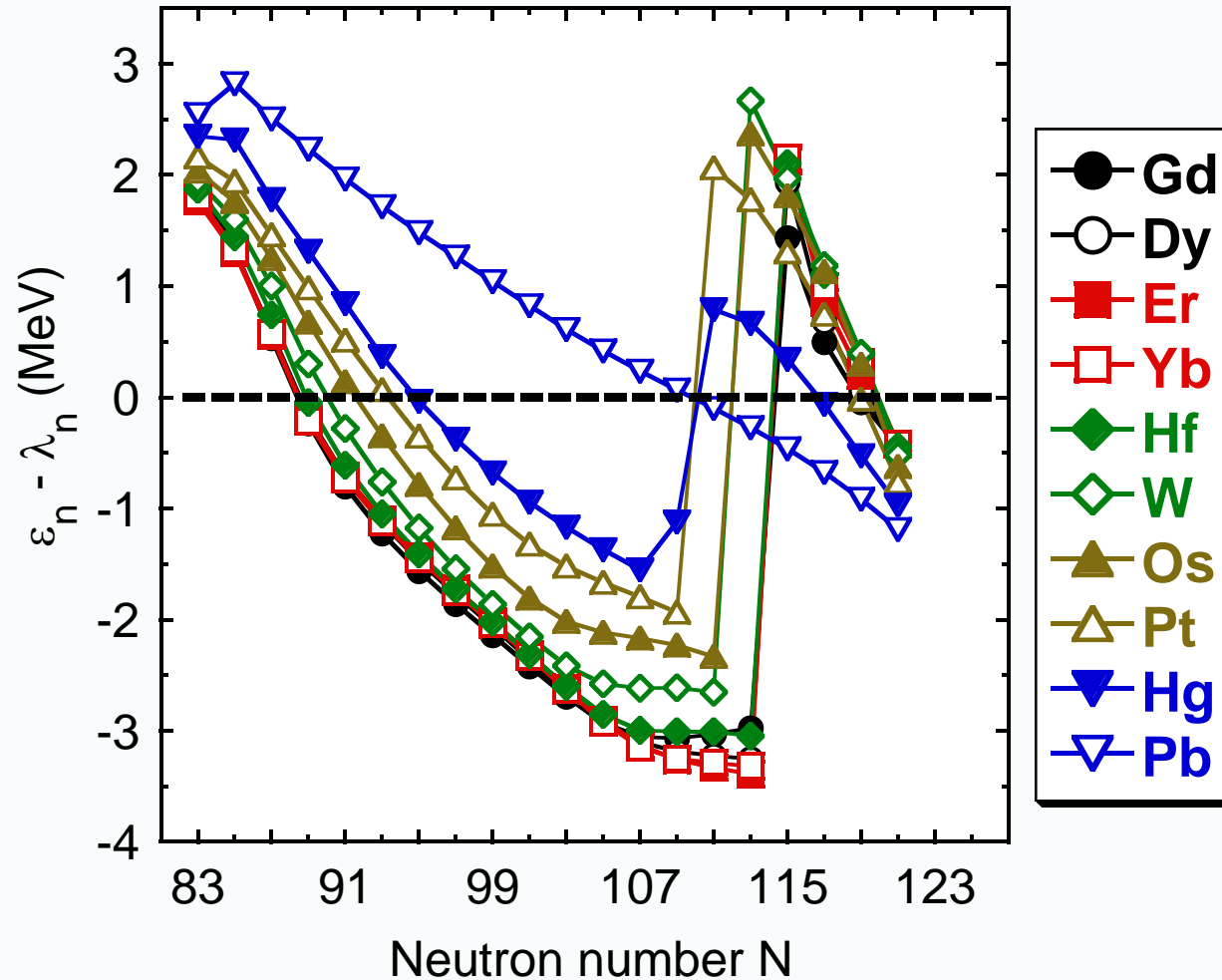
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Heavy deformed $v13/2^+$ odd-N nuclei



Conclusion:

Rules of particle and hole polarizations do not extend from the magicity towards the open shell systems.

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



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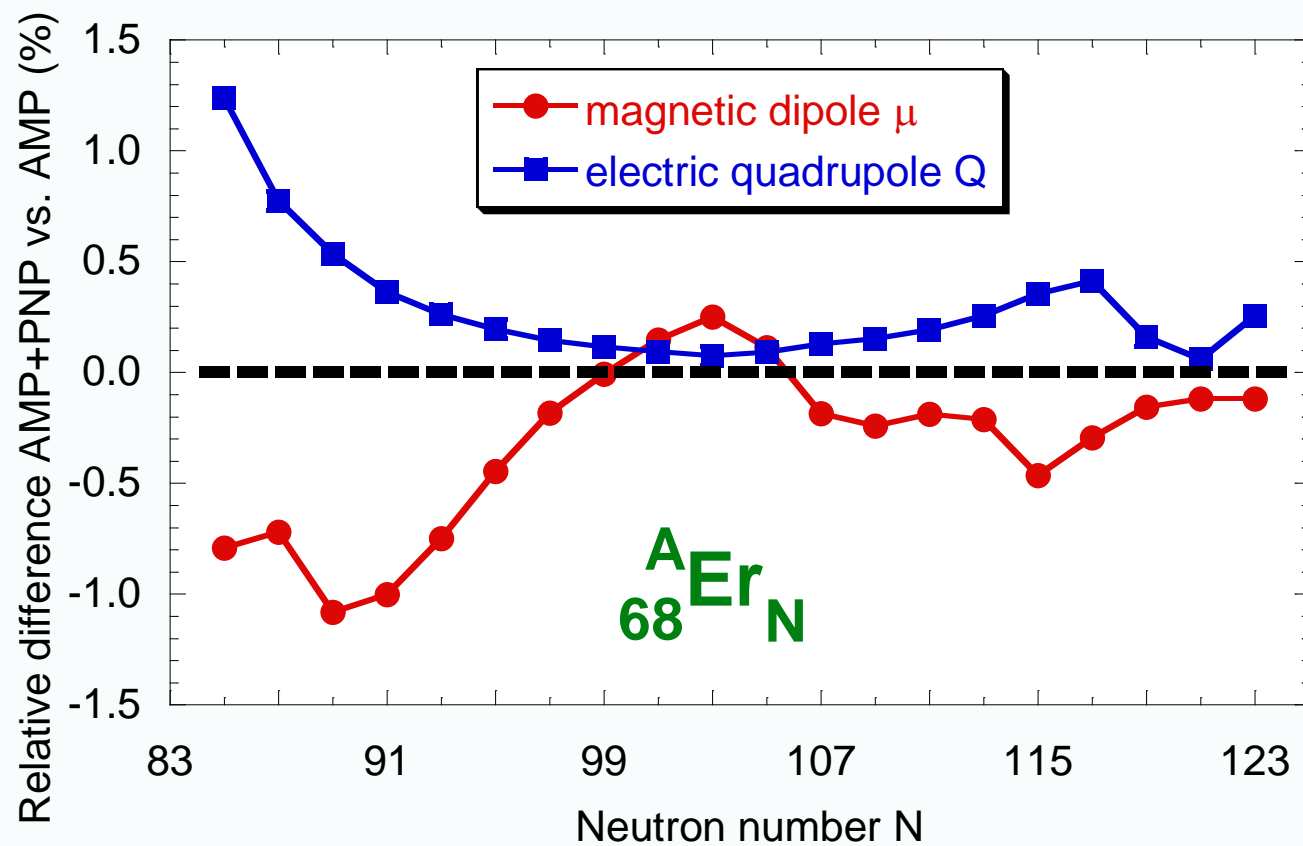


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Insignificant impact of the PNP

UNEDF1, $g'_0=1.7$



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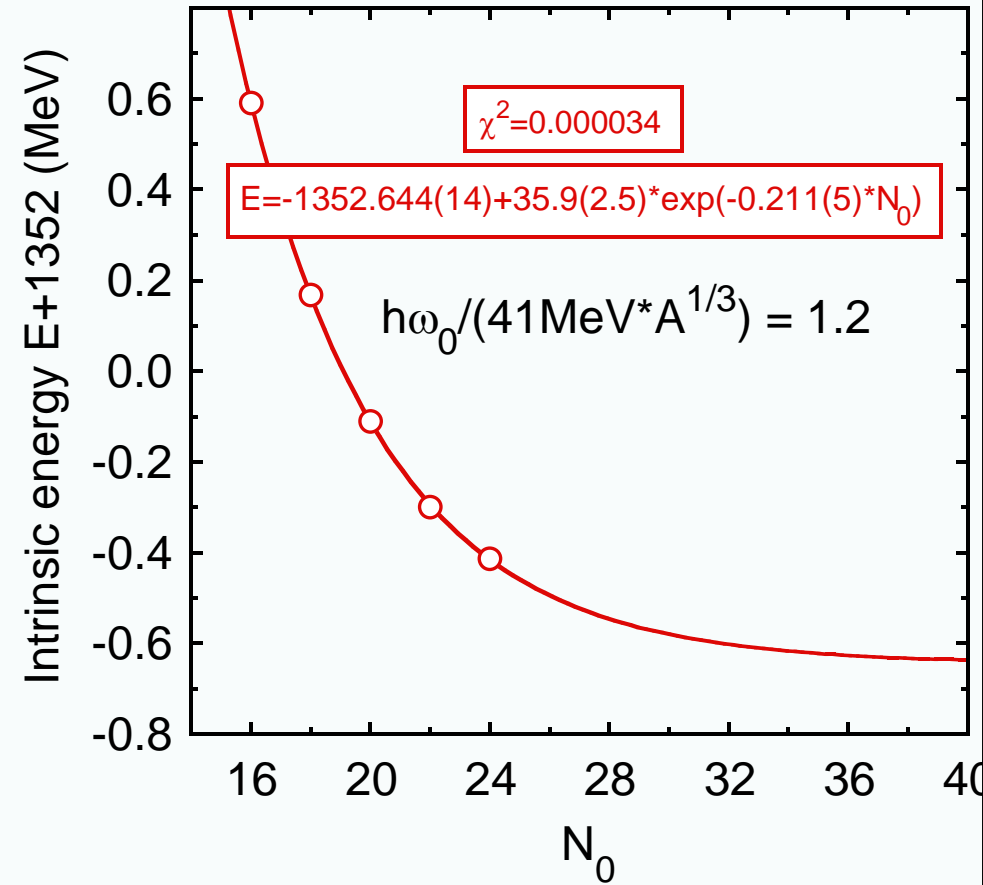
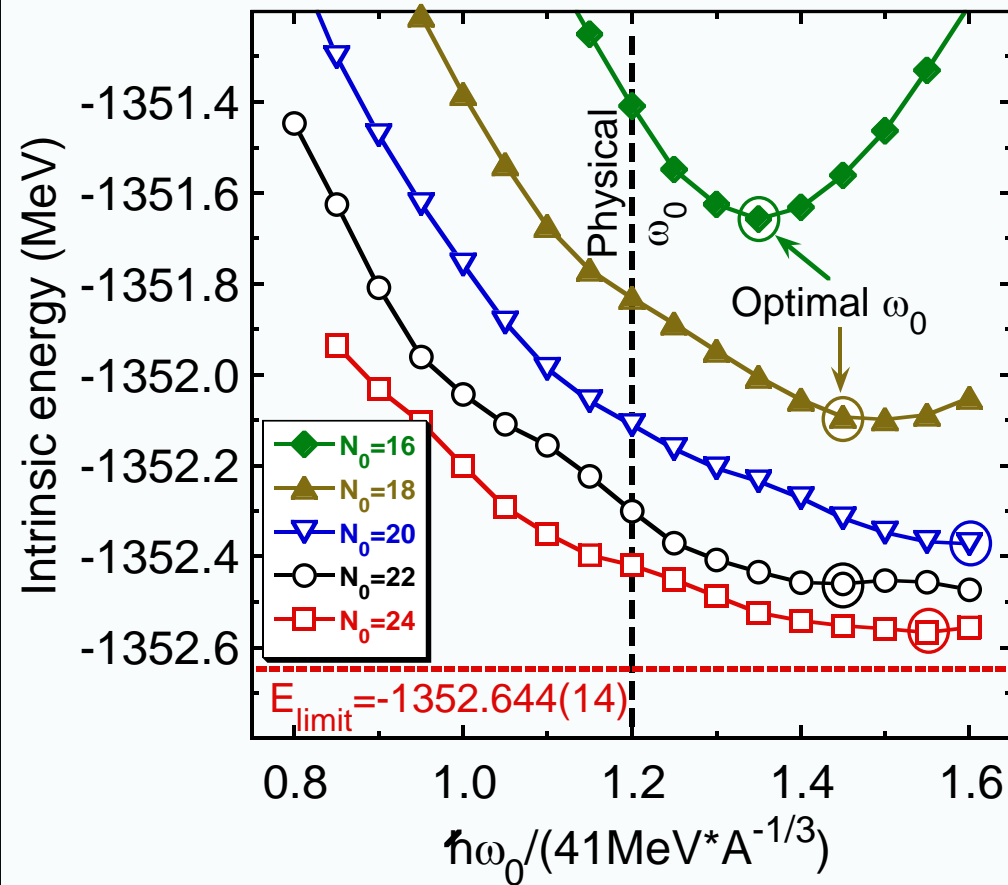


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Convergence of the total HFB intrinsic energy

^{167}Ho 11/2-, UNEDF1, $g'_0=1.7$



$E_{\text{exp}} = -1357.77346$



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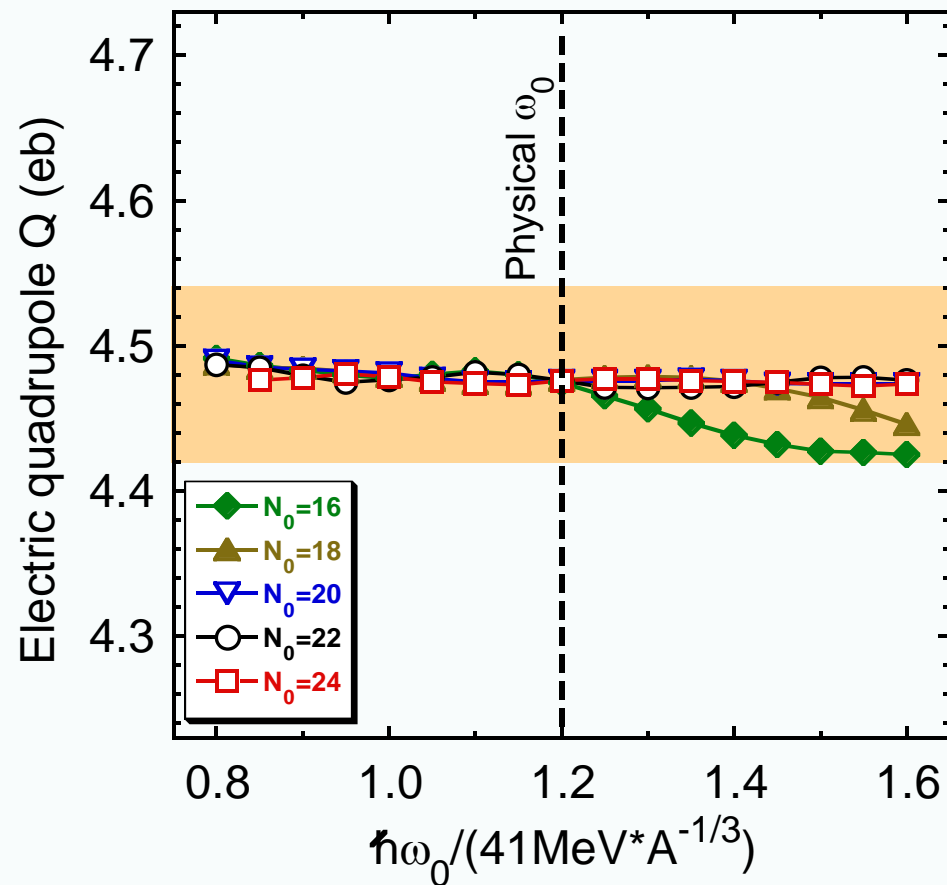
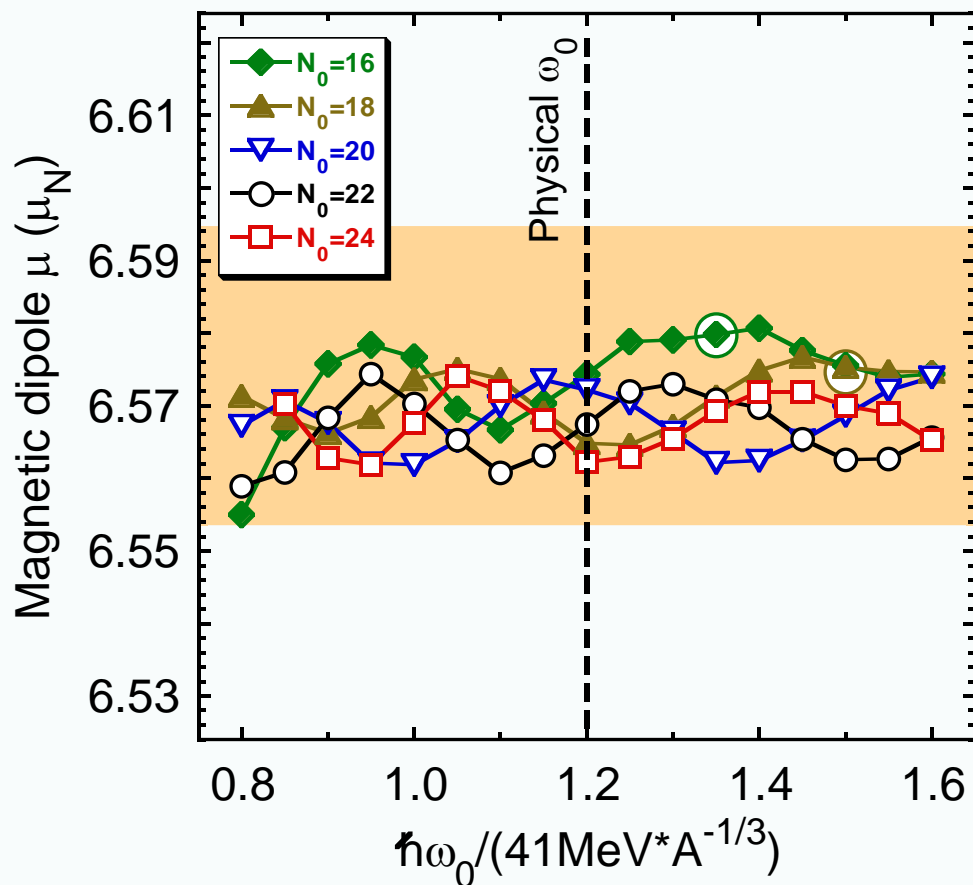


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Convergence of the spectroscopic moments

^{167}Ho 11/2-, UNEDF1, $g'_0=1.7$



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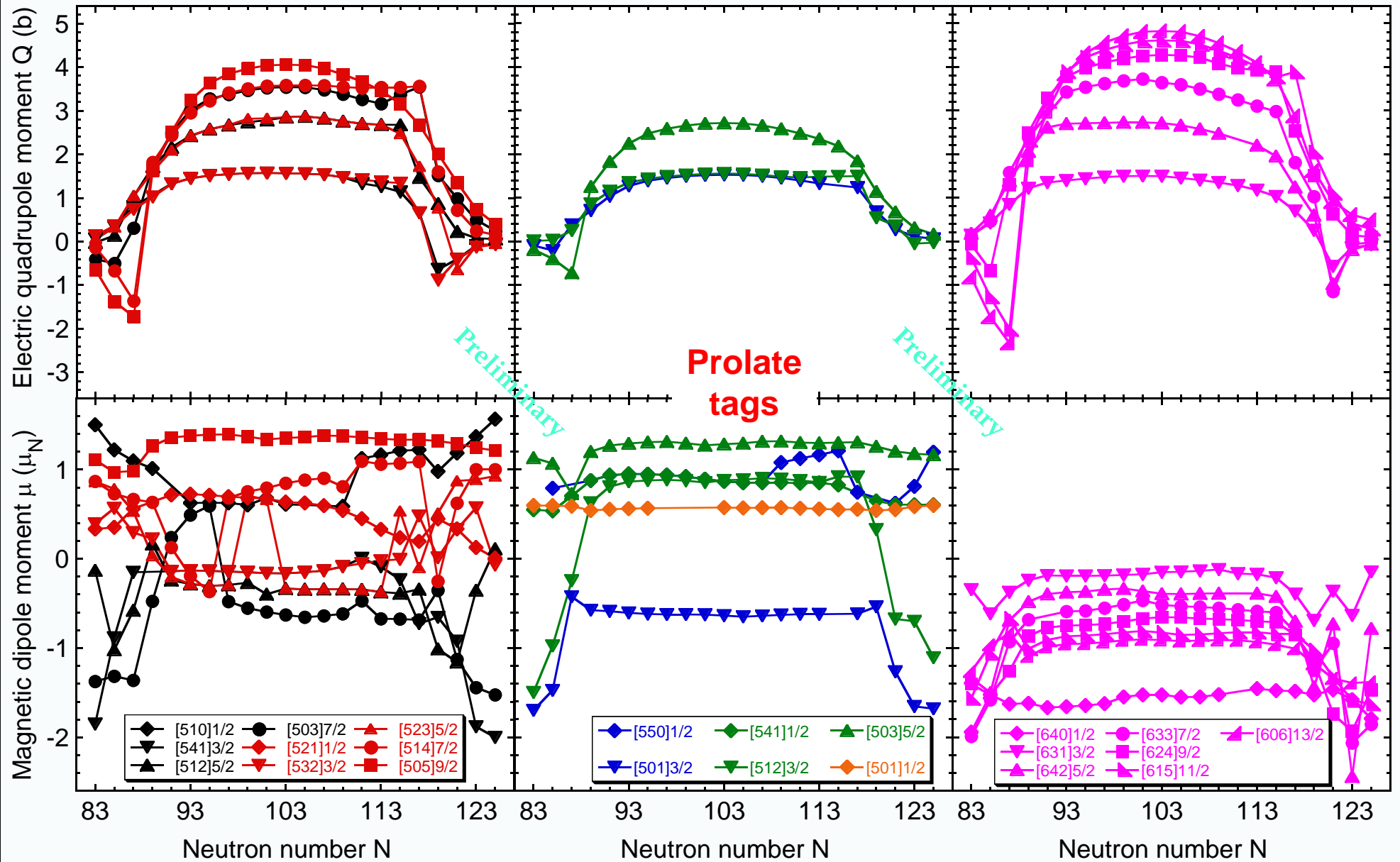
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Electromagnetic moments of odd dysprosium isotopes



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