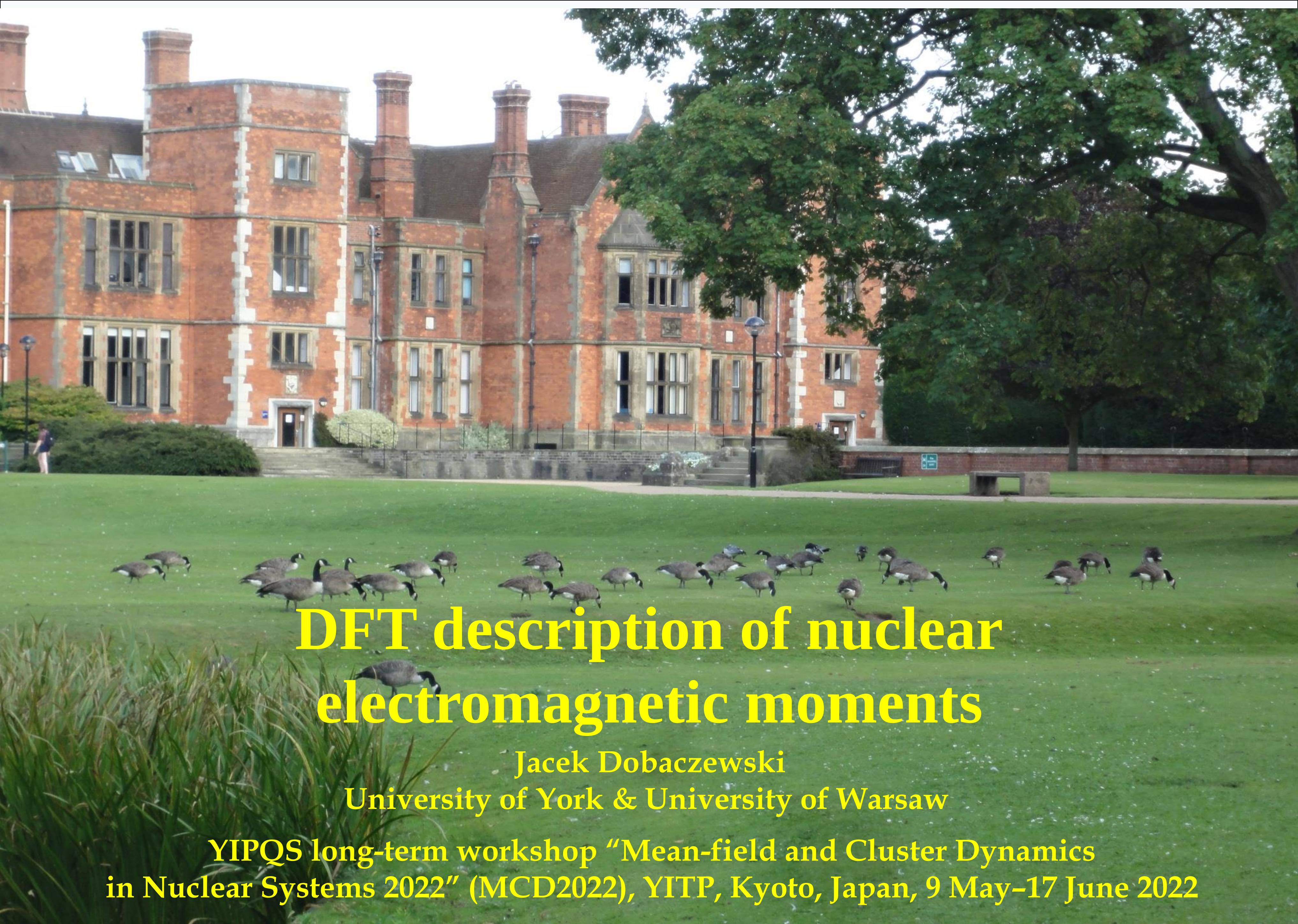

DFT description of nuclear electromagnetic moments

Jacek Dobaczewski

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YIPQS long-term workshop "Mean-field and Cluster Dynamics in Nuclear Systems 2022" (MCD2022), YITP, Kyoto, Japan, 9 May–17 June 2022

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In collaboration with

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Outline

1. Recap on nuclear electromagnetic moments
2. Odd near doubly magic nuclei
3. Indium isotopes
4. Particle-core coupling
5. Antimony, tin, silver
6. Heavy deformed open-shell odd nuclei
   $82 \leq N \leq 126$ & $63 \leq Z \leq 82$
7. Magnetic octupole moments
8. Bohr-Weisskopf correction
9. Conclusions

Recap

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:

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

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

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: $Q_{\lambda\mu}(\vec{r}) = r^\lambda Y_{\lambda\mu}(\theta,\phi)$.
Function $m_{\lambda\mu}(\vec{r})$ is called magnetization density and its higher radial moments

$$M^{(n)}_{\lambda\mu} = \int r^n\, m_{\lambda\mu}(\vec{r})\, d^3\vec{r},$$

define the Bohr-Weisskopf hyperfine splitting corrections.

Mechanism of the e-m moments generation

- In nuclear DFT, properties of odd nuclei can be analysed in terms of the self-consistent polarisation effects caused by the presence of the unpaired nucleon.
- A non-zero quadrupole moment of the odd nucleon induces deformation of the total mean field and thus generates quadrupole moments of all remaining nucleons.

$$V=-\lambda Q_1 Q_2$$

- The latter moments enhance the deformation of the mean field even more, which in turn influences the quadrupole moment of the odd nucleon.
- In a self-consistent solution, these mutual polarisation are effectively summed up to infinity, whereupon the final total quadrupole deformation and electric quadrupole moment Q of the system are generated.
- A non-zero spin and current distributions of the odd particle influence those of all other nucleons and in the self-consistent solution lead to a specific polarisation of the system and its non-zero magnetic dipole moment μ.

$$V=-\lambda \sigma_1 \sigma_2$$

- All nucleons contribute to the moments Q and μ of the system, with individual contributions of nucleons depending on their individual polarisation responses to the deformed and polarised mean field.

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- J. Li and J. Meng, Front. Phys. 13 (2018) 132109
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- P.L. Sassarini *et al*, arXiv:2111.04675 (2021)
- V. Tselyaev *et al.*, arXiv:2201.08838 (2022)

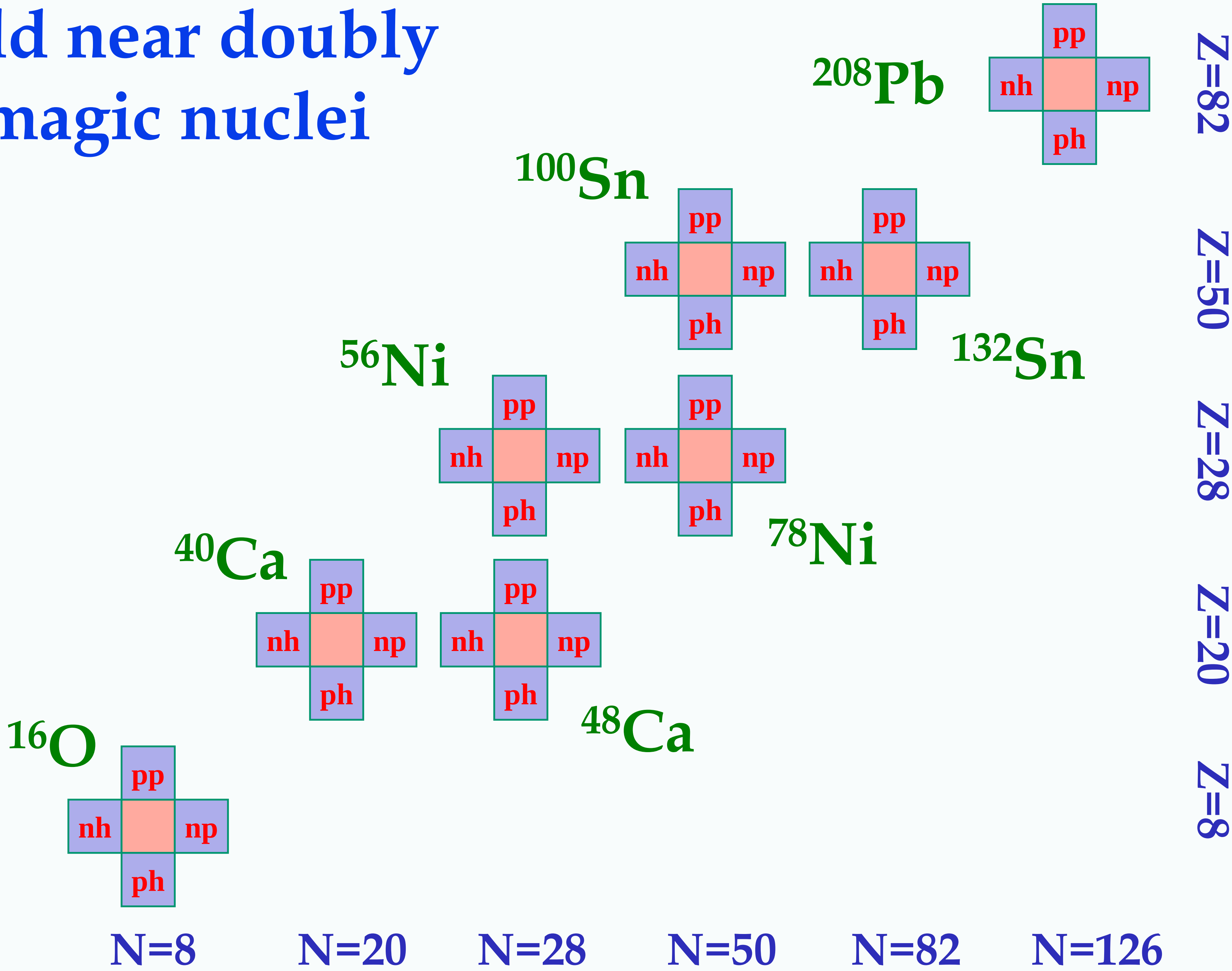
So far …

	Borrajo and Egido	Péru et al.	Bonneau et al.	Li and Meng	Co' et al.	Sassarini et al.
Nuclei Region	Mg Isotopes	Hg Isotopes	A≈50, 100, 178, 236	A≈16, 40, 208	Doubly magic	All doubly magic
HF				✓	✓	✓
HF-BCS			✓			
HFB	✓	✓				
s.p Operator	✓	✓	✓	Meson Ex. Current	Meson Ex. Current	✓
Eff. spin g-factor		✓	✓			
Core contribution	Microscopic	Model	Microscopic	Model	Model	Microscopic
Collective Mixing (BMF)	✓					
Blocking	✓	✓	✓	N/A	N/A	N/A
AMP	✓					✓
Skyrme			SIII, SLyIII.0.8			UNEDF1, SLy4, SkO'
Gogny	D1S	D1M			D1S, D1M	D1S
Regularized						N^3LO
Relativistic Lagrangian				✓		
HO Basis	Spherical	Deformed	Cylindrical	Spherical	Space coordinates	Spherical
Oscillator Shells	8	19	13	not specified	N/A	16
Parity	✓	✓	✓	✓	✓	✓
Signature	✓	✓		✓	✓	
Time-reversal	✓	✓		✓	✓	
Spherical				✓	✓	
Axial		✓	✓			✓
Triaxial	✓					
Refrence Frame	Intrinsic	Intrinsic	Intrinsic	Laboratory	Laboratory	Intrinsic

P. L. Sassarini *et al.*, to be published

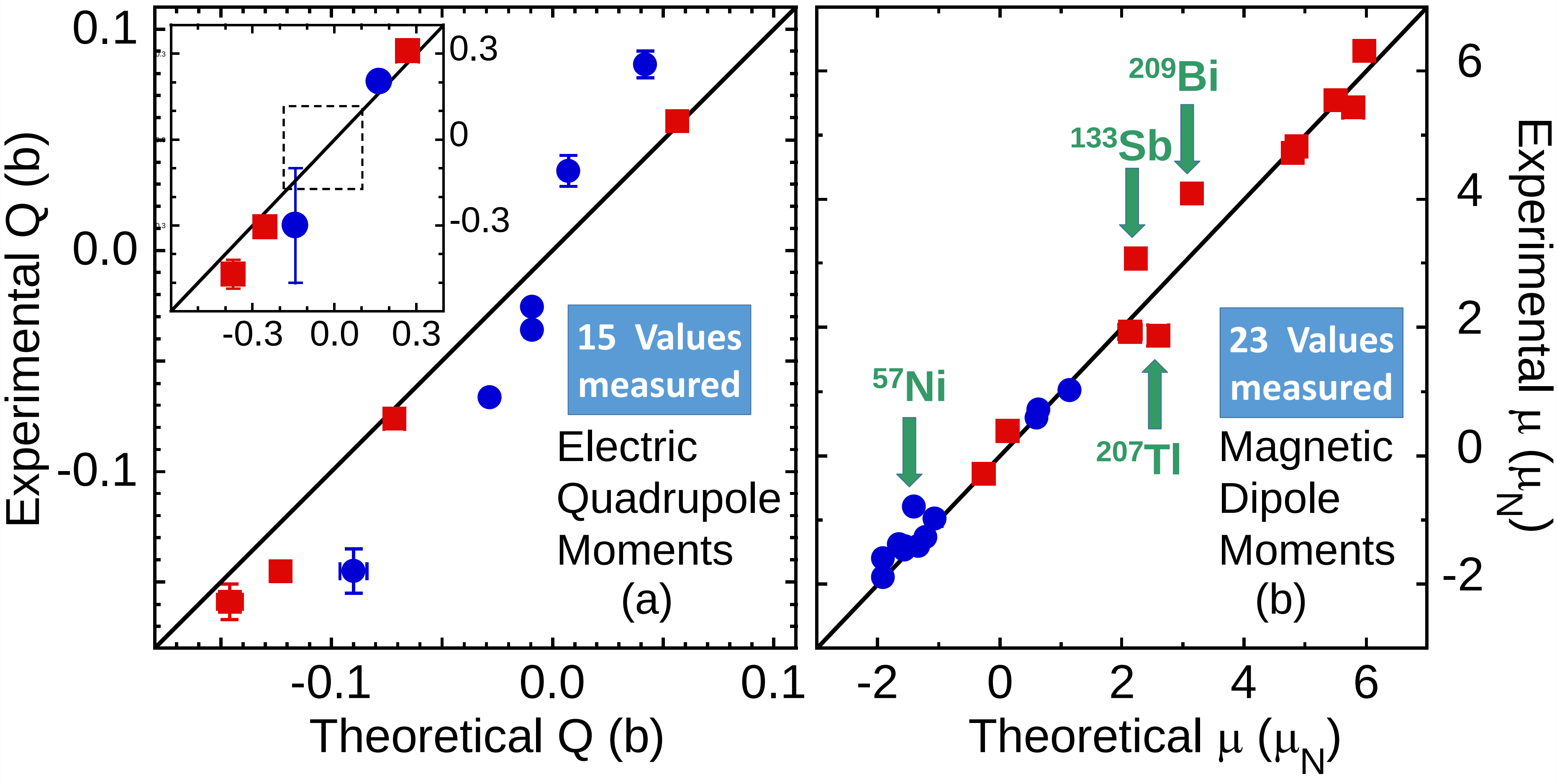
Odd near doubly magic nuclei

Odd near doubly magic nuclei



Quadrupole & dipole moments

P. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



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

Time-odd densities & Landau parameters

- In nuclear DFT, what really matters is not the interaction but the functional, that is, the energy density expressed as a function of local or non-local particle $\rho(\vec{r})$, spin $\vec{s}(\vec{r})$, kinetic $\tau(\vec{r})$, spin-kinetic $\vec{T}(\vec{r})$, current $\vec{j}(\vec{r})$, spin-current $\mathsf{J}(\vec{r})$, . . . , densities.

- In particular, for one-body time-odd observables like magnetic moments, the time-odd densities $\vec{s}(\vec{r})$ and $\vec{j}(\vec{r})$ are essential. For a local functional, the corresponding relevant terms read:

$$
\begin{aligned}
\mathcal{H}(\vec{r}) &= \textstyle\sum_{t=0,1} C_t^s\, \vec{s}_t(\vec{r}) \cdot \vec{s}_t(\vec{r}) \\
&+ \textstyle\sum_{t=0,1} C_t^\tau \Big(\rho_t(\vec{r})\tau_t(\vec{r}) - \vec{j}_t(\vec{r}) \cdot \vec{j}_t(\vec{r})\Big) \\
&+ \textstyle\sum_{t=0,1} C_t^T \Big(\vec{s}_t(\vec{r}) \cdot \vec{T}_t(\vec{r}) - \mathsf{J}_t^2\Big)
\end{aligned}
$$

where $t = 0, 1$ stands for the isoscalar and isovector terms, respectively.

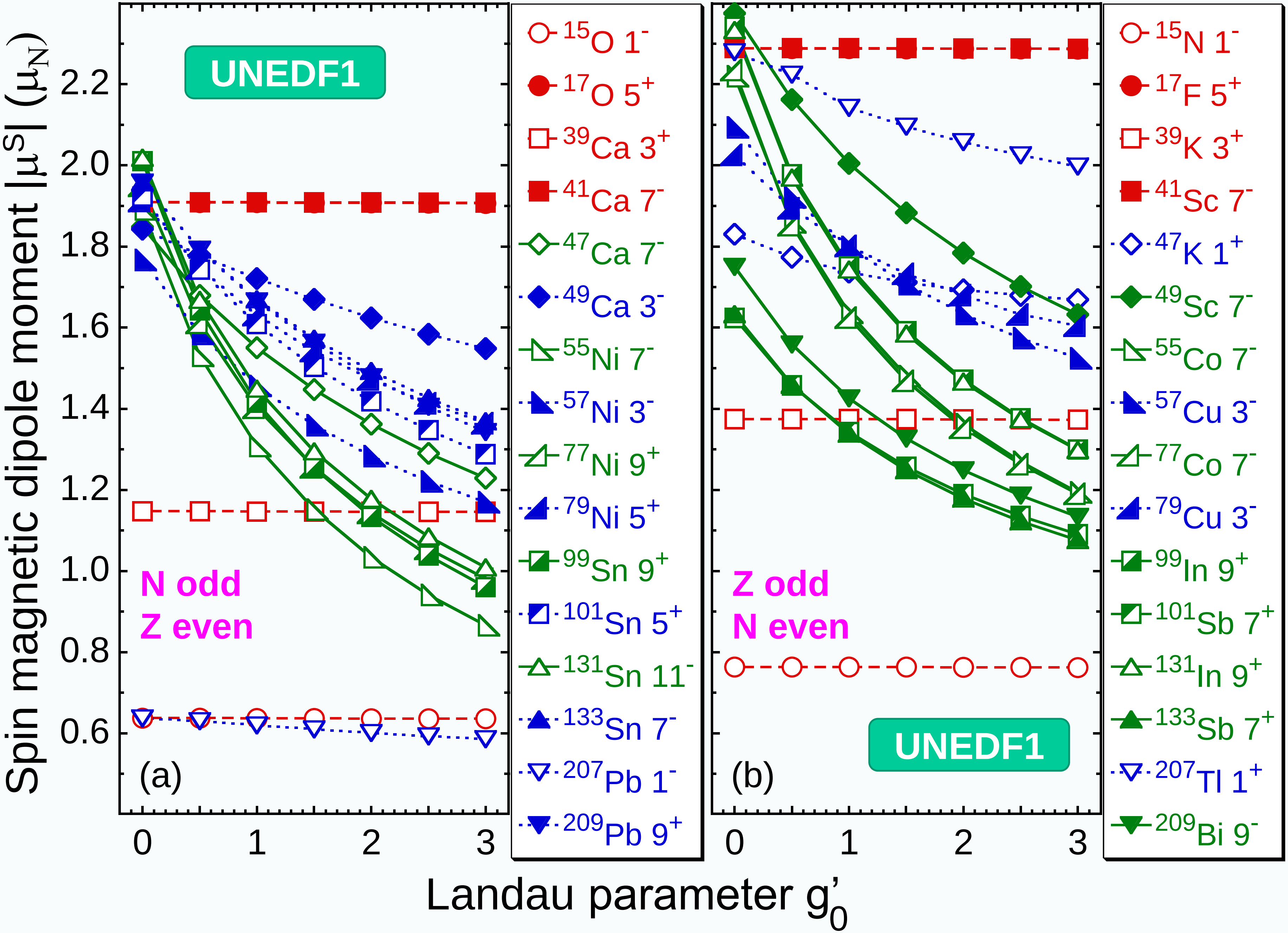
- In the present study, we analyse the isovector spin-spin term only and we parameterise it by the Landau parameter g_0' as

$$
g_0' = N_0\Big(2C_1^s + 2C_1^T\,(3\pi^2\rho_0/2)^{2/3}\Big),
$$

where the normalization factor N_0 is the level density at the Fermi surface

$$
\frac{1}{N_0} = \frac{\pi^2\hbar^2}{2m^* k_\mathrm{F}} \approx 150\,\frac{m}{m^*}\ \mathrm{MeV\ fm}^3.
$$

P.L. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



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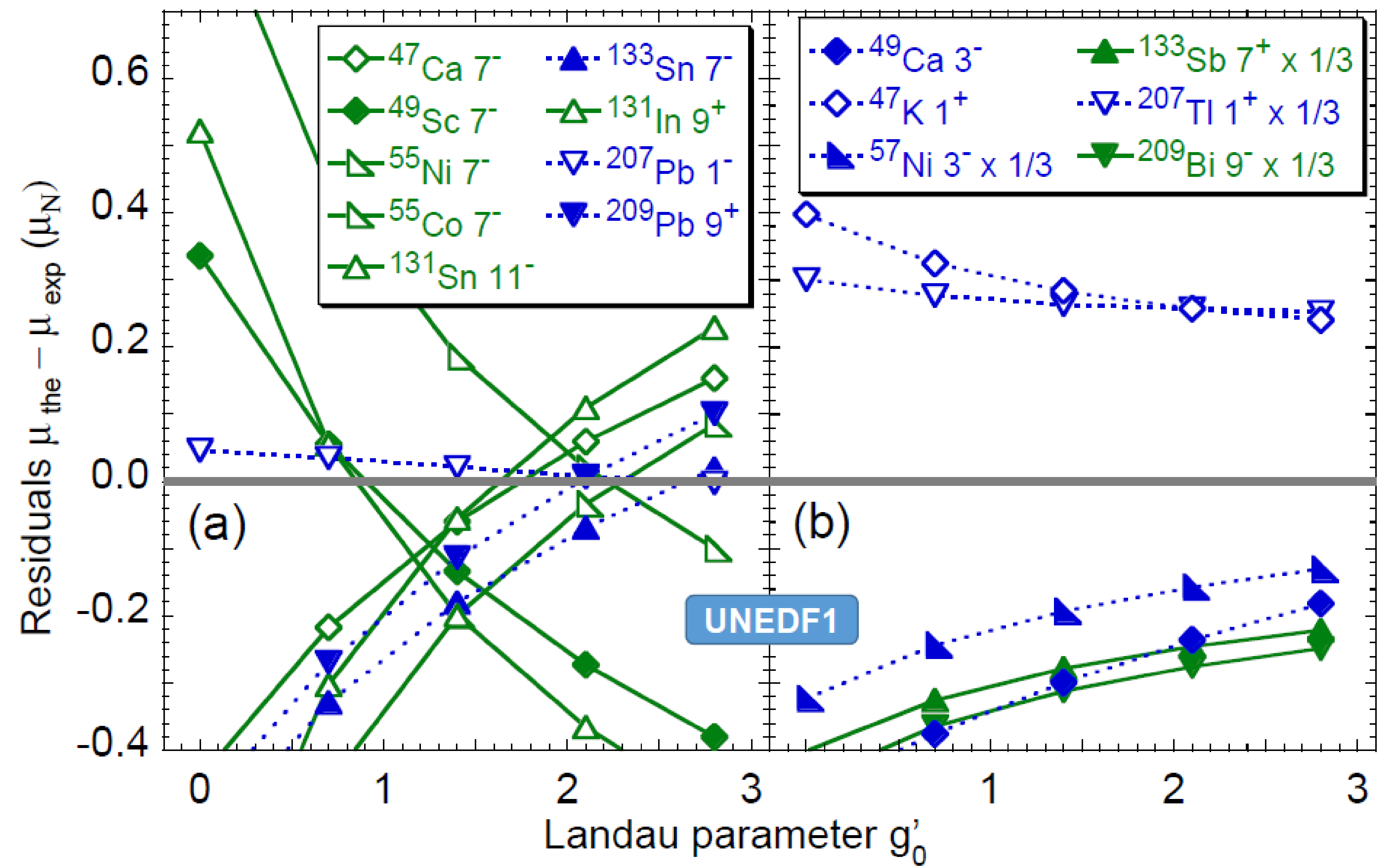
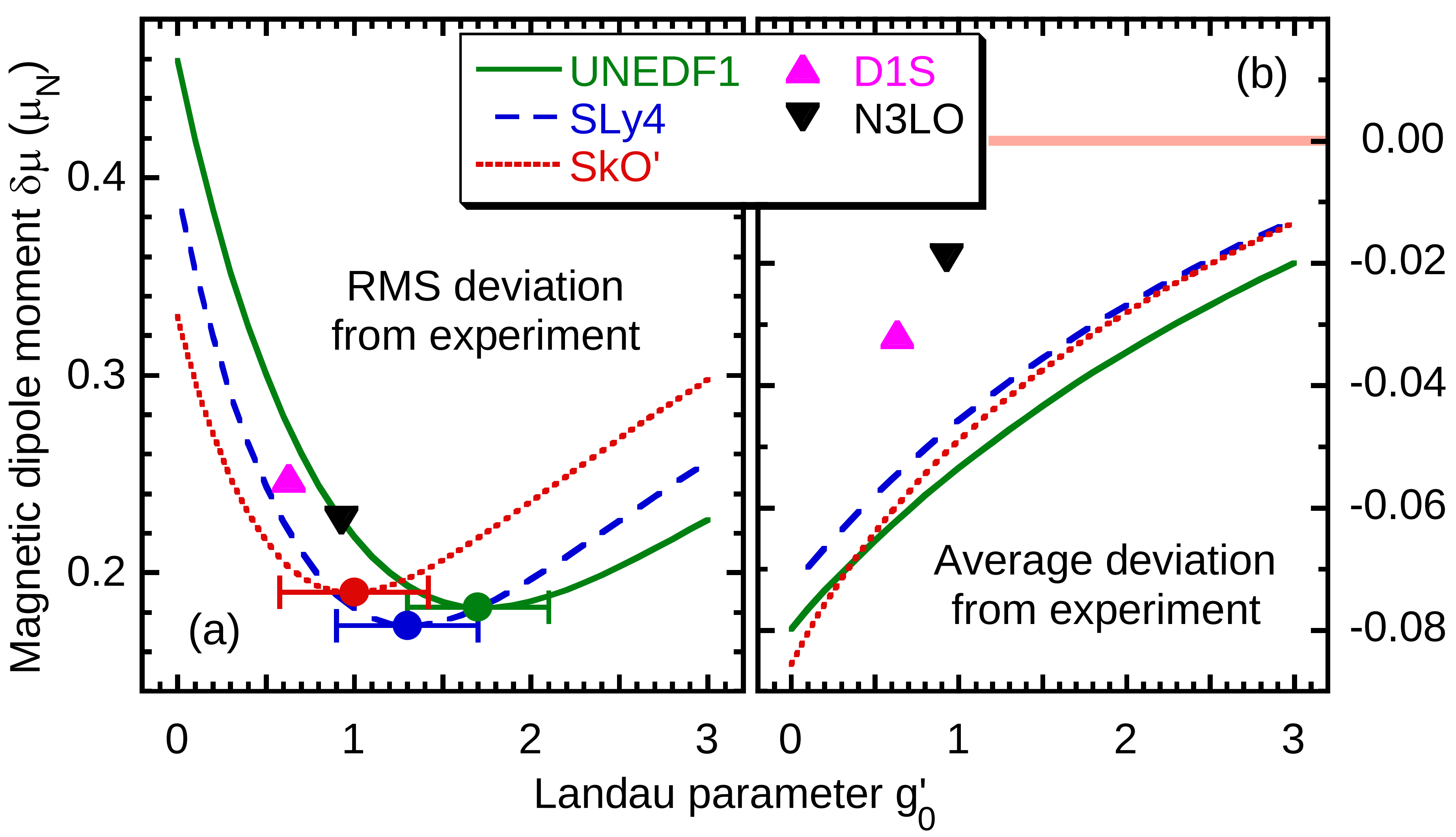
Magnetic dipole moments vs. experiment

P.L. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



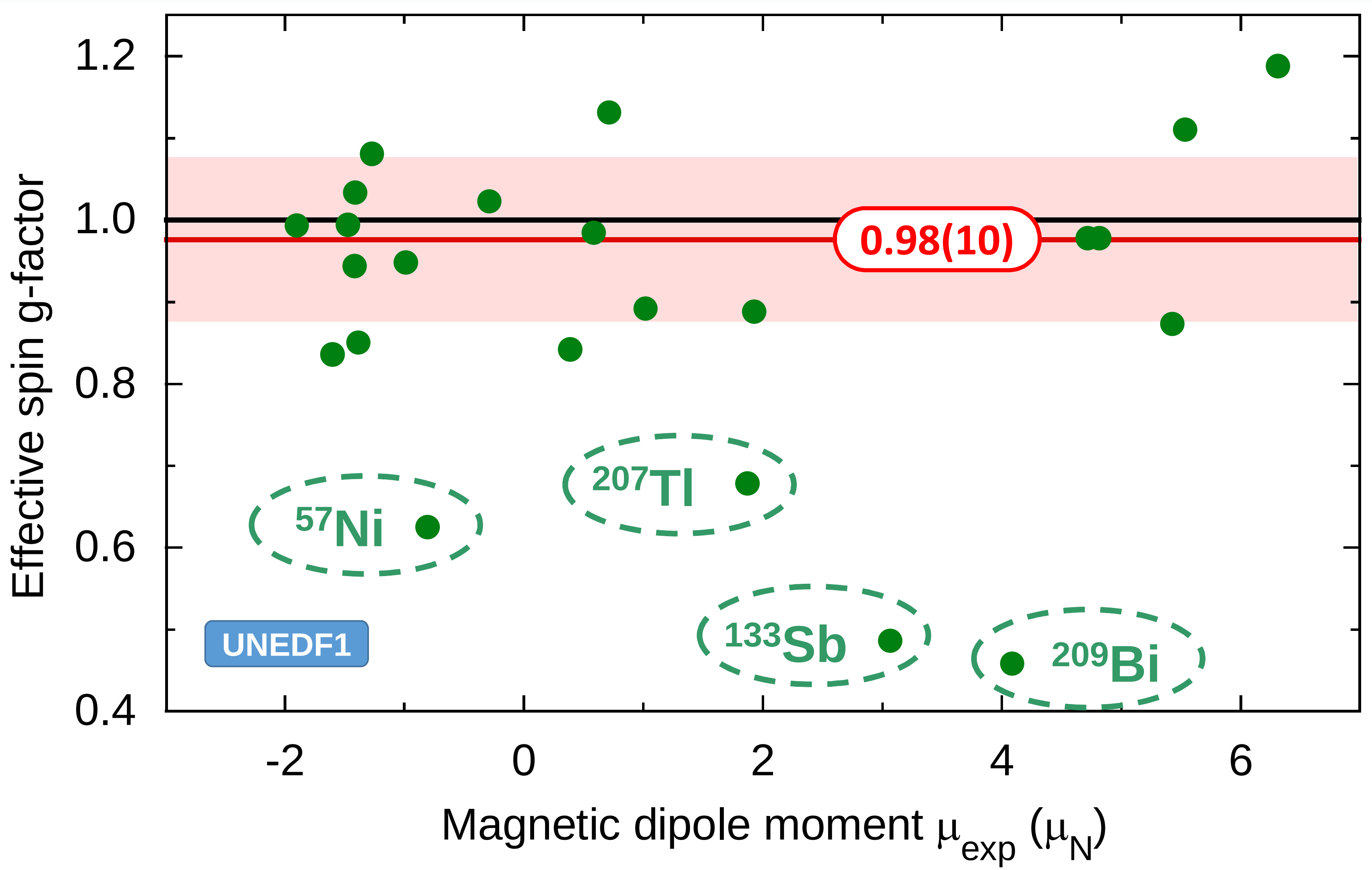
Optimisation of the spin-spin term

P.L. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



Effective spin g-factor?

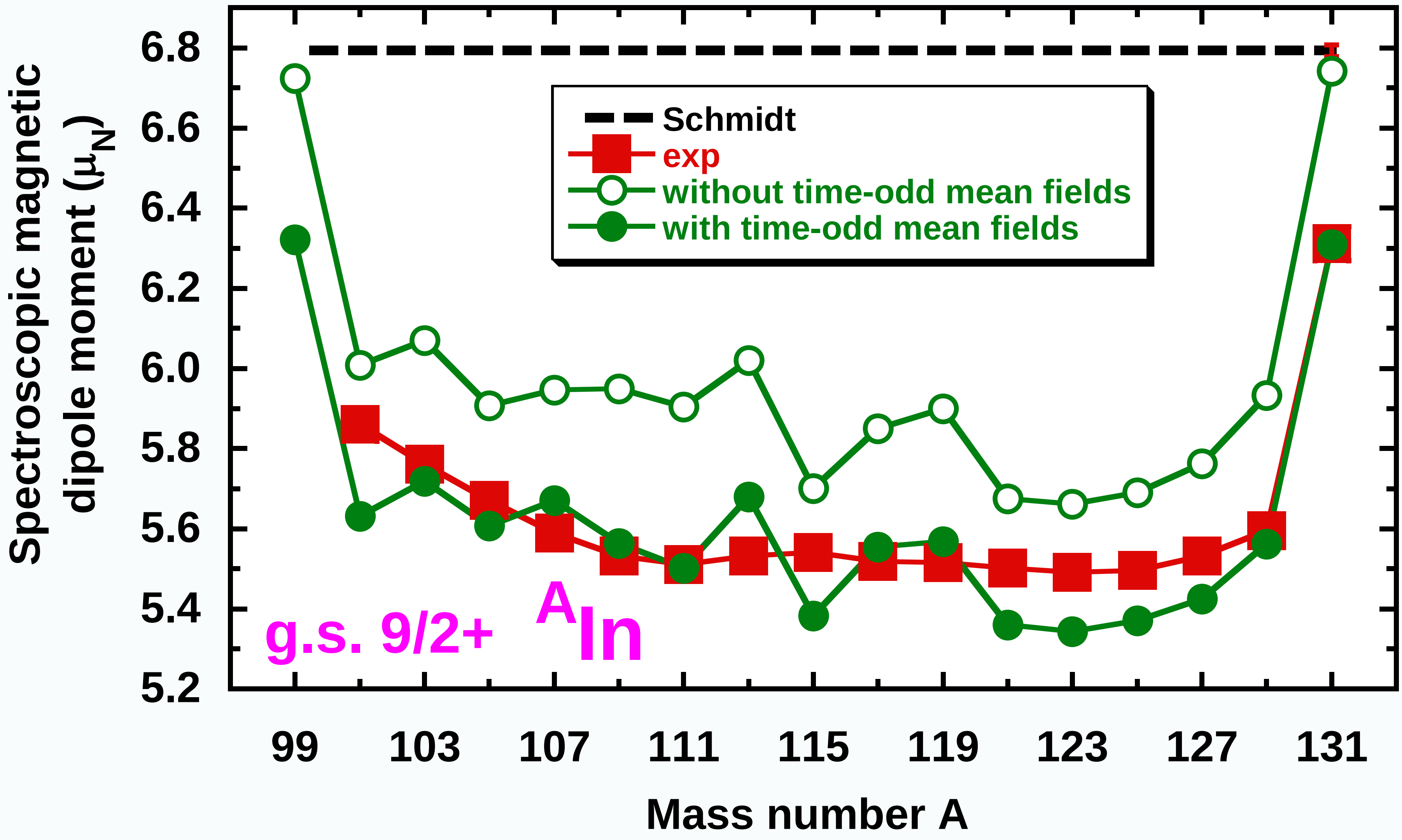
P.L. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



Indium

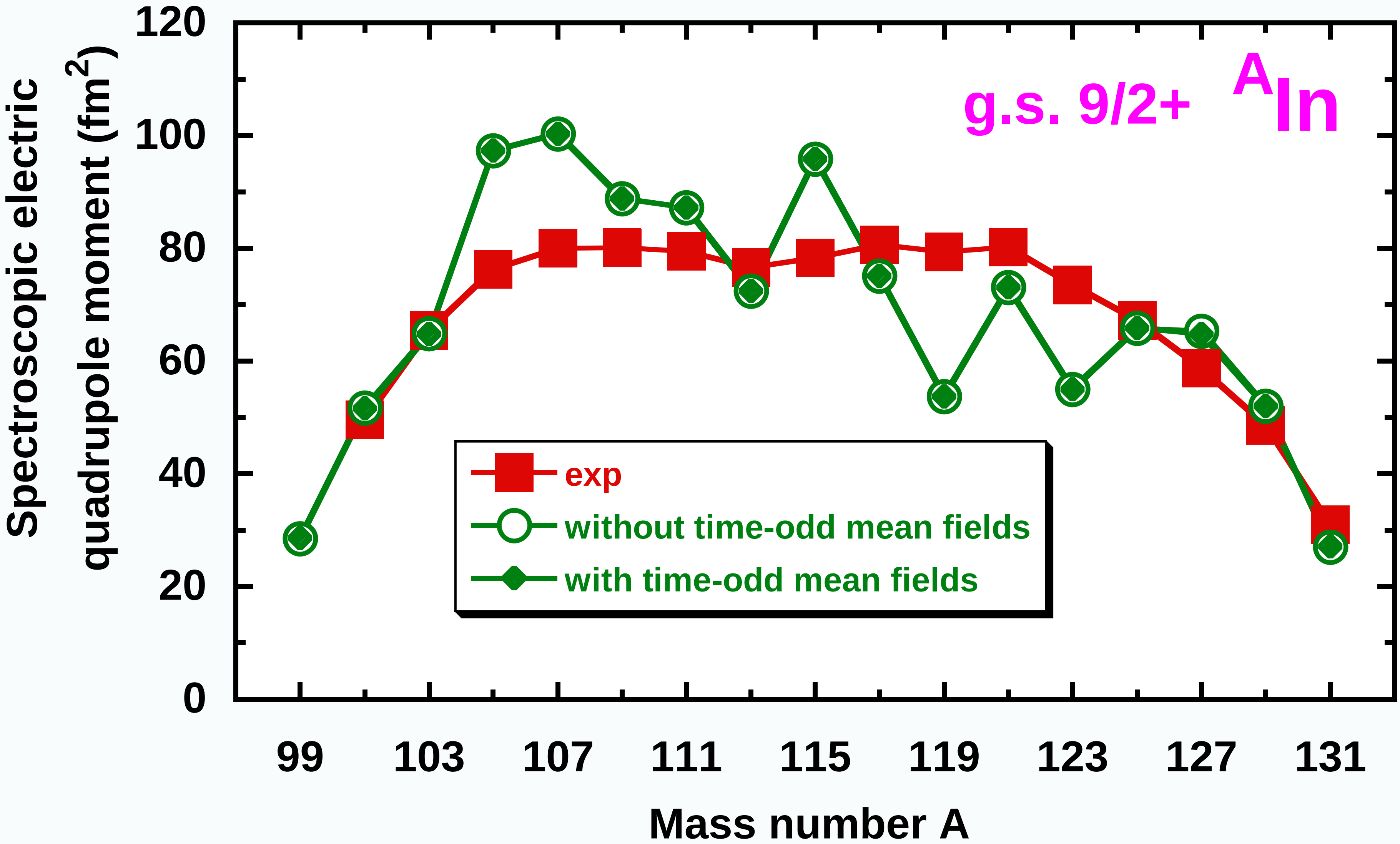
Magnetic dipole moments in indium

A.R. Vernon *et al.*, accepted in Nature



Electric quadrupole moments in indium

A.R. Vernon *et al.*, accepted in Nature



Particle-core coupling

Particle-core-coupling analysis

Consider three HF states:

- 1° $|\Phi_K\rangle$: the Indium self-consitent state with projection $K = +9/2$ of the angular momentum on the z axis,
- 2° $|\phi_\Omega\rangle$: the polarized $g_{9/2}$ orbital with $\Omega = -9/2$ (a hole orbital extracted from the self-consistent results for Indium),
- 3° $|\Psi\rangle$: the Tin-like polarized core state obained by adding orbital $|\phi_\Omega\rangle$ to the Indium state $|\Phi_K\rangle$.

The particle-core model neglects the Pauli principle between the particle and the core and assumes that $|\Psi\rangle = |\Phi_K\rangle \times |\phi_\Omega\rangle$. We perform the angular-momentum restoration for the three states:

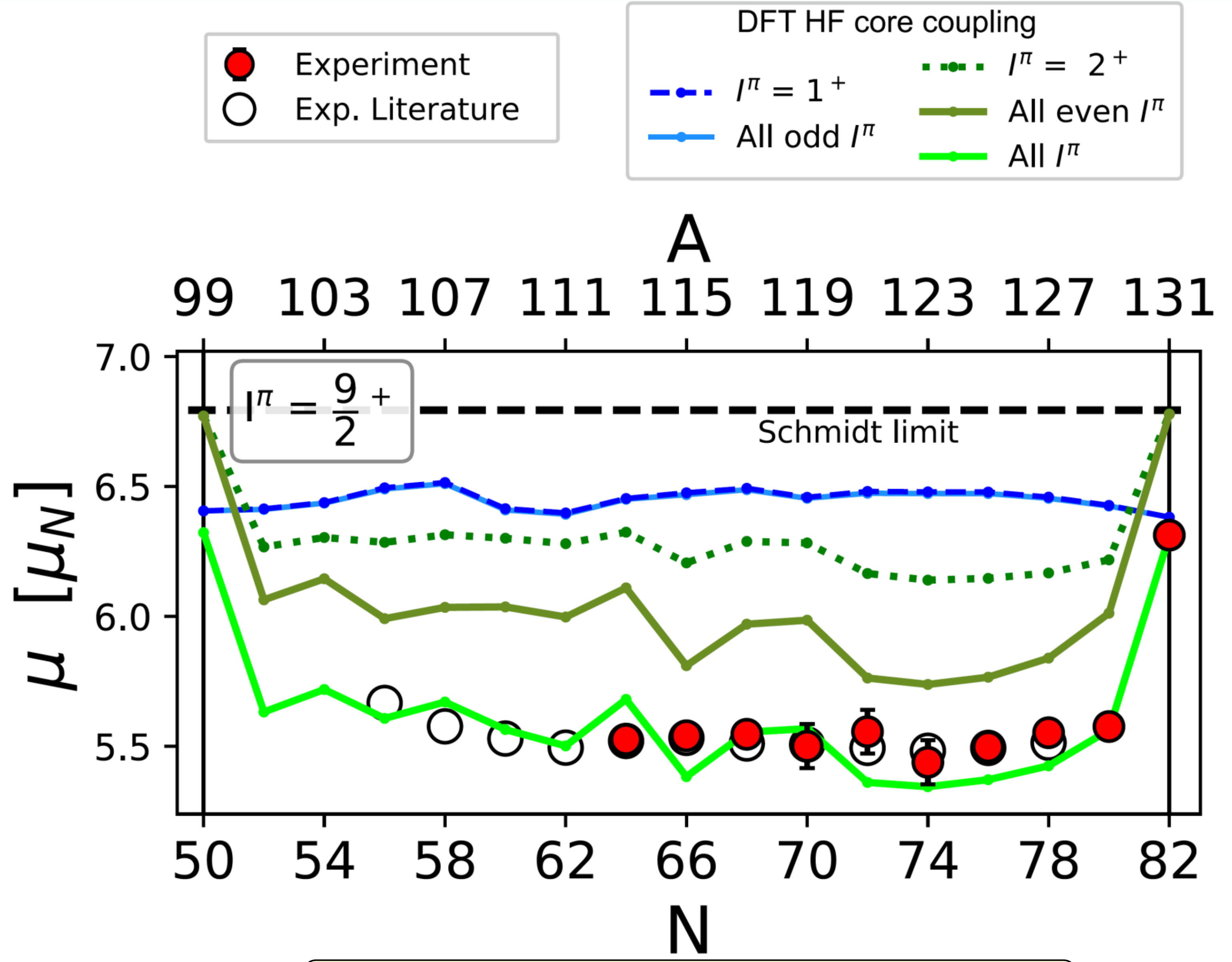
1° $|\Phi_K\rangle = \sum_I g_I |\Phi_{IK}\rangle$,
2° $|\phi_\Omega\rangle = \sum_j c_j |\phi_{j\Omega}\rangle$,
3° $|\Psi\rangle = \sum_J C_J |\Psi_{J0}\rangle$.

where g_I, c_j, and C_J are normalization factors. This gives:

$$
\begin{aligned}
\langle \Phi_{IK} | \hat{O}_{\lambda\mu} | \Phi_{IK} \rangle \quad = \quad & |g_I|^2 [I]^4 \begin{pmatrix} I & \lambda & I \\ K & \mu & -K \end{pmatrix} \\
\times \quad & \Bigg\{ \sum_{J,j,J'} C_J^* C_{J'} |c_j|^2 (-1)^{J'+j-K} \begin{pmatrix} J & j & I \\ M & m & -K \end{pmatrix} \begin{pmatrix} J' & j & I \\ M & m & -K \end{pmatrix} \begin{Bmatrix} I & \lambda & I \\ J & j & J' \end{Bmatrix} \langle J || \hat{O}^c_\lambda || J' \rangle \\
+ \quad & \sum_{J,j,j'} |C_J|^2 c_j^* c_{j'} (-1)^{J+j-K} \begin{pmatrix} J & j & I \\ M & m & -K \end{pmatrix} \begin{pmatrix} J & j' & I \\ M & m & -K \end{pmatrix} \begin{Bmatrix} I & \lambda & I \\ j & J & j' \end{Bmatrix} \langle j || \hat{O}^{sp}_\lambda || j' \rangle \Bigg\}
\end{aligned}
$$

J. Bonnard, J.D., W. Nazarewicz, to be published

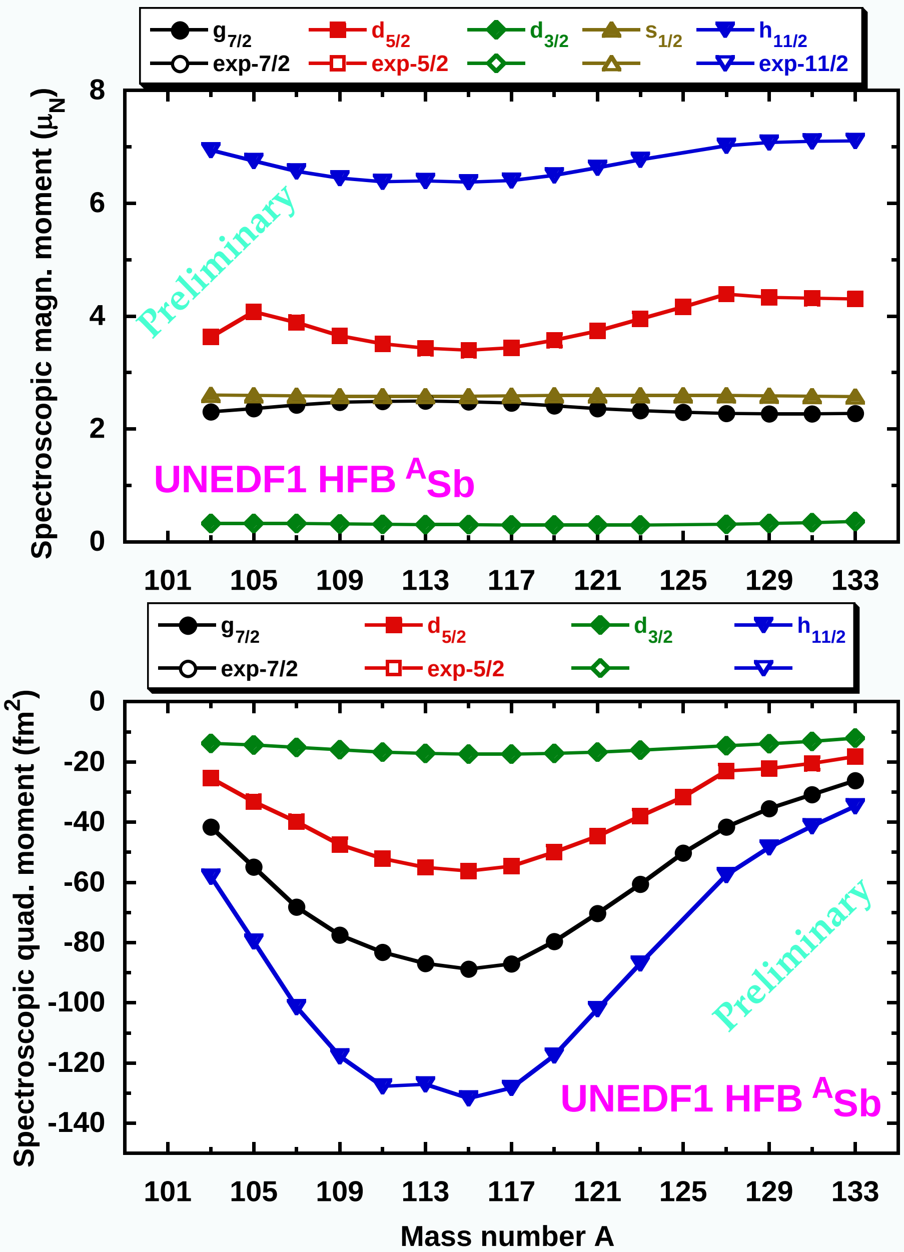
Particle-core-coupling analysis



A.R. Vernon *et al.*, accepted in Nature

Antimony

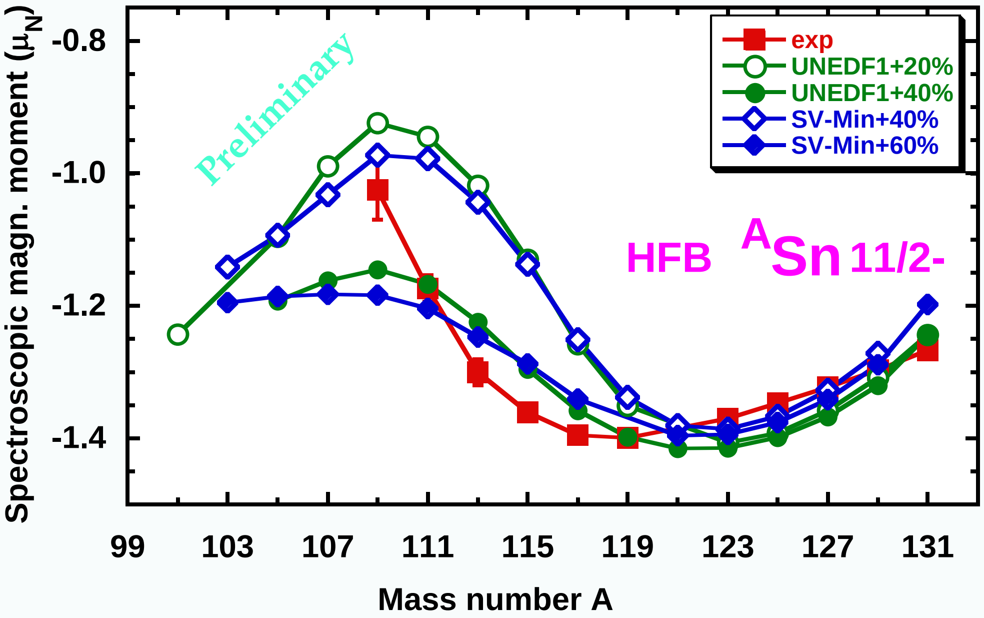
Dipole and quadrupole moments in antimony

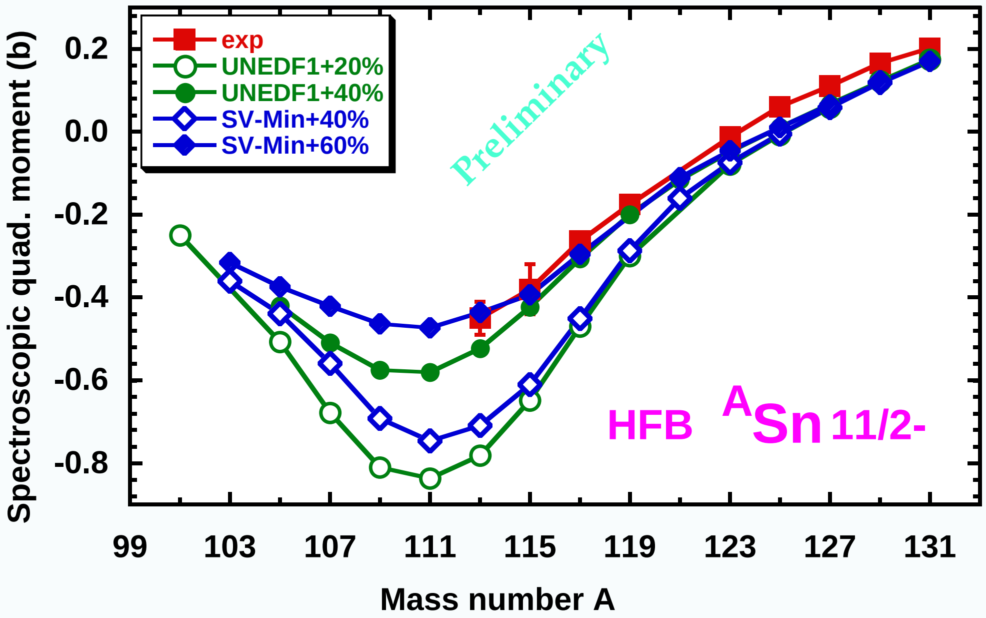


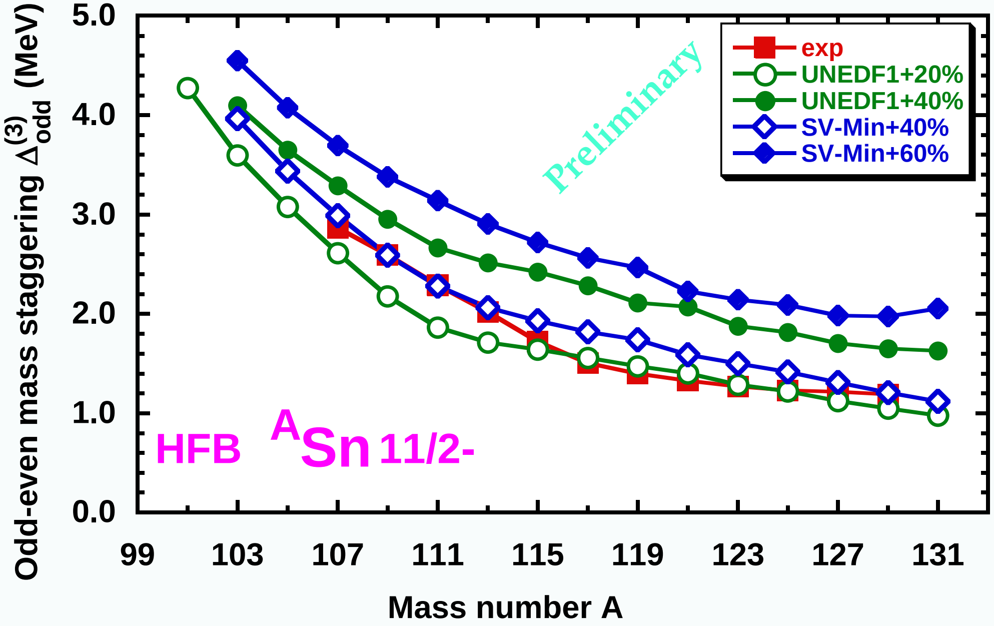
Experimental data exist:
S. Lechner *et al.*, to be published

Tin

Dipole and quadrupole moments in tin



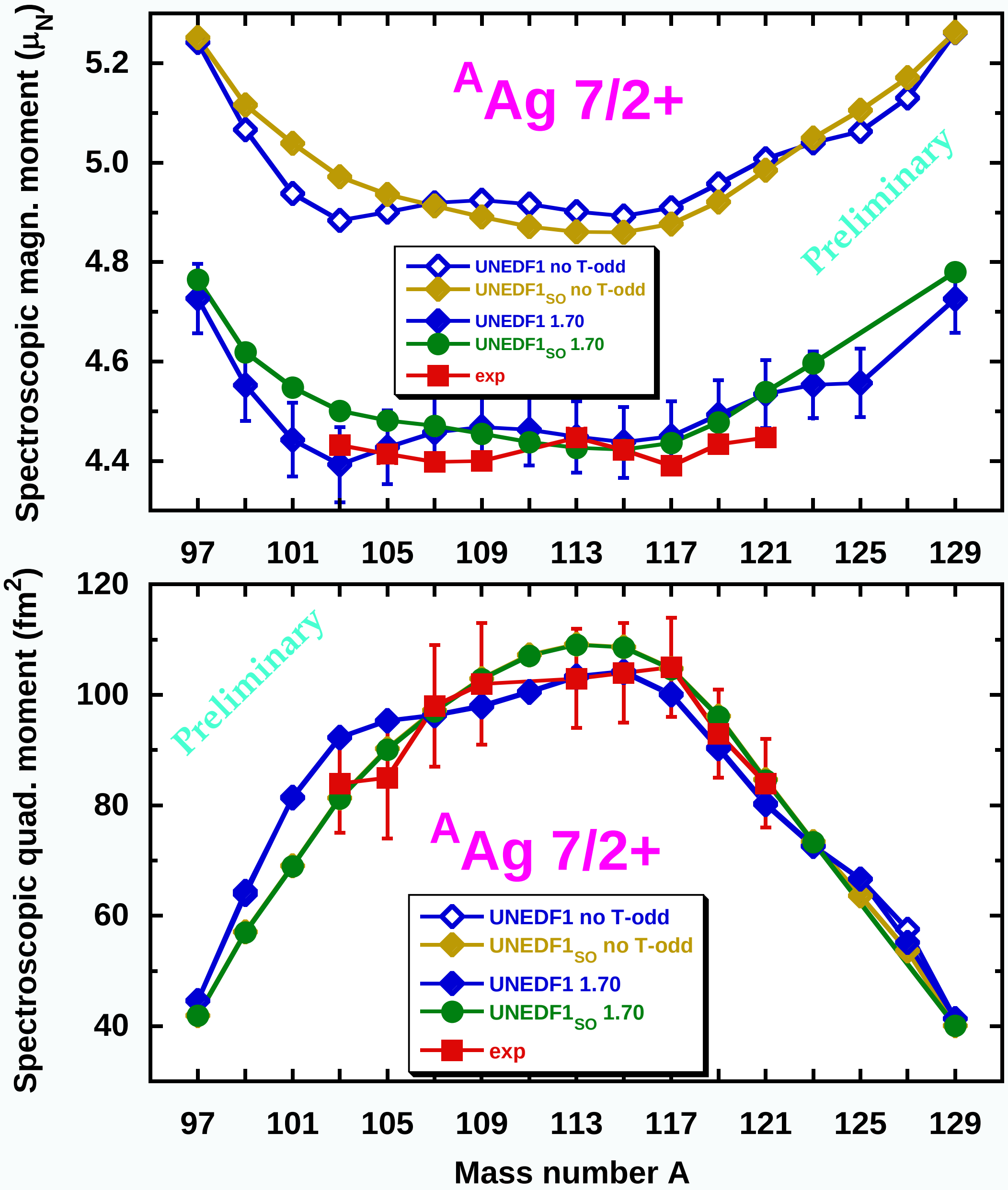




T. J. Gray, A. E. Stuchbery,
J. Dobaczewski, ... , J. Bonnard
et al., to be published

Silver

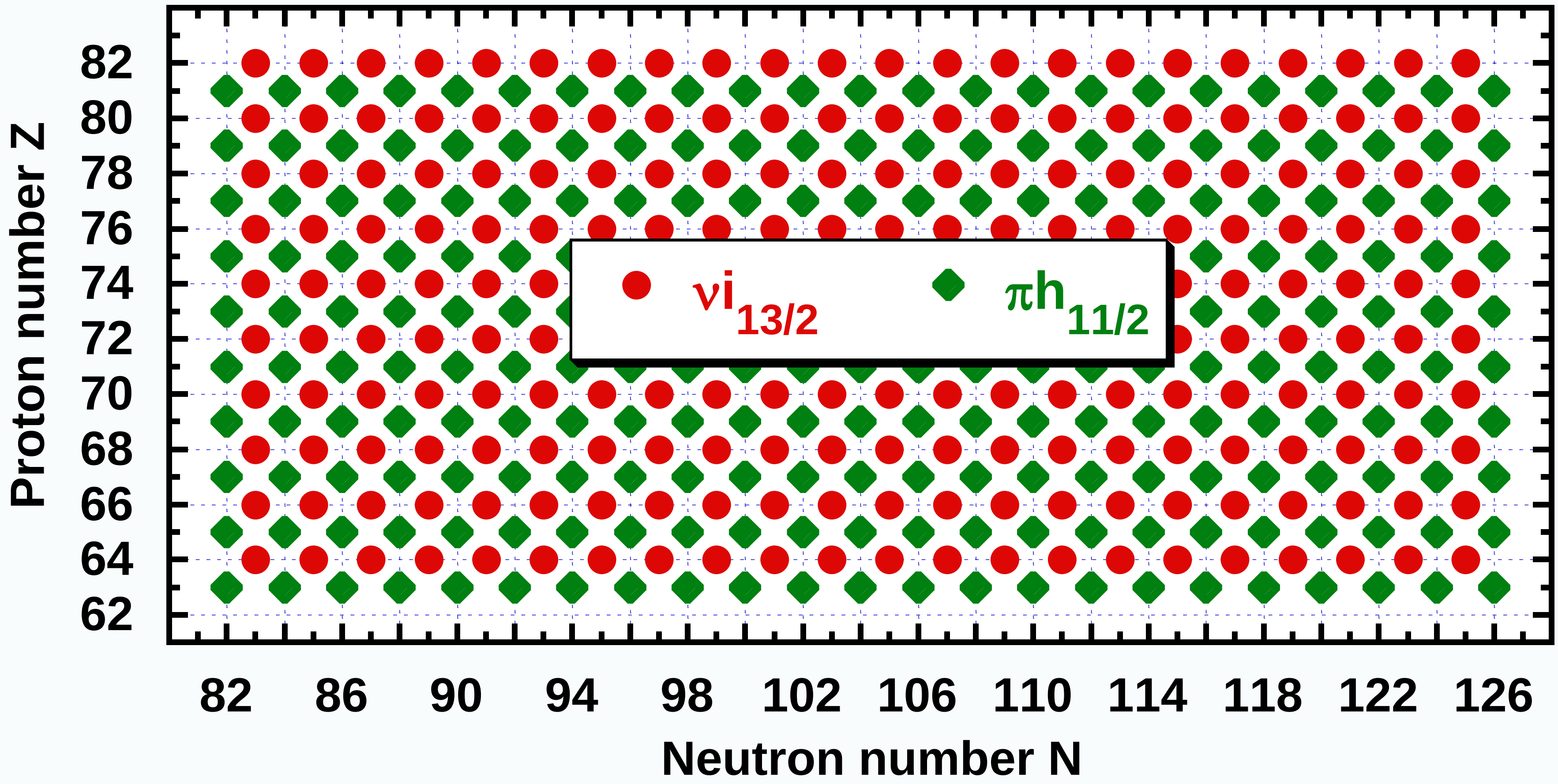
Dipole and quadrupole moments in silver



R. P. de Groote, D. A. Nesterenko, A. Kankainen, … , J. Bonnard, … , J. Dobaczewski *et al.*, to be published

$$82 \leq N \leq 126$$
$$63 \leq Z \leq 82$$

First systematic nuclear-DFT analysis of electromagnetic moments in heavy deformed open-shell odd nuclei



J. Bonnard & J.D, to be published

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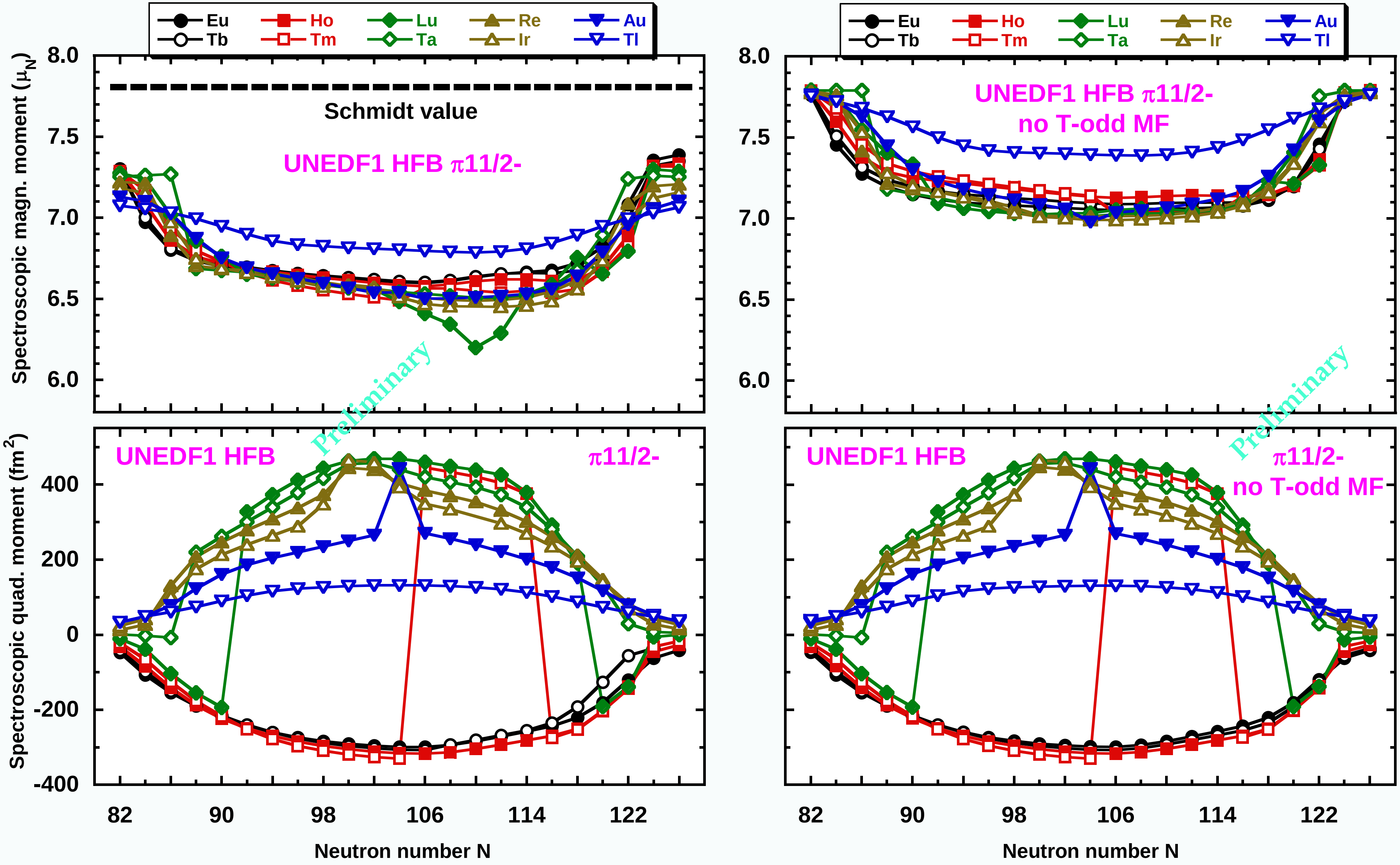
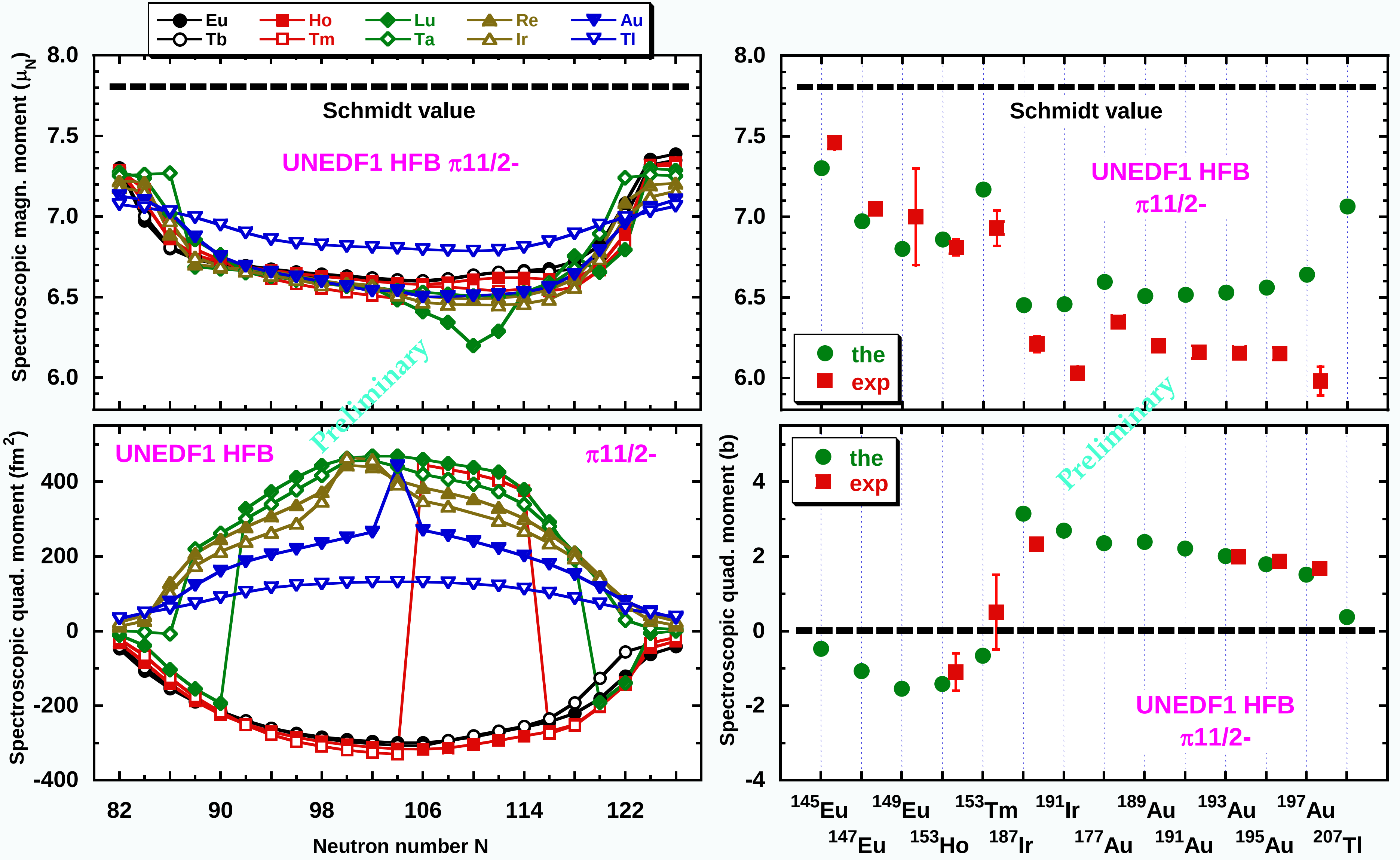
Heavy deformed π11/2- odd-Z nuclei



J. Bonnard & J.D, to be published

Heavy deformed π11/2- odd-Z nuclei



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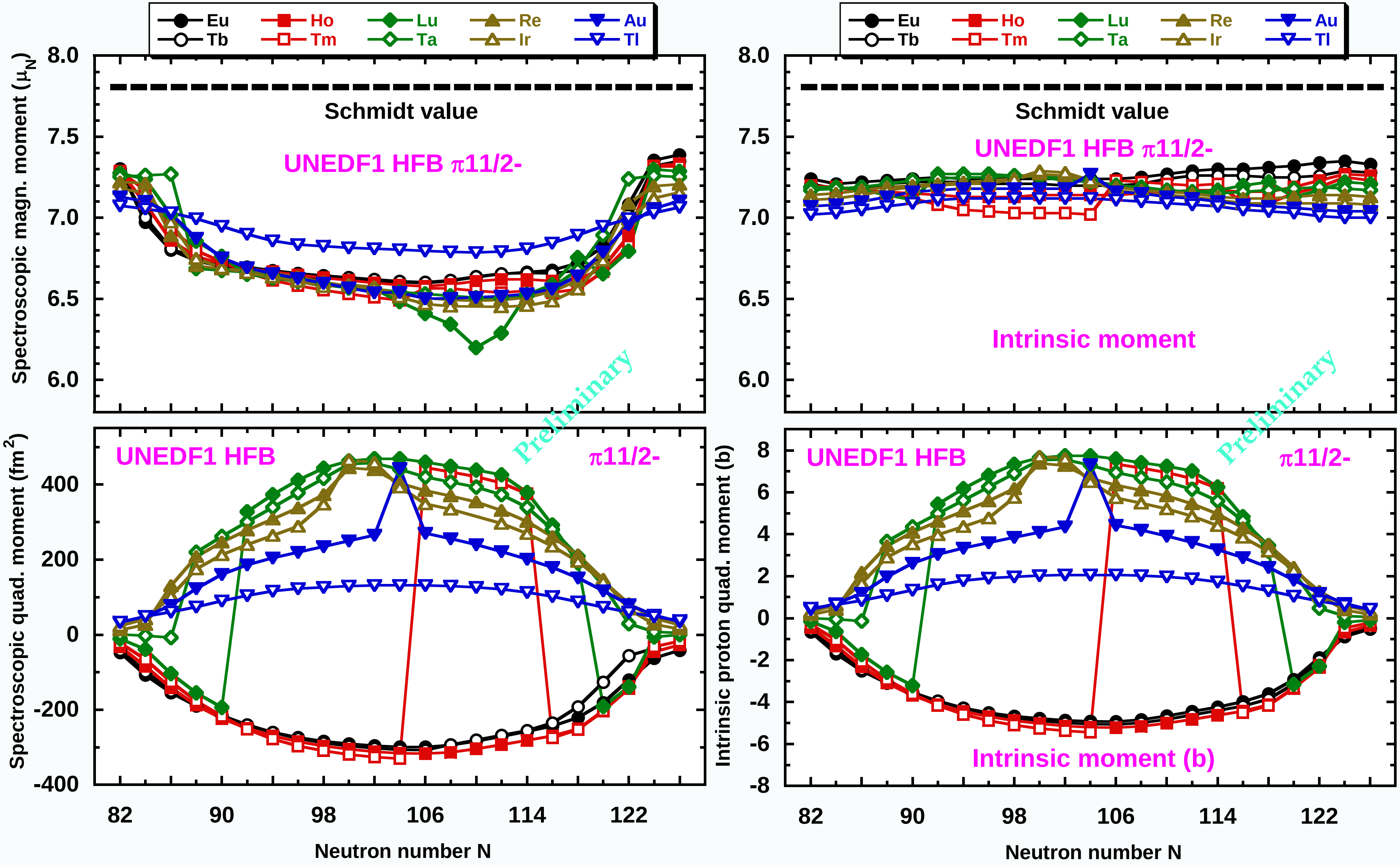
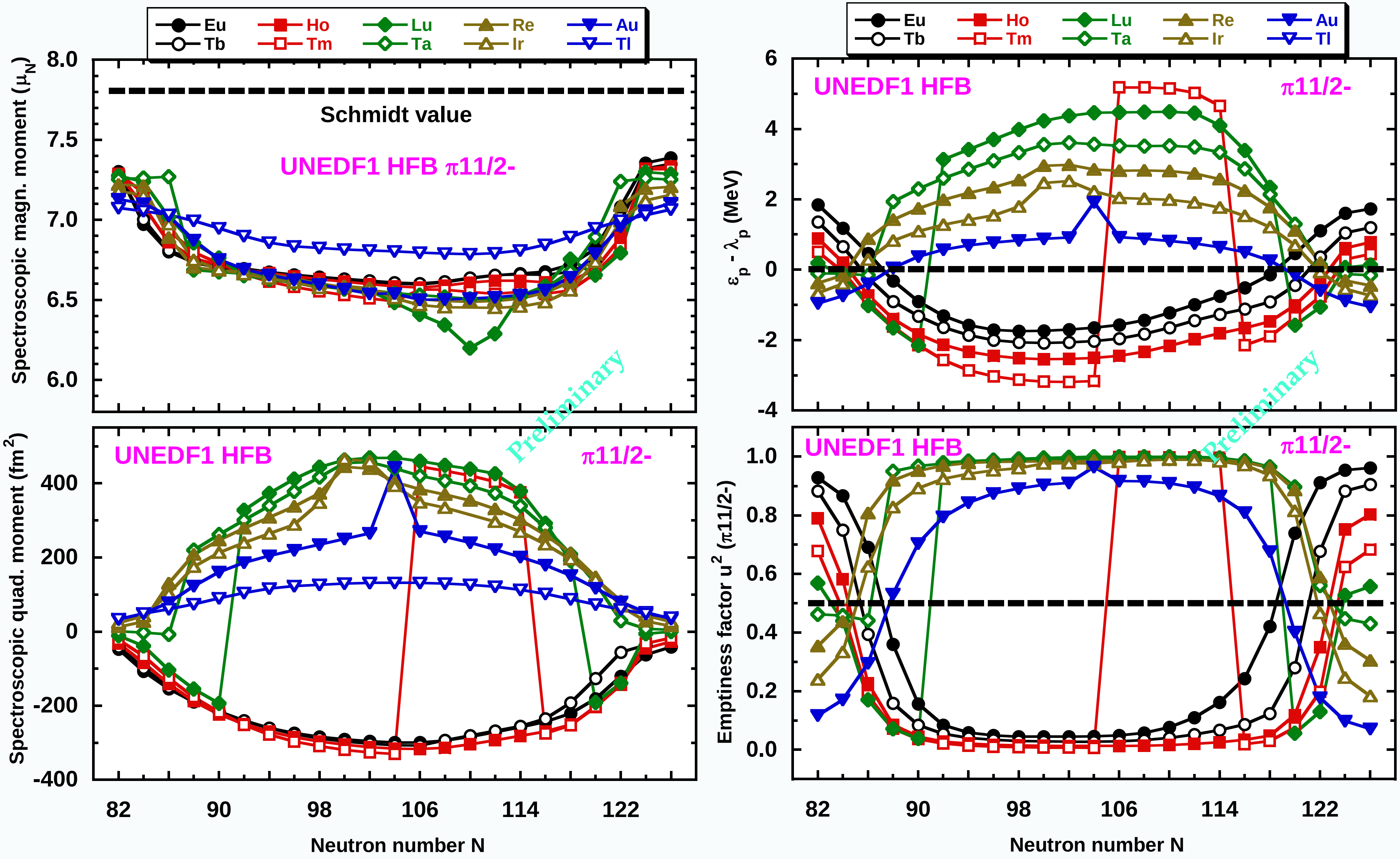
Heavy deformed π11/2- odd-Z nuclei



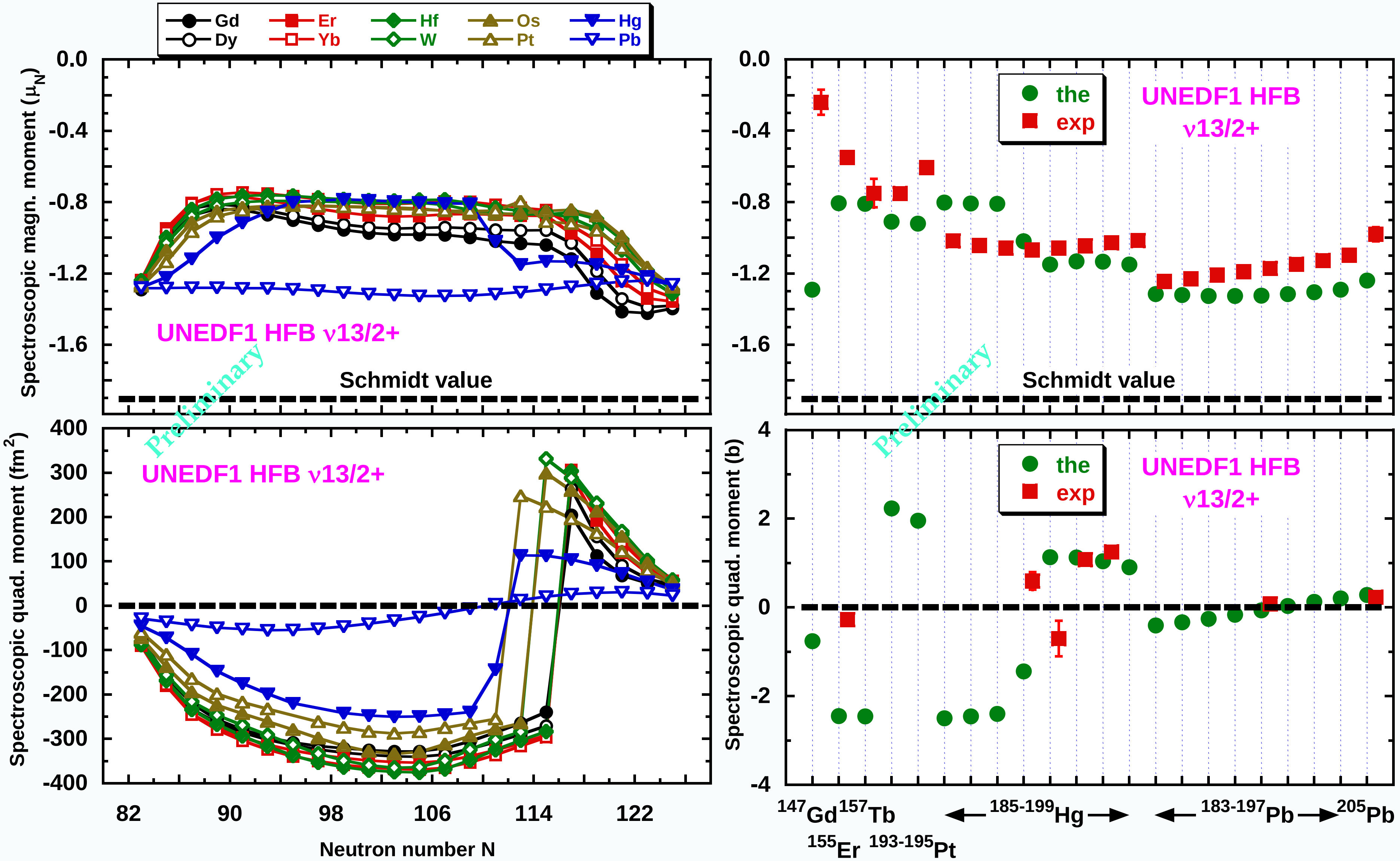
J. Bonnard & J.D, to be published

Heavy deformed π11/2- odd-Z nuclei



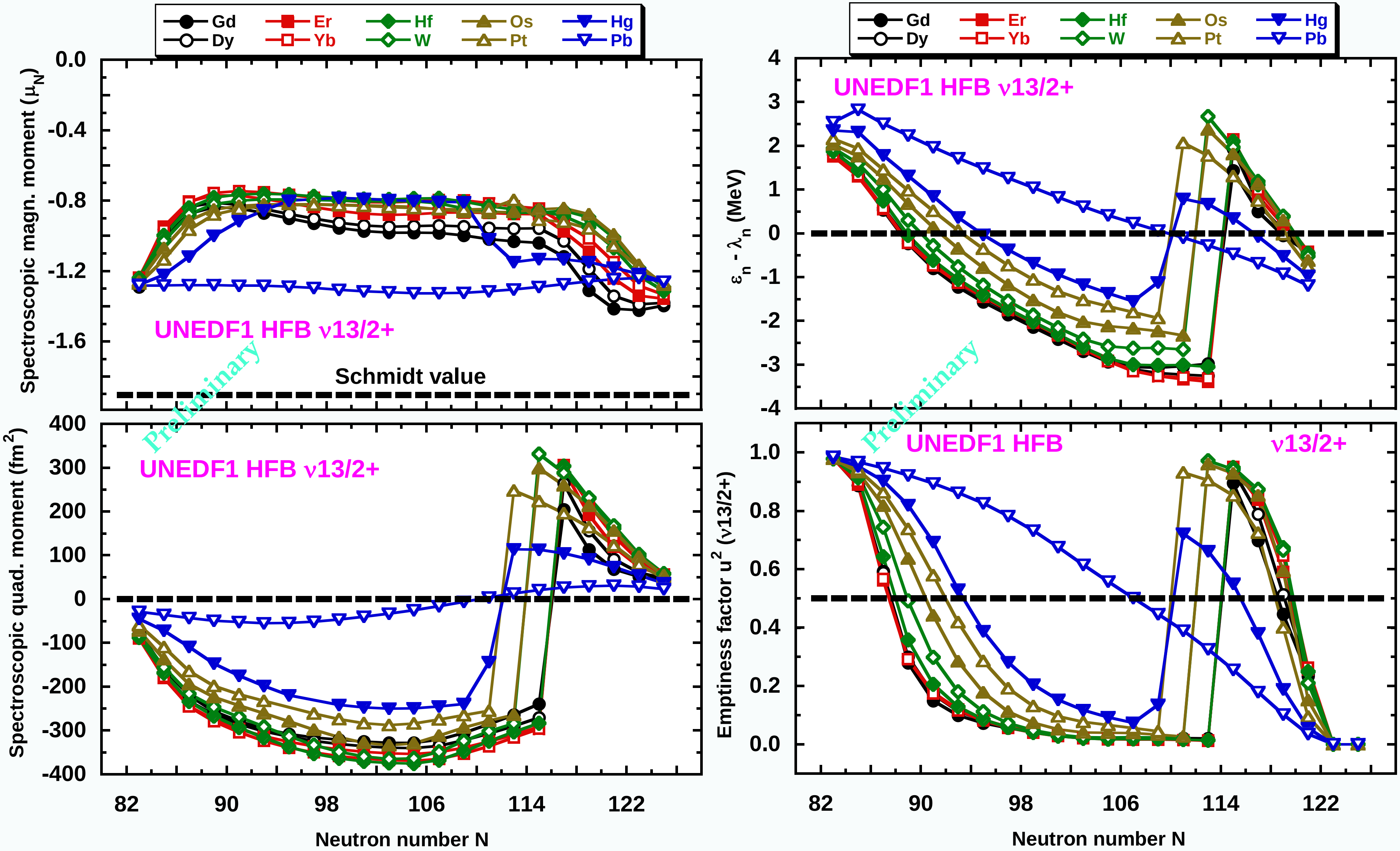
J. Bonnard & J.D, to be published

Heavy deformed ν13/2+ odd-N nuclei



J. Bonnard & J.D, to be published

Heavy deformed ν13/2+ odd-N nuclei

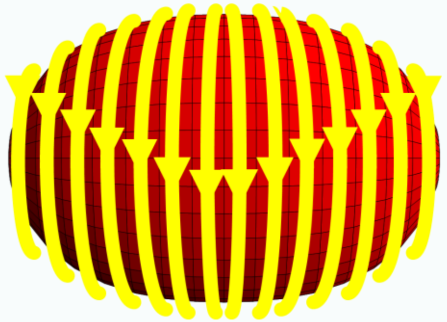


J. Bonnard & J.D, to be published

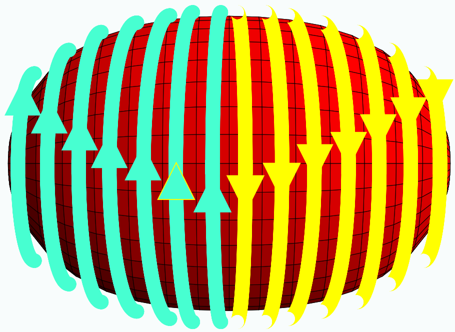
Magnetic octupole moments

Visualisation of the magnetic multipole moments in axial symmetry

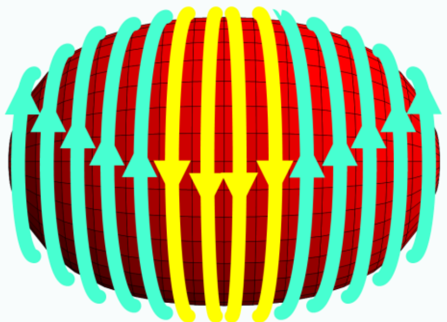
λ=1



λ=2



λ=3



Axial solid harmonics:

$\lambda\mu$	$Q_{\lambda\mu}$	$\nabla_z Q_{\lambda\mu}$
00	$\sqrt{\frac{1}{4\pi}}$	0
10	$\sqrt{\frac{3}{4\pi}}z$	$\sqrt{\frac{3}{4\pi}} \quad = \sqrt{3}Q_{00}$
20	$\sqrt{\frac{5}{16\pi}}\left(2z^2 - x^2 - y^2\right)$	$\sqrt{\frac{5}{\pi}}z \quad = \sqrt{\frac{20}{3}}Q_{10}$
30	$\sqrt{\frac{7}{16\pi}}\left(2z^3 - 3x^2z - 3y^2z\right)$	$\sqrt{\frac{7}{16\pi}}3\left(2z^2 - x^2 - y^2\right) \quad = \sqrt{\frac{63}{5}}Q_{20}$

Axial electric and magnetic-moment densities:

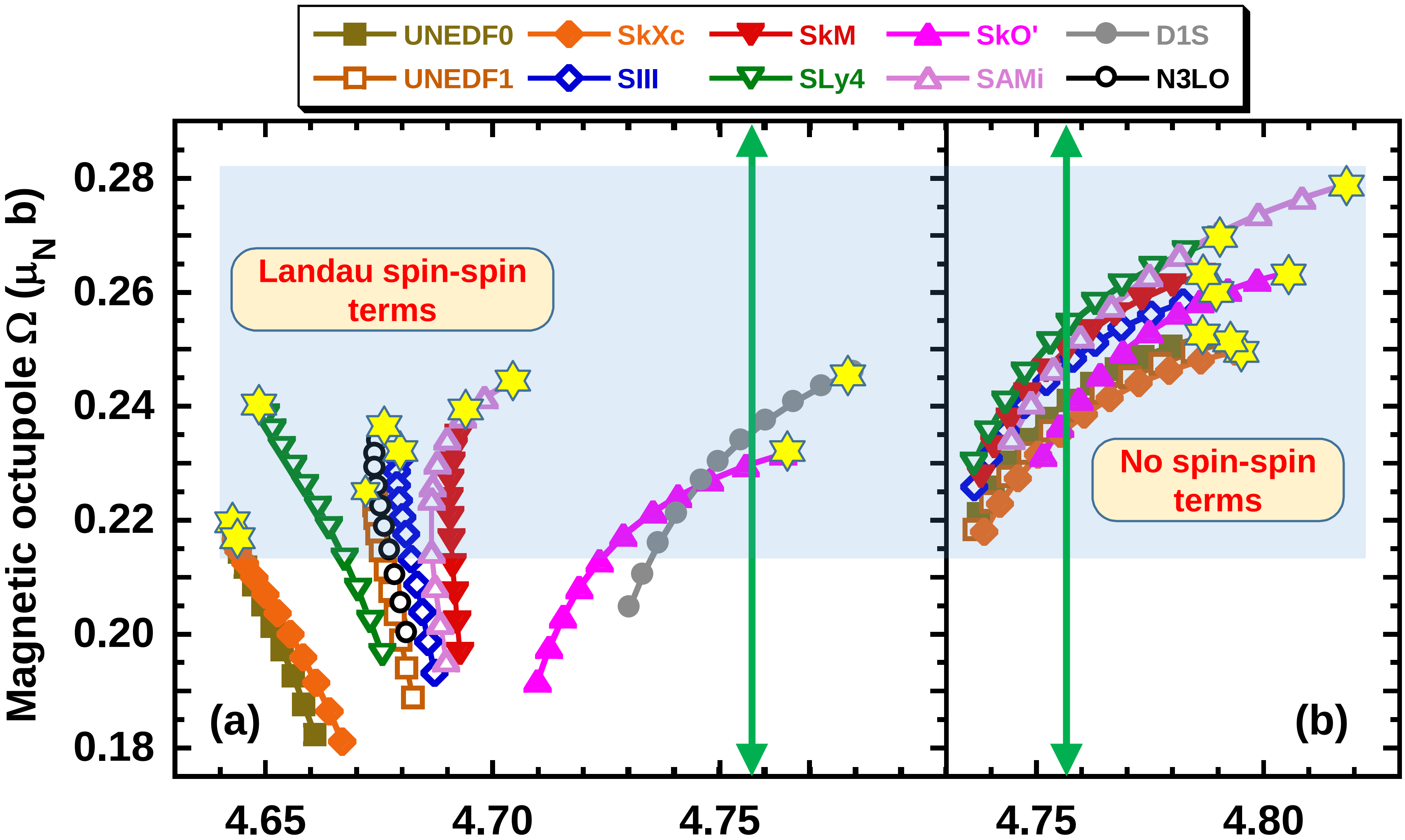
$$q_{\lambda 0}(r,\theta) = e\rho(r,\theta)Q_{\lambda 0}(r,\theta),$$

$$m_{\lambda 0}(r,\theta) = \mu_N\left[g_s s_z(r,\theta) + \tfrac{2}{\lambda+1}g_l\left(\vec{r}\times\vec{j}\right)_z(r,\theta)\right]\cdot\nabla_z Q_{\lambda 0}(r,\theta),$$

or

$$m_{\lambda 0}(r,\theta) = \mu_N\left[g_s s_z(r,\theta) + \tfrac{2}{\lambda+1}g_l I_z(r,\theta)\right]C_\lambda Q_{(\lambda-1)0}(r,\theta),$$

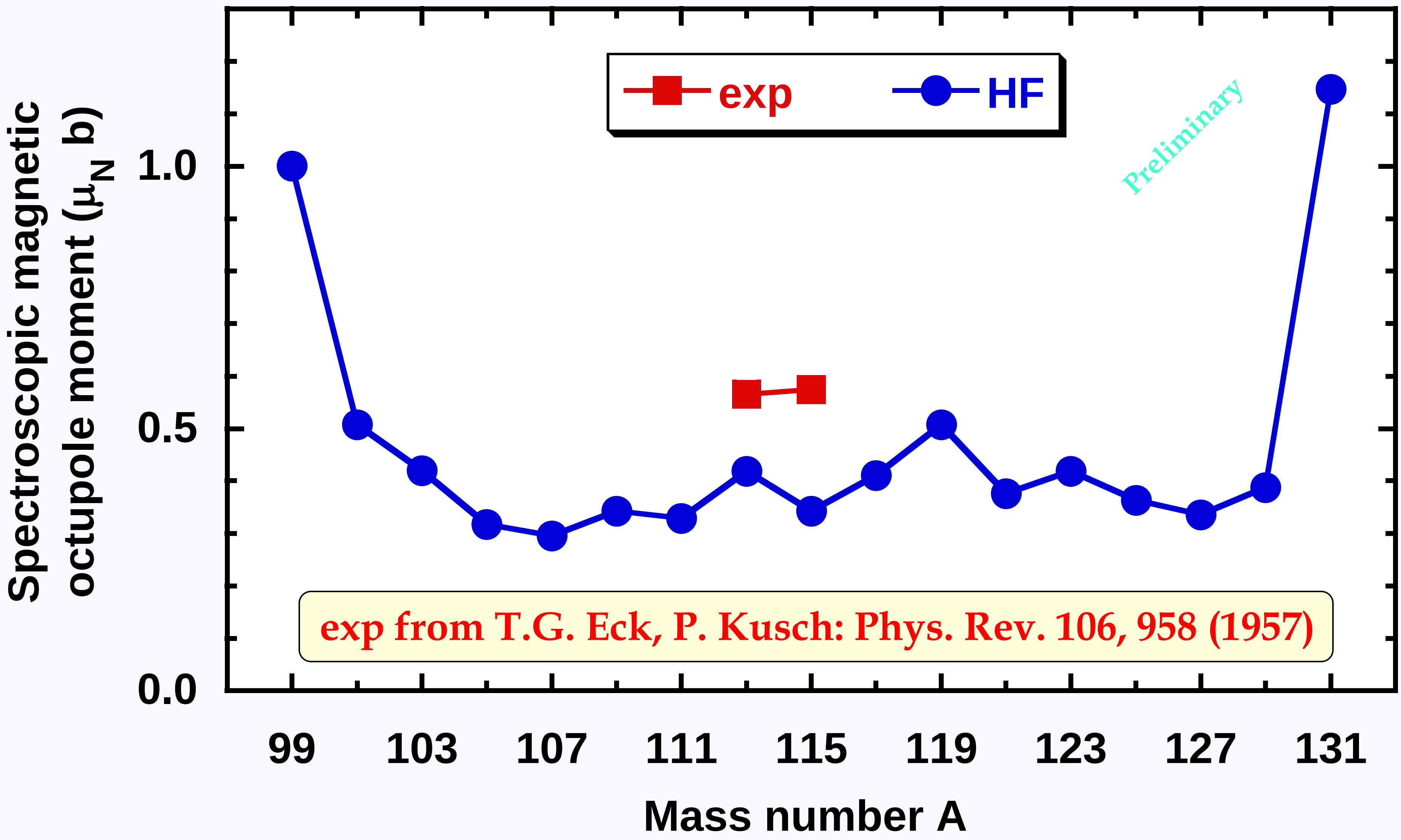
Magnetic moments in ^{45}Sc



$\Omega^{exp} = -0.07(53)\mu_N b$

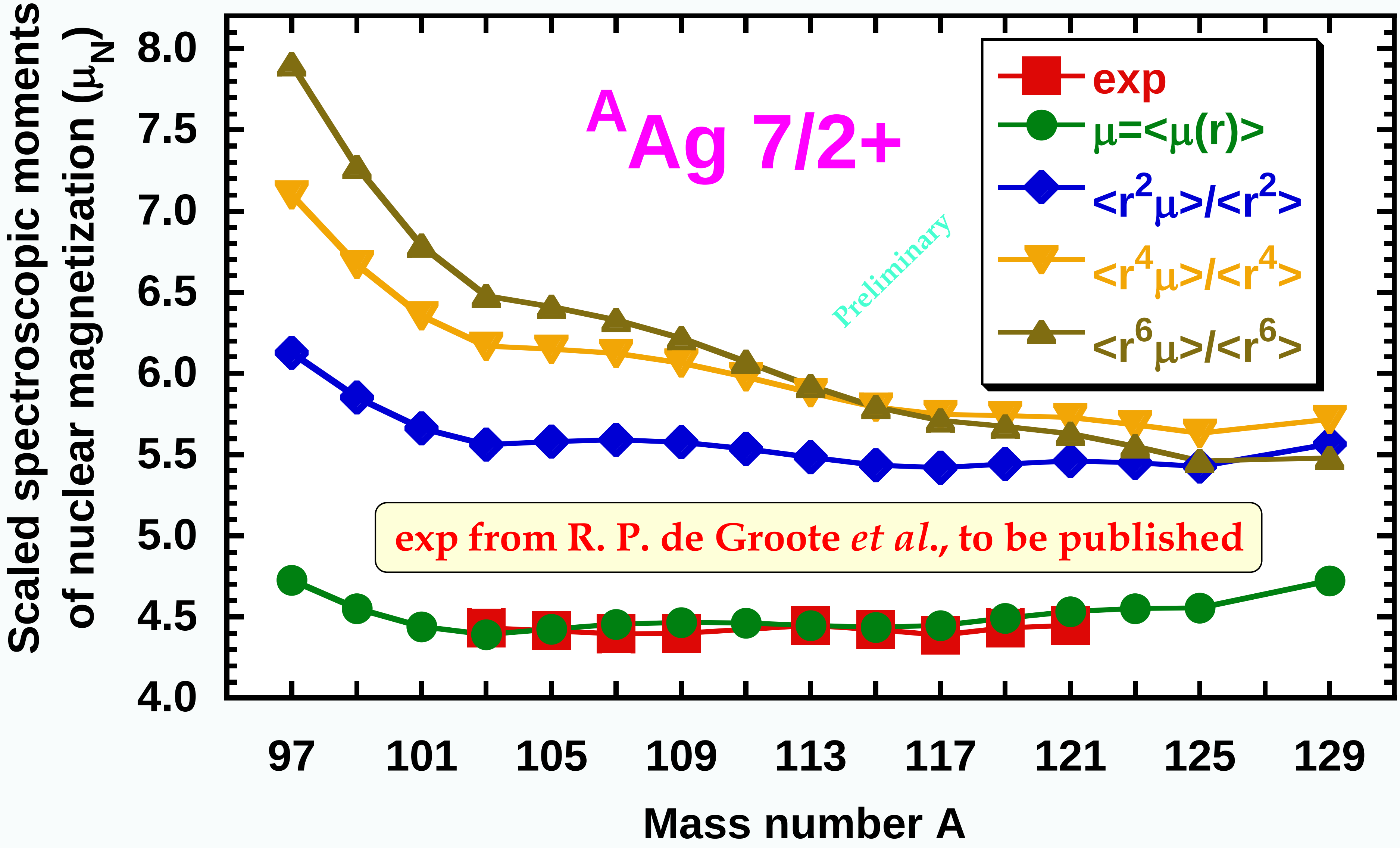
R. P. de Groote *et al.*, Phys. Lett. B827 (2022) 136930

Magnetic octupole moments in indium



Bohr-Weisskopf correction

Moments of magnetization in silver



Conclusions

1. Nuclear DFT:
   - An approach of choice to calculate electromagnetic moments in nuclei.
   - Takes into account polarization effects by odd particles to infinite order in full single-particle space.
   - Unified approach with no limits on mass.
2. Time-odd mean fields and symmetry restoration are essential.
3. Effective charges and effective g-factors not needed.
4. Applications in semi-magic & open-shell nuclei, excited states.
5. Future applications to exotic moments: Schiff, anapole, weak… provide links to particle, atomic, and molecular physics.
6. Adjustments of the nuclear DFT coupling constants to data should take the magnetic moments into account.
7. Terms beyond $\sigma\sigma$? T-odd spin-orbit? tensor? higher order?
8. Triaxiality? K-mixing? Configuration interaction?

Thank you

„Spin” magnetic dipole moment

In this study we use the single-particle magnetic-dipole-moment operator for neutron and proton bare orbital and spin gyroscopic factors,

$$g_\ell^p = \mu_N, \;\; g_s^n = -3.826\,\mu_N, \;\; g_s^p = +5.586\,\mu_N,$$

which reads

$$\hat{\mu} = g_\ell^p \hat{L}_p + g_s^n \hat{S}_n, + g_s^p \hat{S}_p,$$

where $\hat{L}_\nu$ **and** $\hat{S}_\nu$ **for** $\nu = n, p$ **are the operators of orbital and spin angular momenta, respectively. Since the total angular momentum** $\hat{J} = \sum_{\nu=n,p}(\hat{L}_\nu + \hat{S}_\nu)$ **is conserved, it is convenient to subtract its eigenvalue from the spectroscopic magnetic moments of odd-**Z **nuclei and to define "spin" magnetic moments** $\mu^{\mathbf{S}}$ **as**

$$\mu^{\mathbf{S}} = \mu = g_\ell^p \langle \hat{L}_p \rangle + g_s^n \langle \hat{S}_n \rangle + g_s^p \langle \hat{S}_p \rangle \quad \textbf{for } Z \textbf{ even},$$

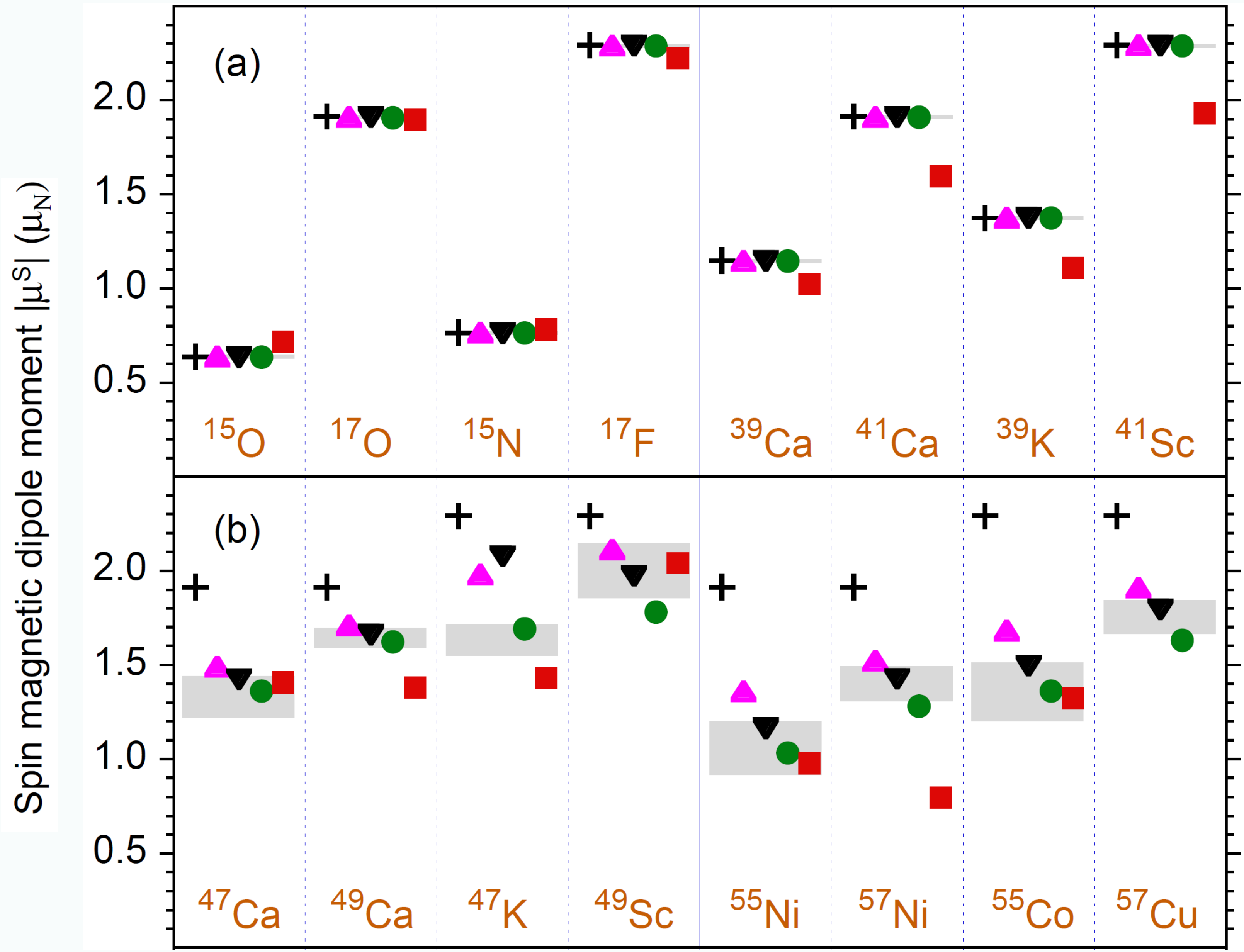
$$\mu^{\mathbf{S}} = \mu - J\,\mu_N$$
$$= g_\ell'^n \langle \hat{L}_n \rangle + g_s'^n \langle \hat{S}_n \rangle + g_s'^p \langle \hat{S}_p \rangle \quad \textbf{for } Z \textbf{ odd}.$$

with

$$g_\ell'^n = -\mu_N, \;\; g_s'^n = -4.826\,\mu_N, \;\; g_s'^p = +4.586\,\mu_N.$$

Spin magnetic dipole moments

P.L. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



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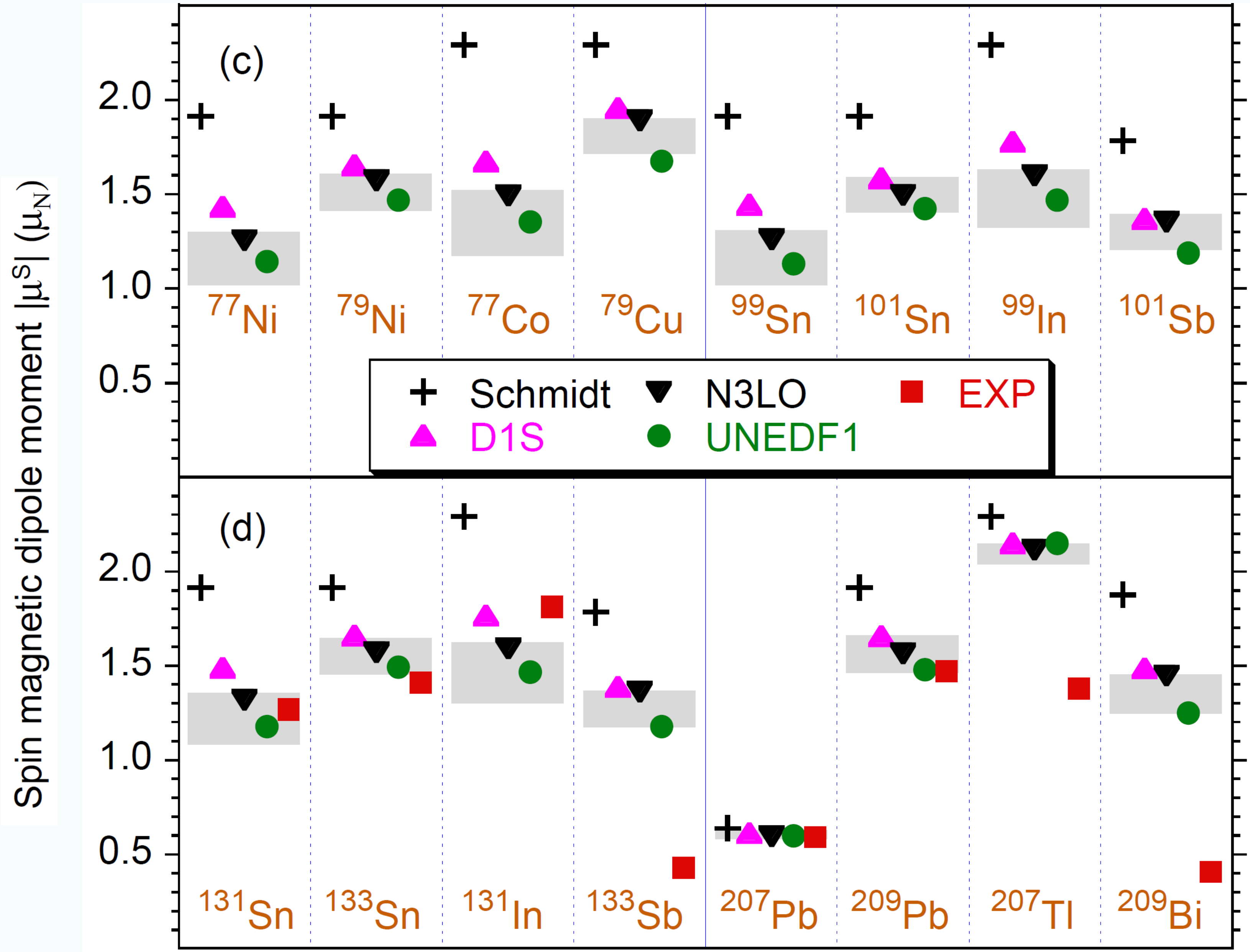

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