Studies of electromagnetic moments in nuclei within nuclear DFT

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Outline

1. Recap on nuclear electromagnetic moments
2. Odd near doubly magic nuclei
3. Indium isotopes
4. Magnetic octupole moments
5. Bohr-Weisskopf correction in silver
6. Antimony
7. Tin
8. Schiff moment in ^{225}Ra
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:

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

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

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: $Q_{\lambda\mu}(\vec{r}) = r^\lambda Y_{\lambda\mu}(\theta,\phi)$.
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 for 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.

Odd near doubly magic nuclei

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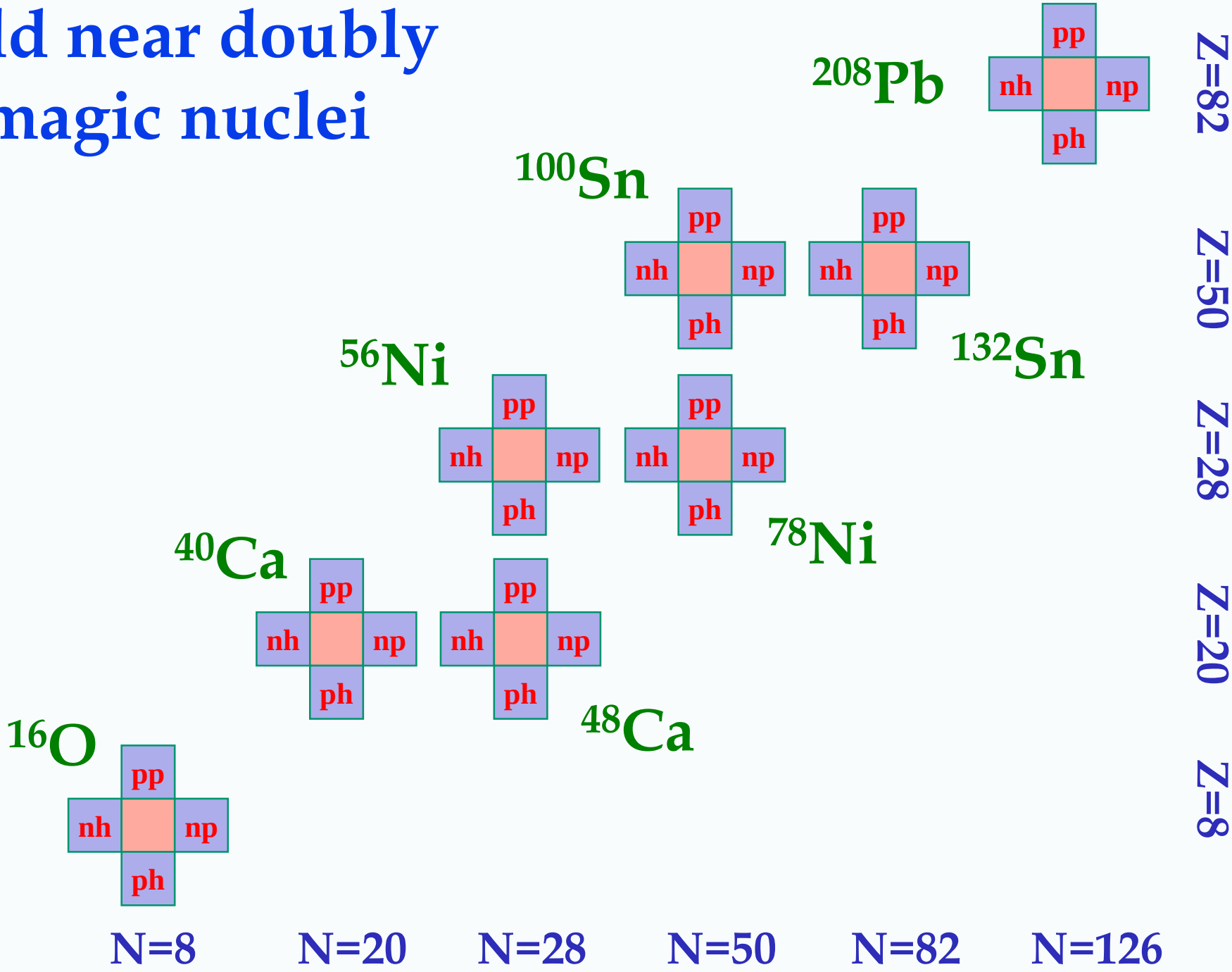
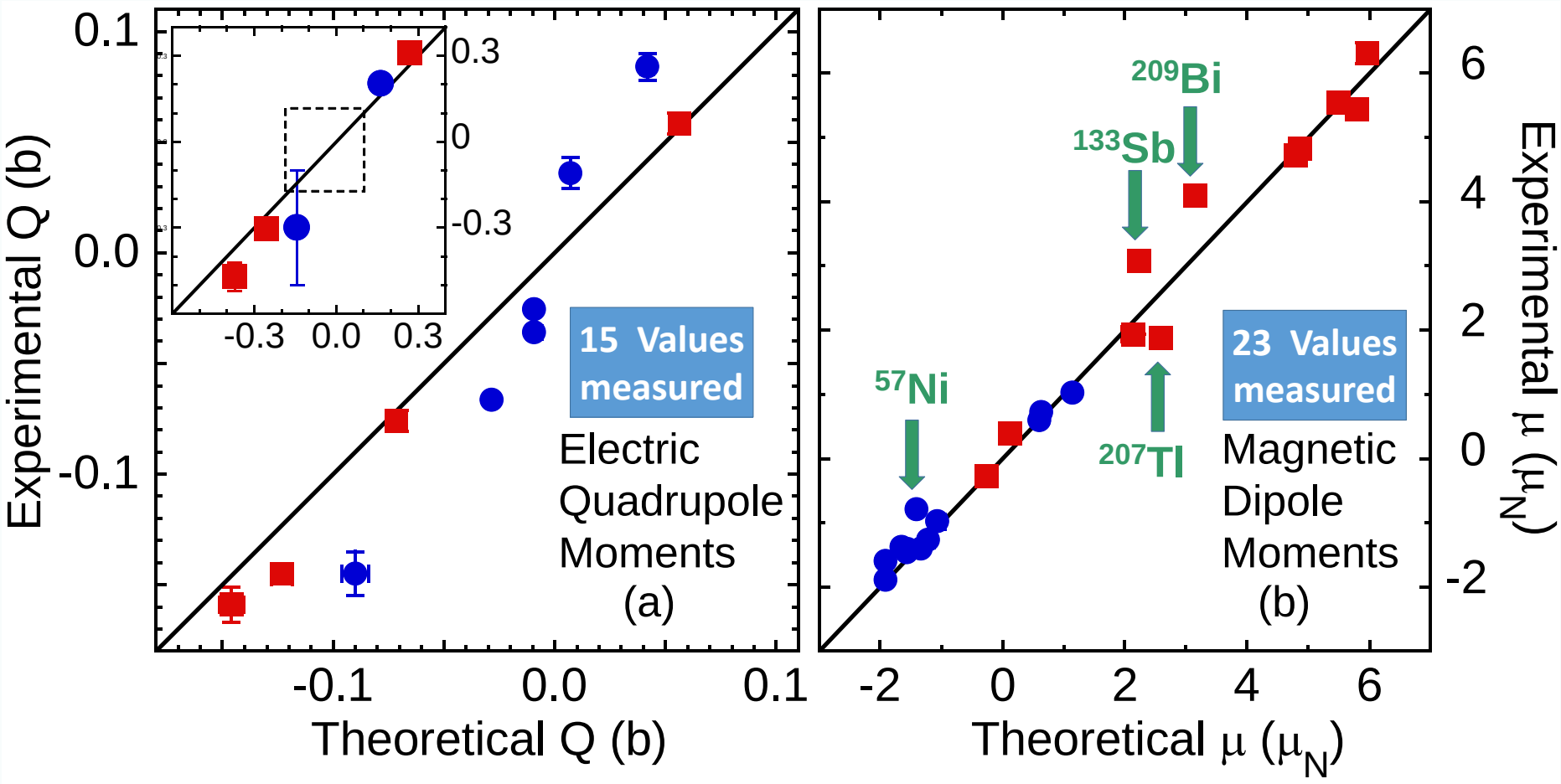
Odd near doubly magic nuclei



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

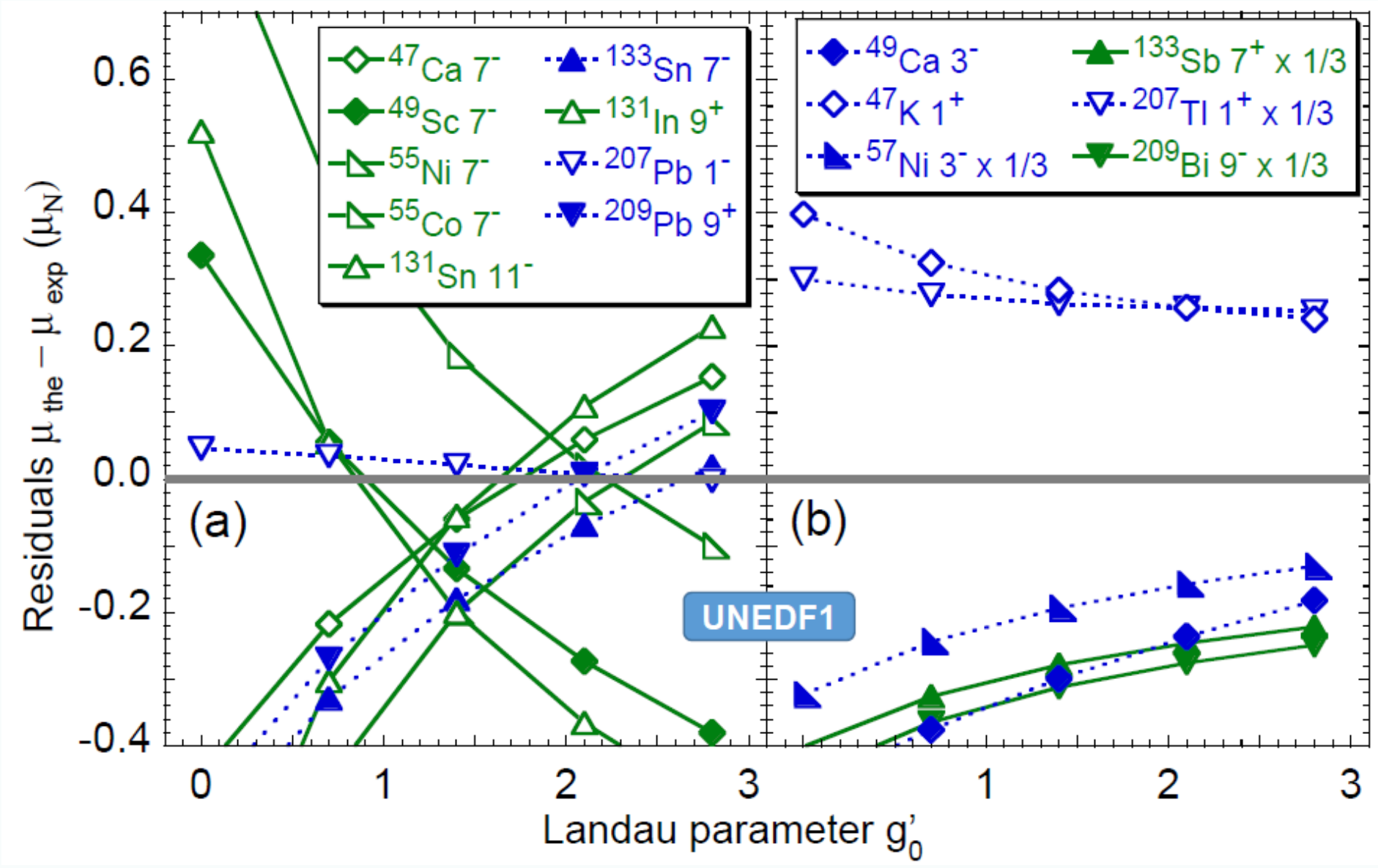
$$g_0' = N_0\Big(2C_1^s + 2C_1^T\,(3\pi^2\rho_0/2)^{2/3}\Big),$$

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

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

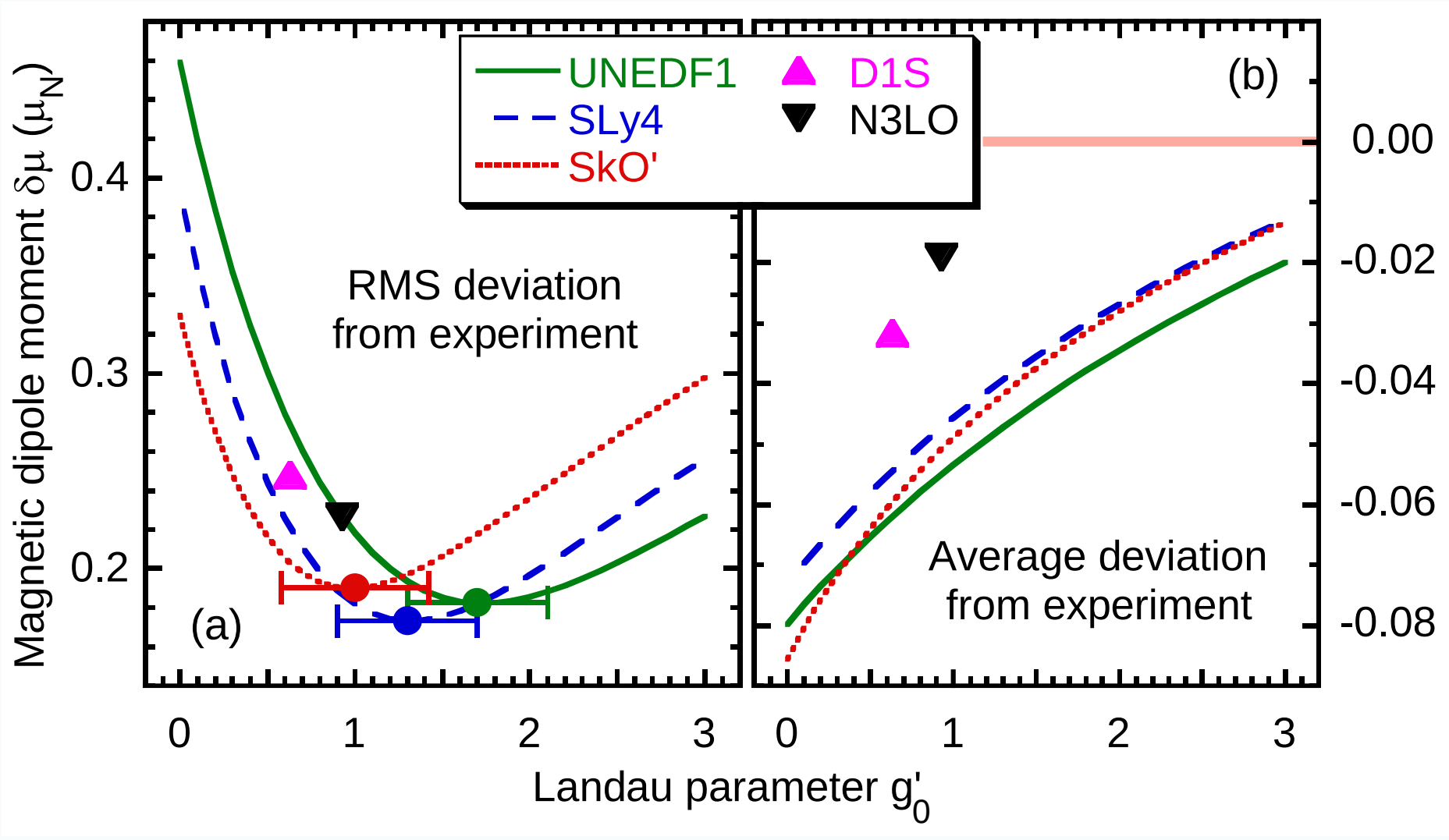
Magnetic dipole moments vs. experiment

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



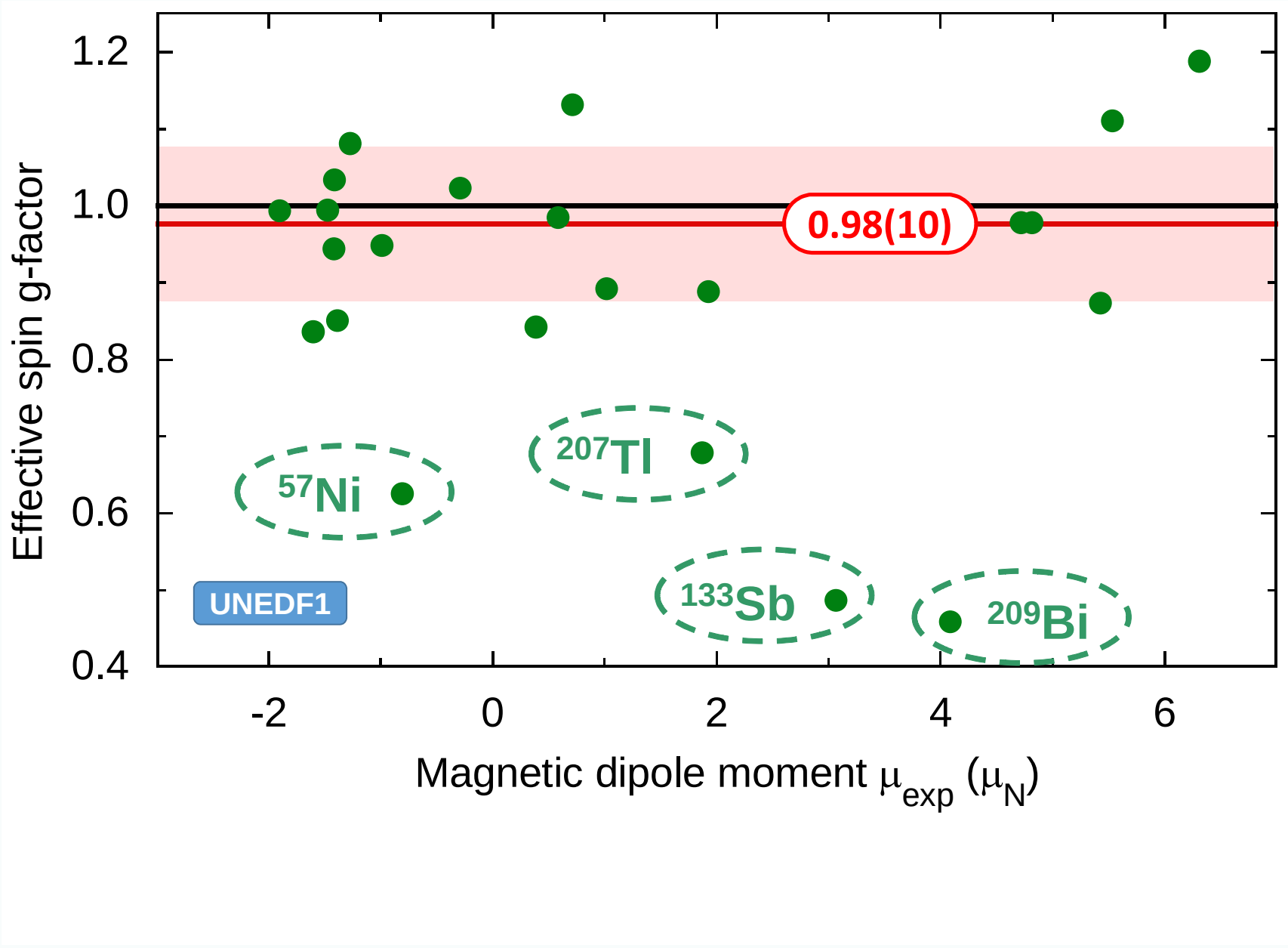
Optimisation of the spin-spin term

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



Effective spin g-factor?

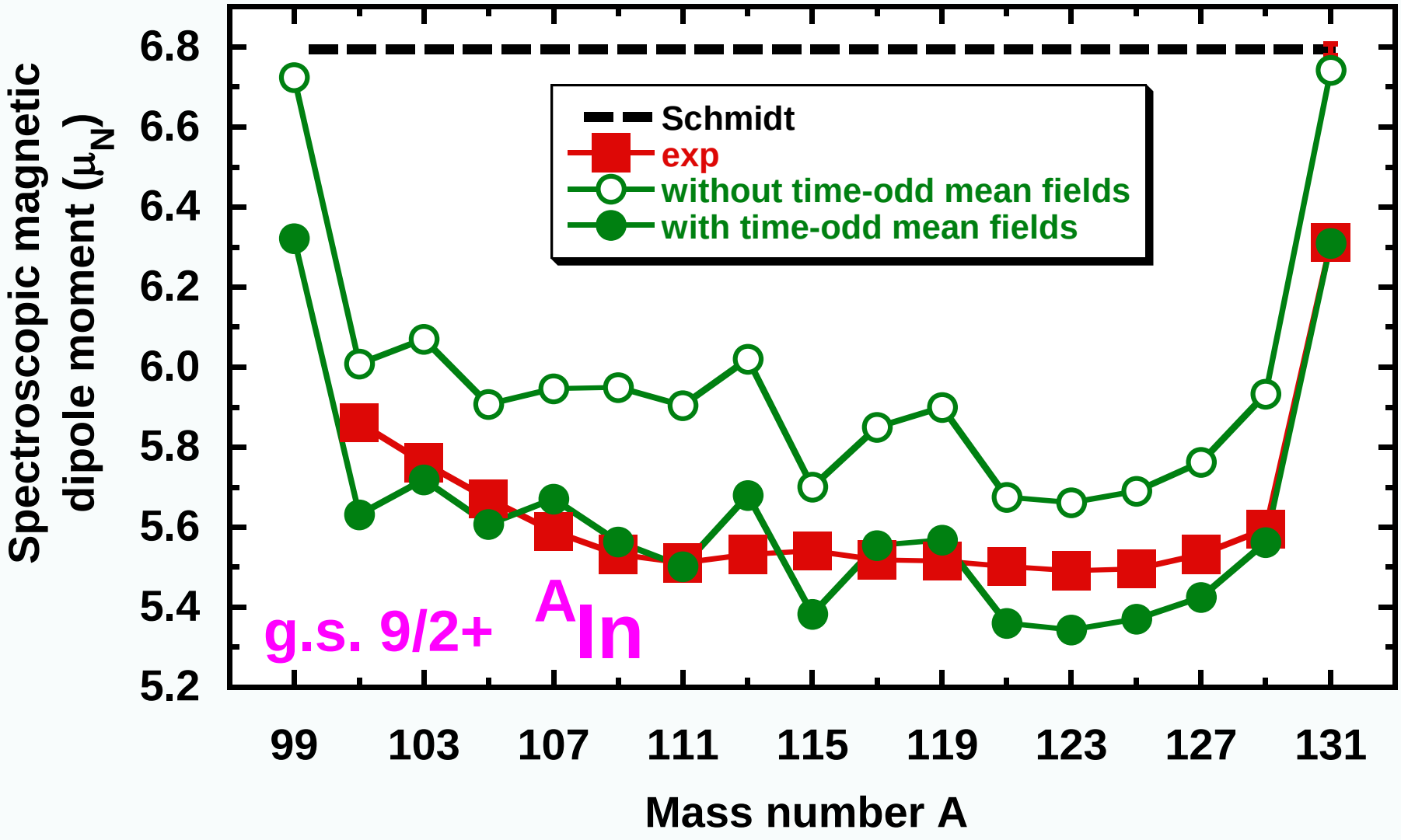
P. Sassarini, J.D., J. Bonnard, R.F. Garcia Ruiz, arXiv:2111.04675



Indium

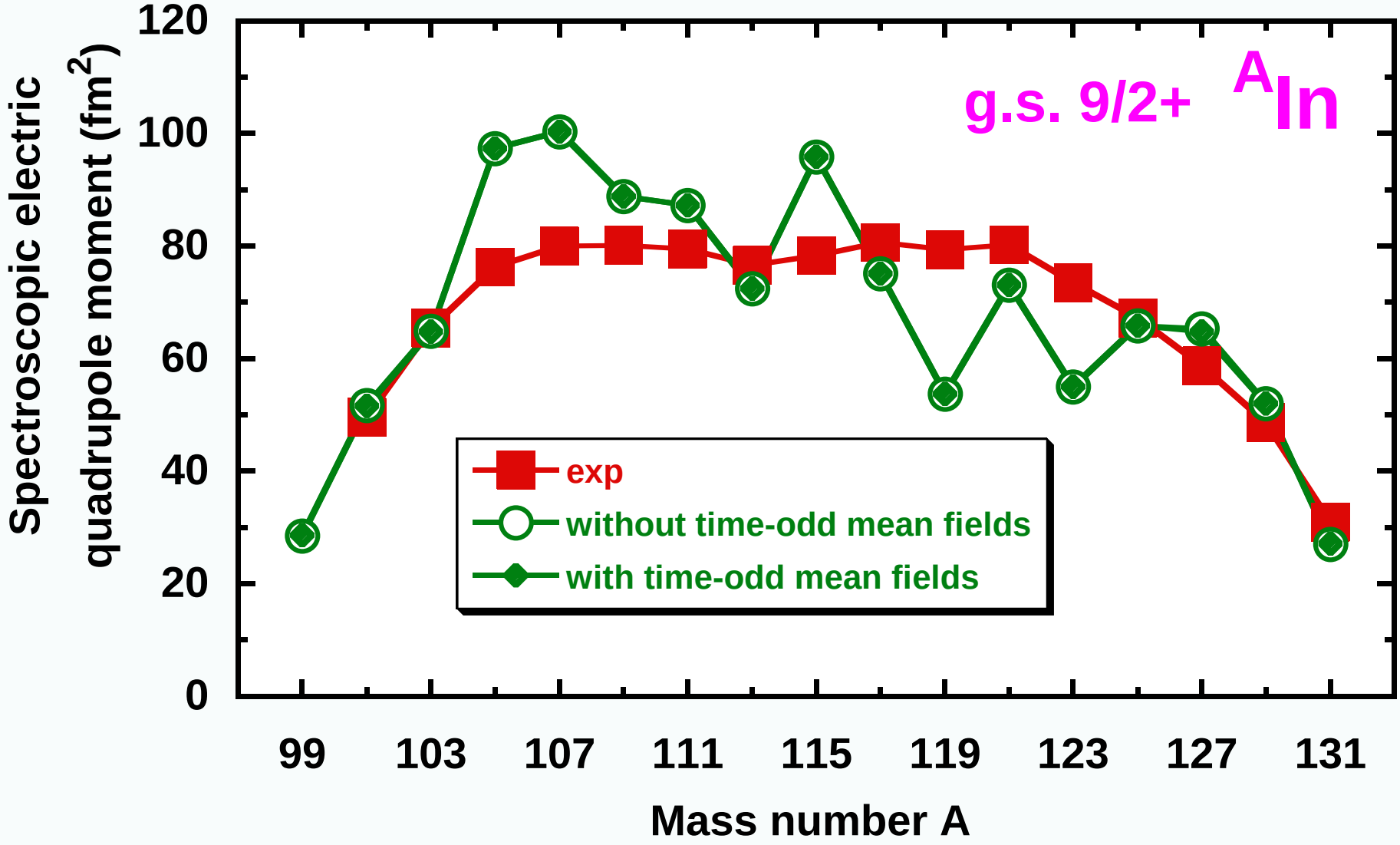
Magnetic dipole moments in indium

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



Electric quadrupole moments in indium

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



Particle-core-coupling 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:

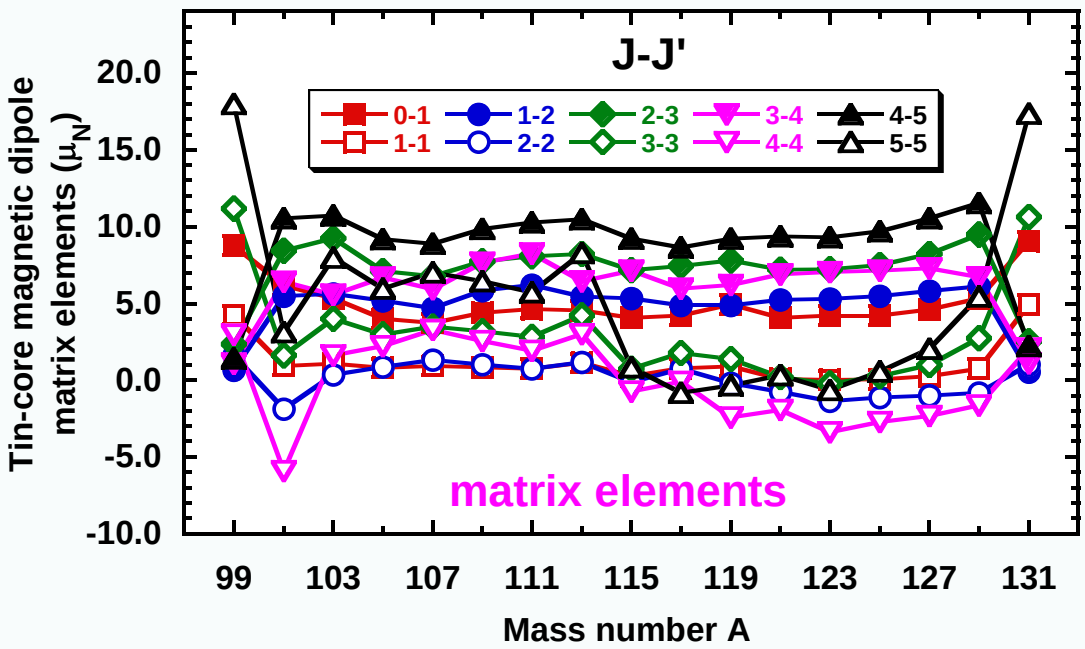
1° $|\Phi_K\rangle = \sum_I g_I |\Phi_{IK}\rangle$,
2° $|\phi_\Omega\rangle = \sum_j c_j |\phi_{j\Omega}\rangle$,
3° $|\Psi\rangle = \sum_J C_J |\Psi_{J0}\rangle$.

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

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

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

Particle-core-coupling analysis



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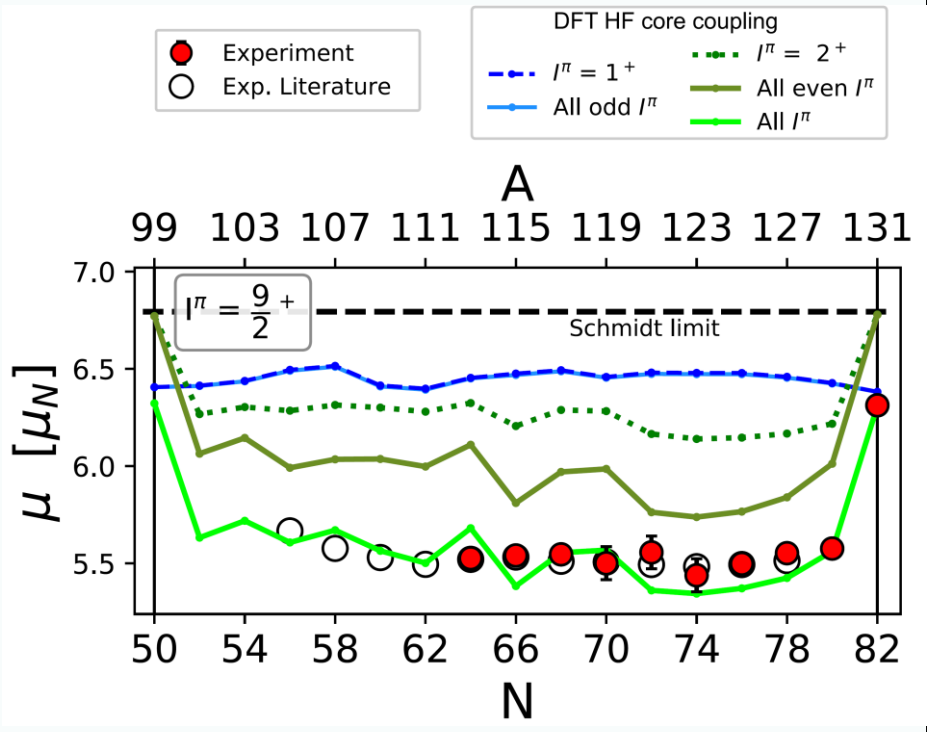
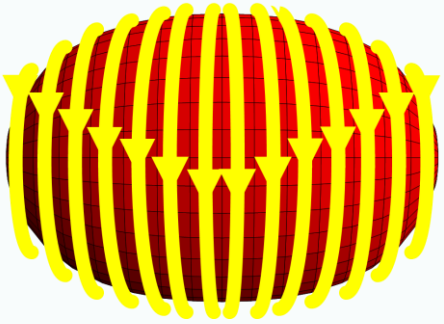


A.R. Vernon et al., accepted in Nature

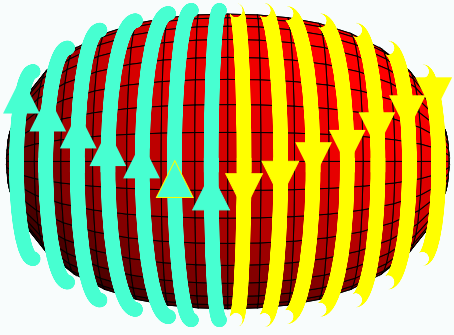
Magnetic octupole moments

Visualisation of the magnetic multipole moments in axial symmetry

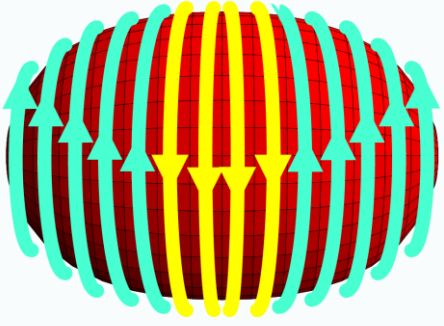
λ=1



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

Axial electric and magnetic-moment densities:

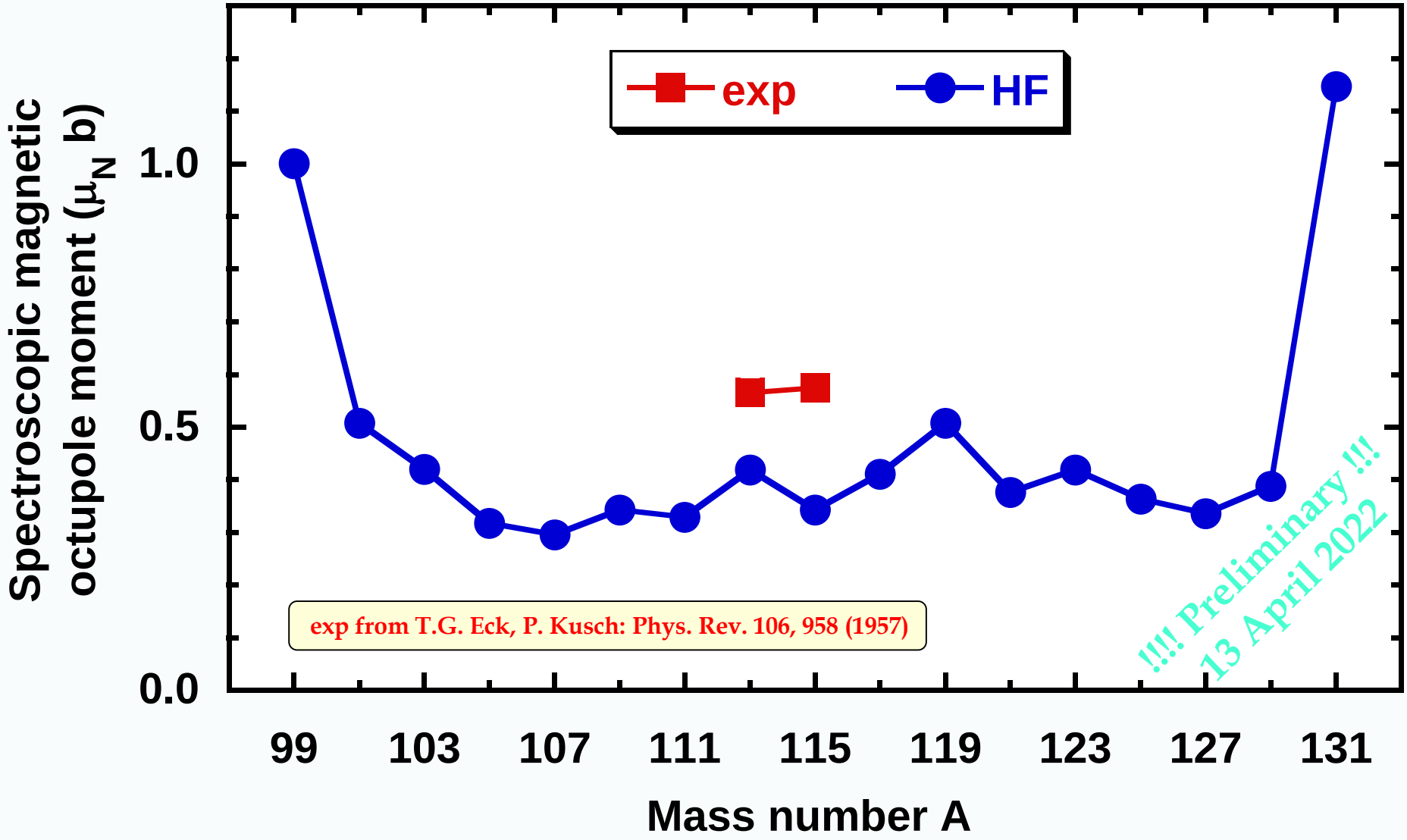
$$q_{\lambda 0}(r,\theta) = e\rho(r,\theta)Q_{\lambda 0}(r,\theta),$$

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

or

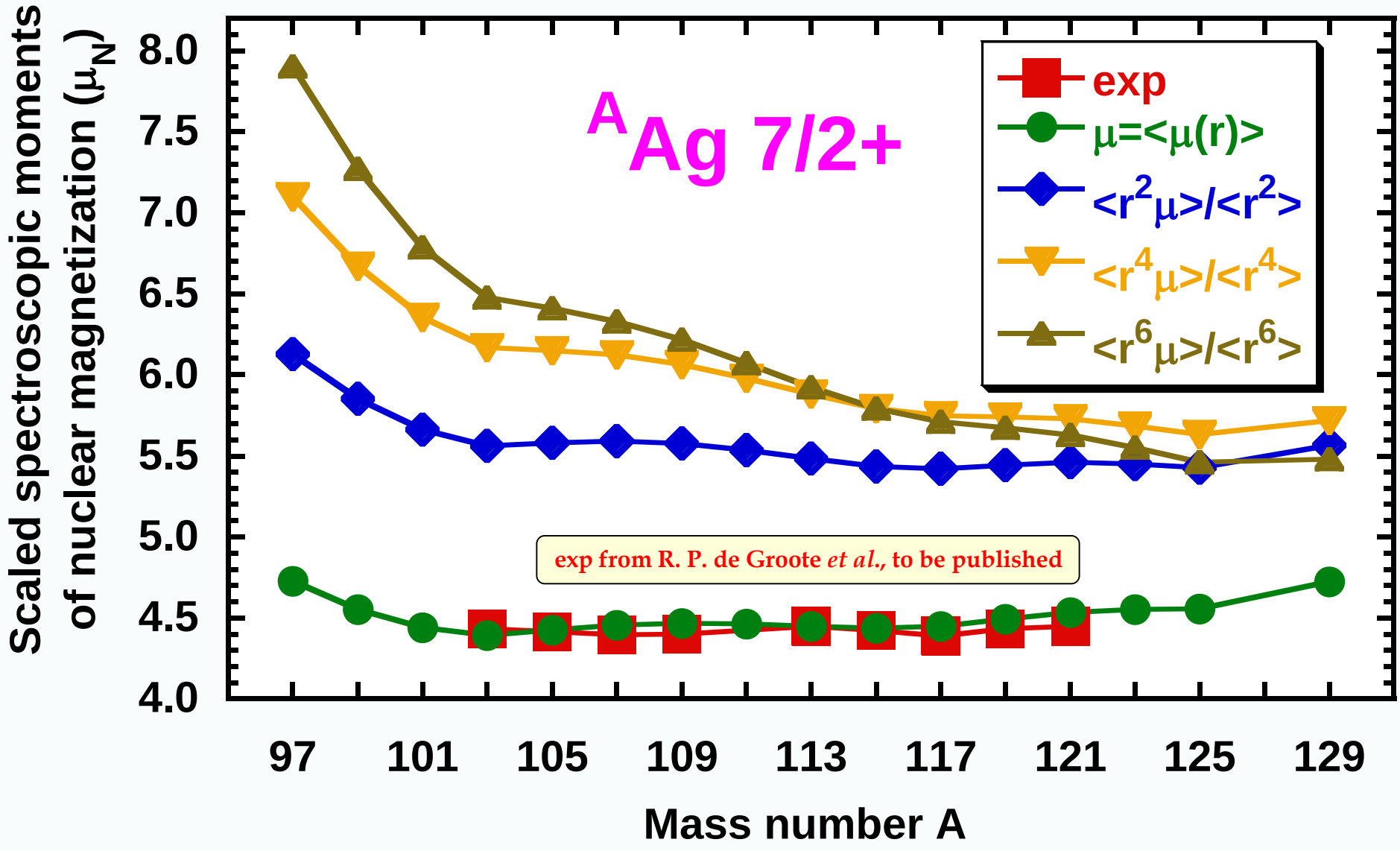
$$m_{\lambda 0}(r,\theta) = \mu_N\left[g_s s_z(r,\theta) + \frac{2}{\lambda+1}g_l I_z(r,\theta)\right]C_\lambda Q_{(\lambda-1)0}(r,\theta),$$

Magnetic octupole moments in indium



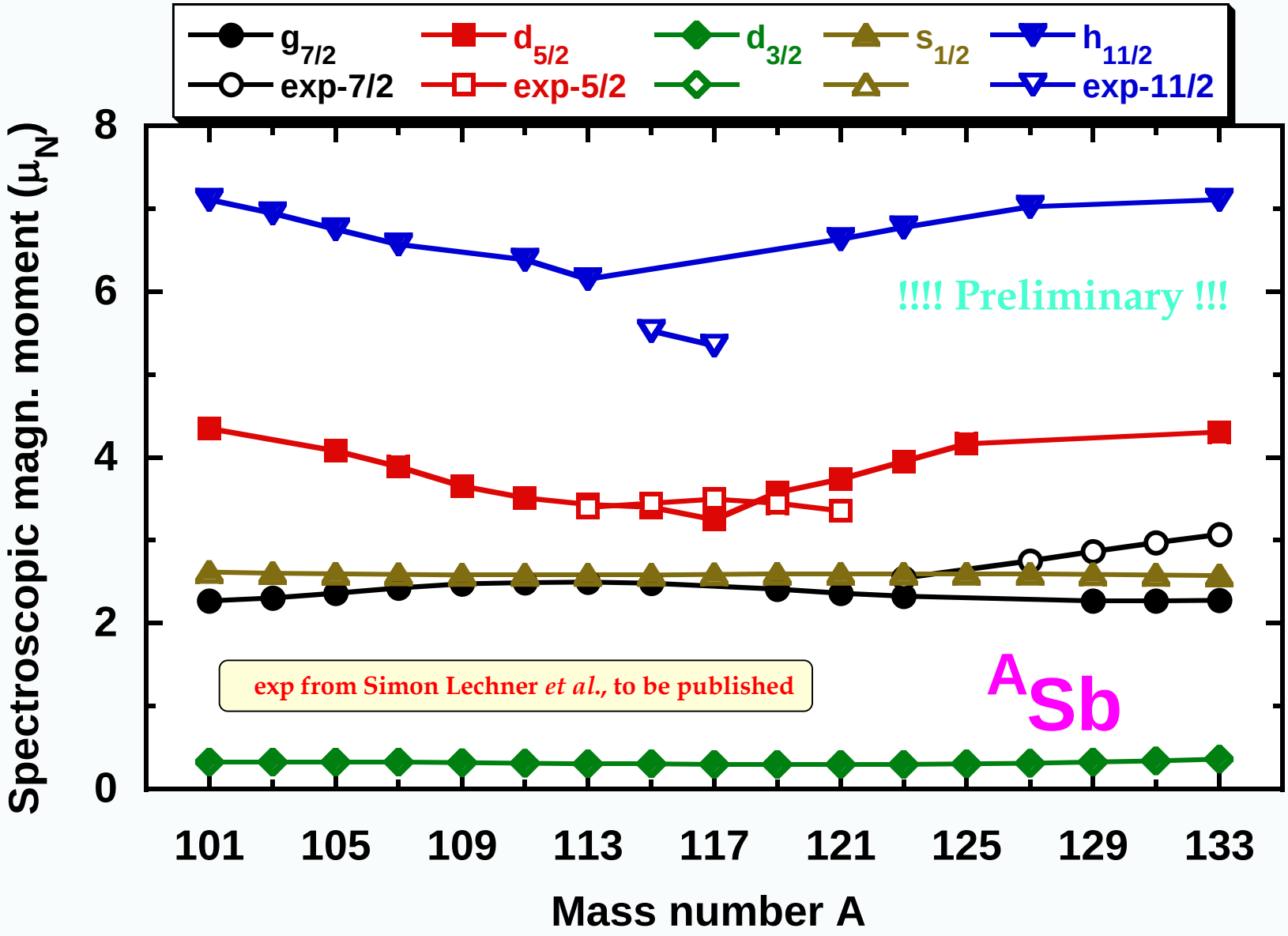
Bohr-Weisskopf correction

Moments of magnetization in silver

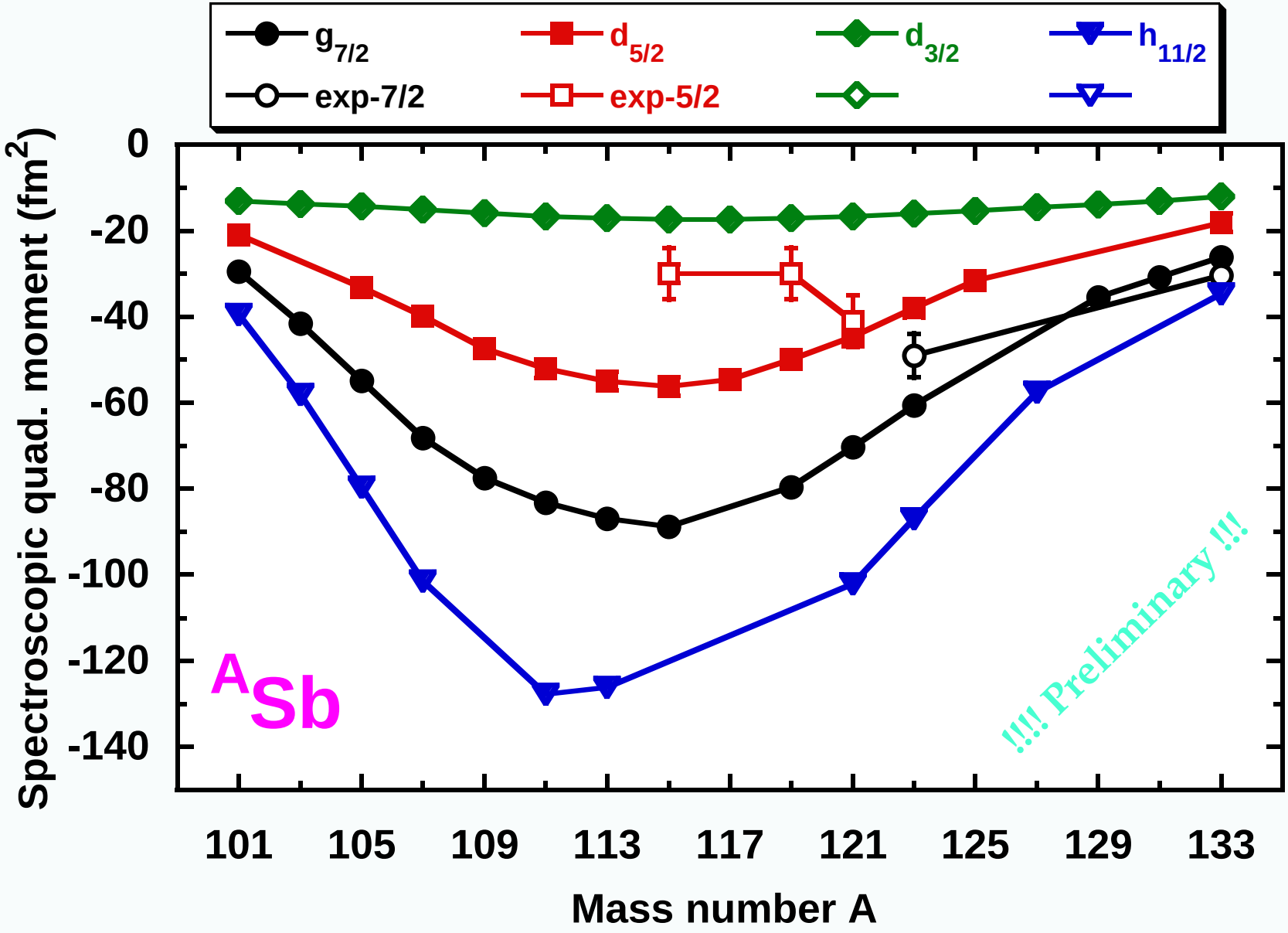


Antimony

Magnetic dipole moments in antimony

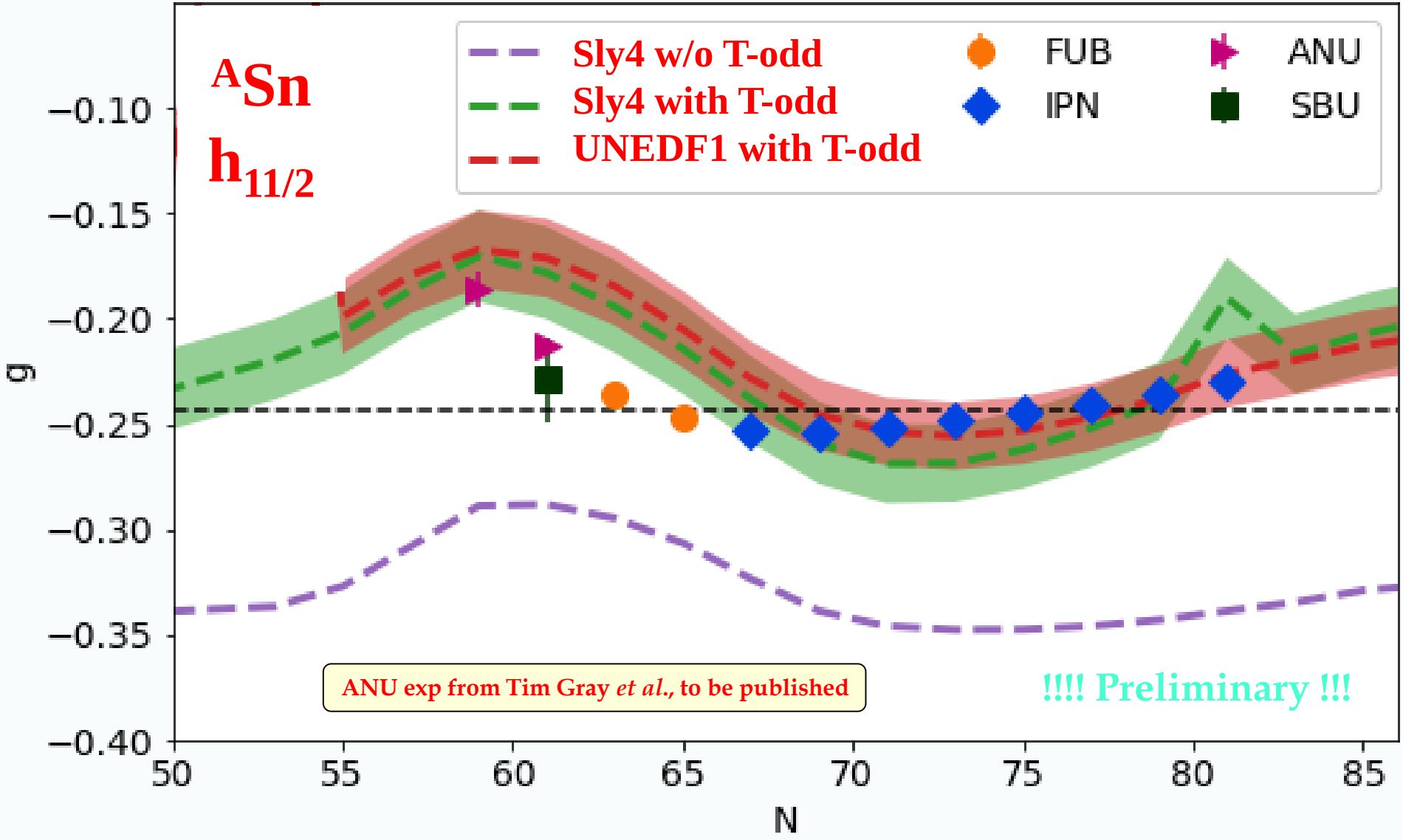


Electric quadrupole moments in antimony



Tin

Magnetic dipole moments in tin



Schiff moment in ^{225}Ra

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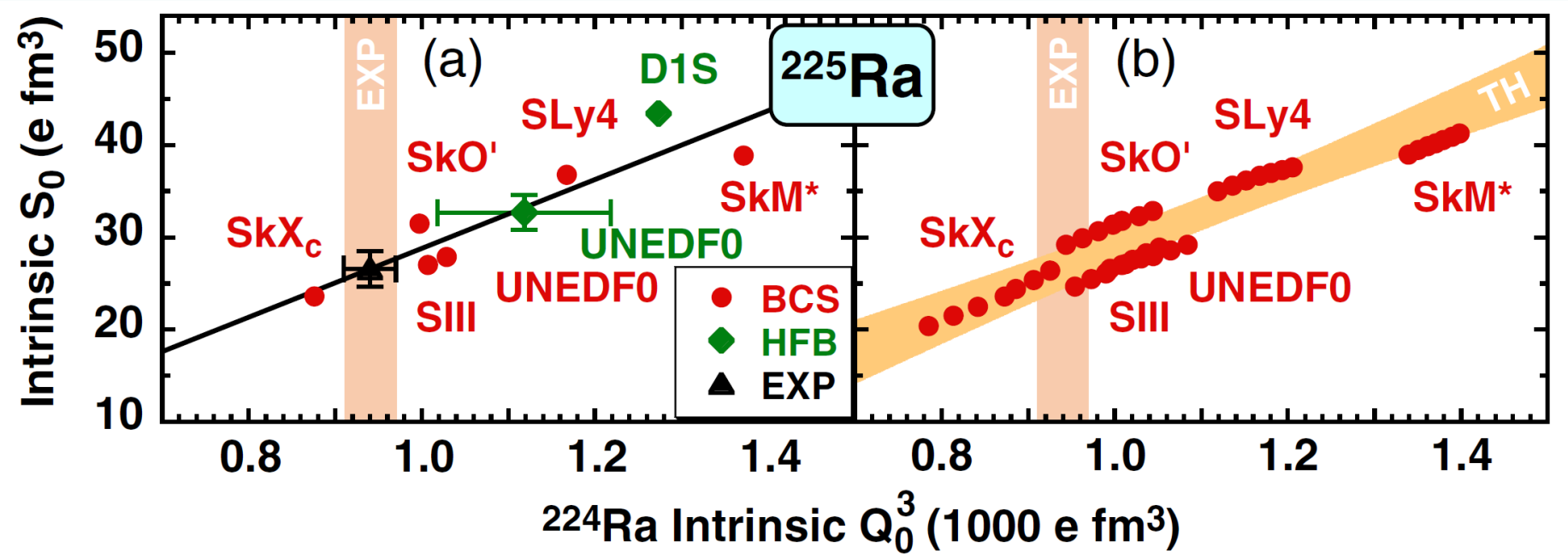
^{225}Ra Schiff moment vs. ^{224}Ra octupole moment



	a_0	a_1	a_2	b_1	b_2
^{221}Rn	*−0.04(10)*	**−1.7(3)**	**0.67(10)**	−0.015(5)	−0.007(4)
^{223}Rn	*−0.08(8)*	**−2.4(4)**	**0.86(10)**	−0.031(9)	*−0.008(8)*
^{223}Fr	*0.07(20)*	*−0.8(7)*	*0.05(40)*	0.018(8)	−0.016(10)
^{225}Ra	*0.2(6)*	−5(3)	3.3(1.5)	*−0.01(3)*	0.03(2)
^{229}Pa	**−1.2(3)**	*−0.9(9)*	*−0.3(5)*	**0.036(8)**	0.032(18)

$$S = a_0 g\bar{g}_0 + a_1 g\bar{g}_1 + a_2 g\bar{g}_2 + b_1\bar{c}_1 + b_2\bar{c}_2.$$

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.
   - Allows for analysing physical effects.
   - Unified approach with no limits on mass.
2. Symmetry restoration is essential.
3. Effective charges and effective g-factors not needed.
4. Future systematic applications to semi-magic nuclei, excited states, open-shell systems.
5. Future applications to exotic moments: Schiff, anapole, weak…
6. Links to particle, atomic, and molecular physics.
7. Adjustments of the nuclear DFT coupling constants to data should take the magnetic moments into account.

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

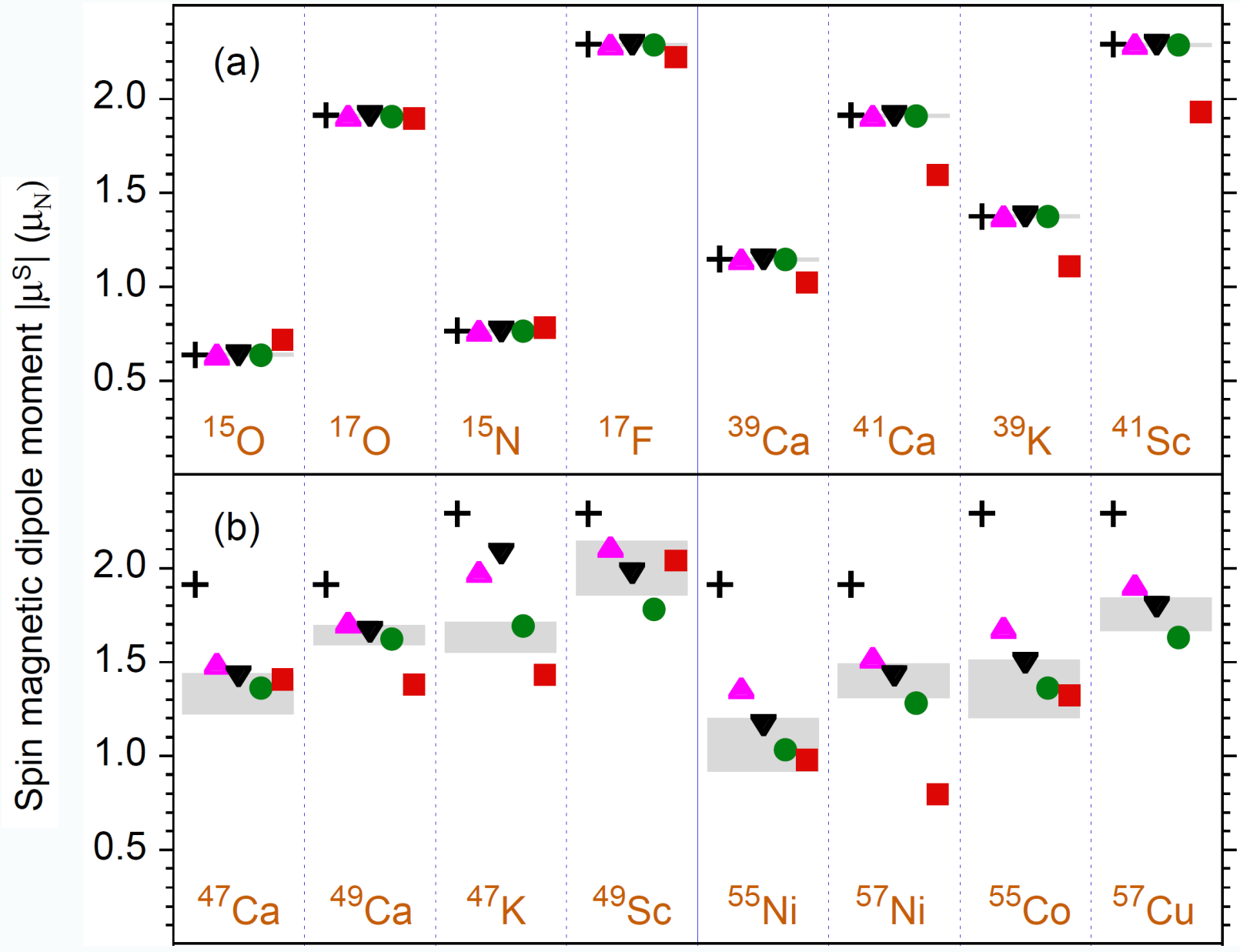
$$\begin{aligned}
\mu^{\mathbf{S}} &= \mu = g_\ell^p \langle \hat{L}_p \rangle + g_s^n \langle \hat{S}_n \rangle + g_s^p \langle \hat{S}_p \rangle \quad \text{for } Z \text{ even,} \\
\mu^{\mathbf{S}} &= \mu - J\,\mu_N \\
&= g_\ell'^n \langle \hat{L}_n \rangle + g_s'^n \langle \hat{S}_n \rangle + g_s'^p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

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



Spin magnetic dipole moments

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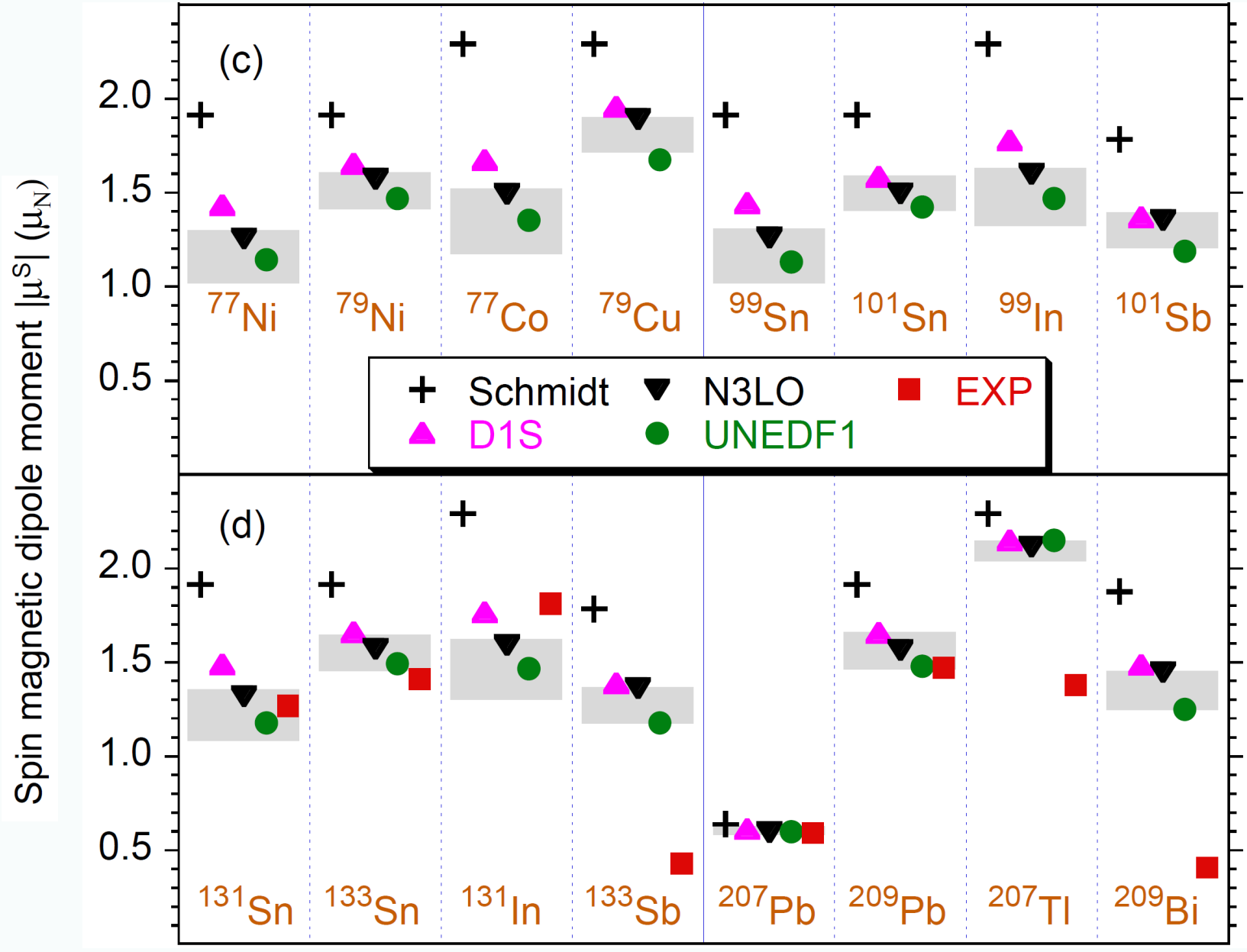
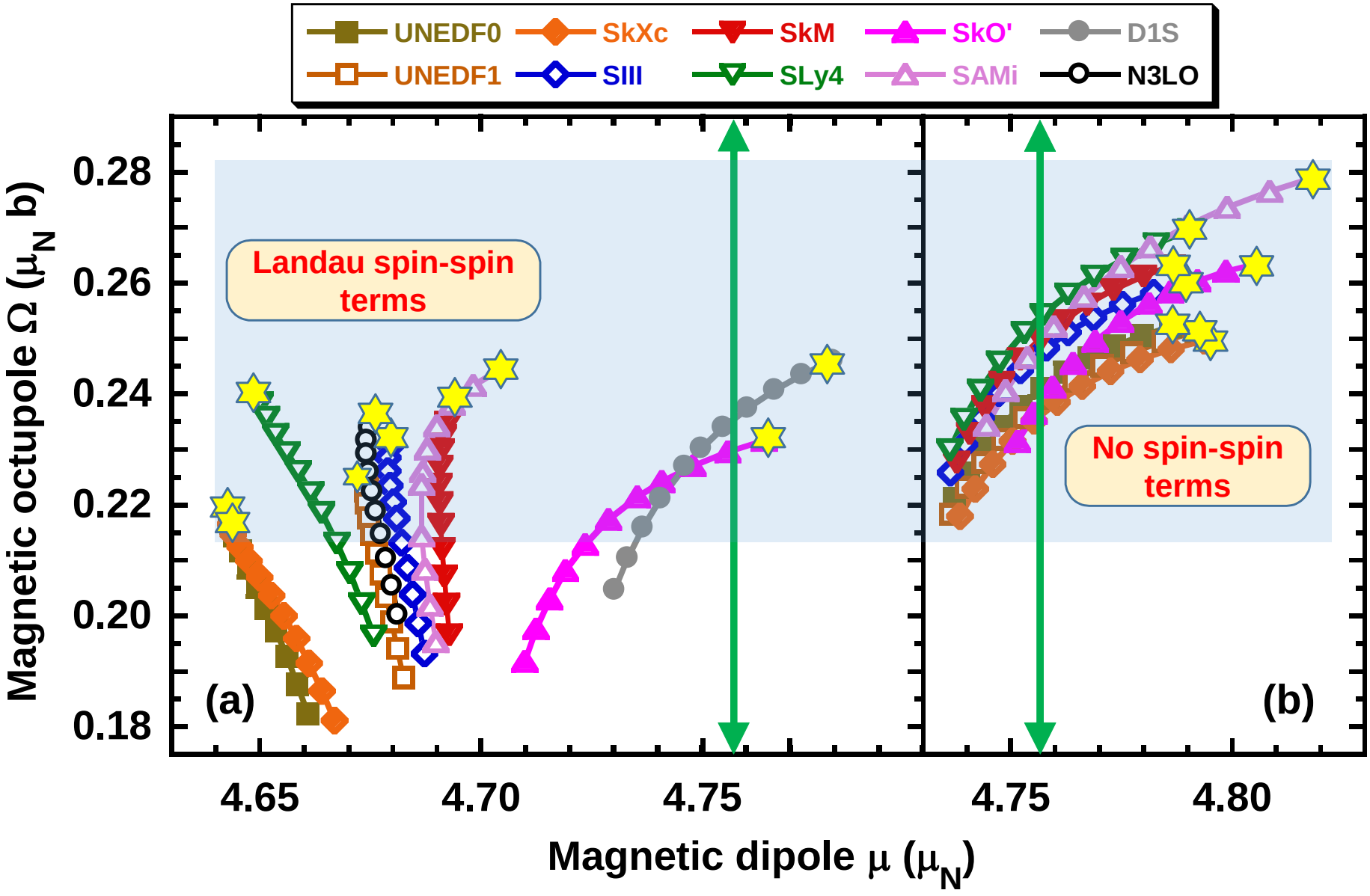
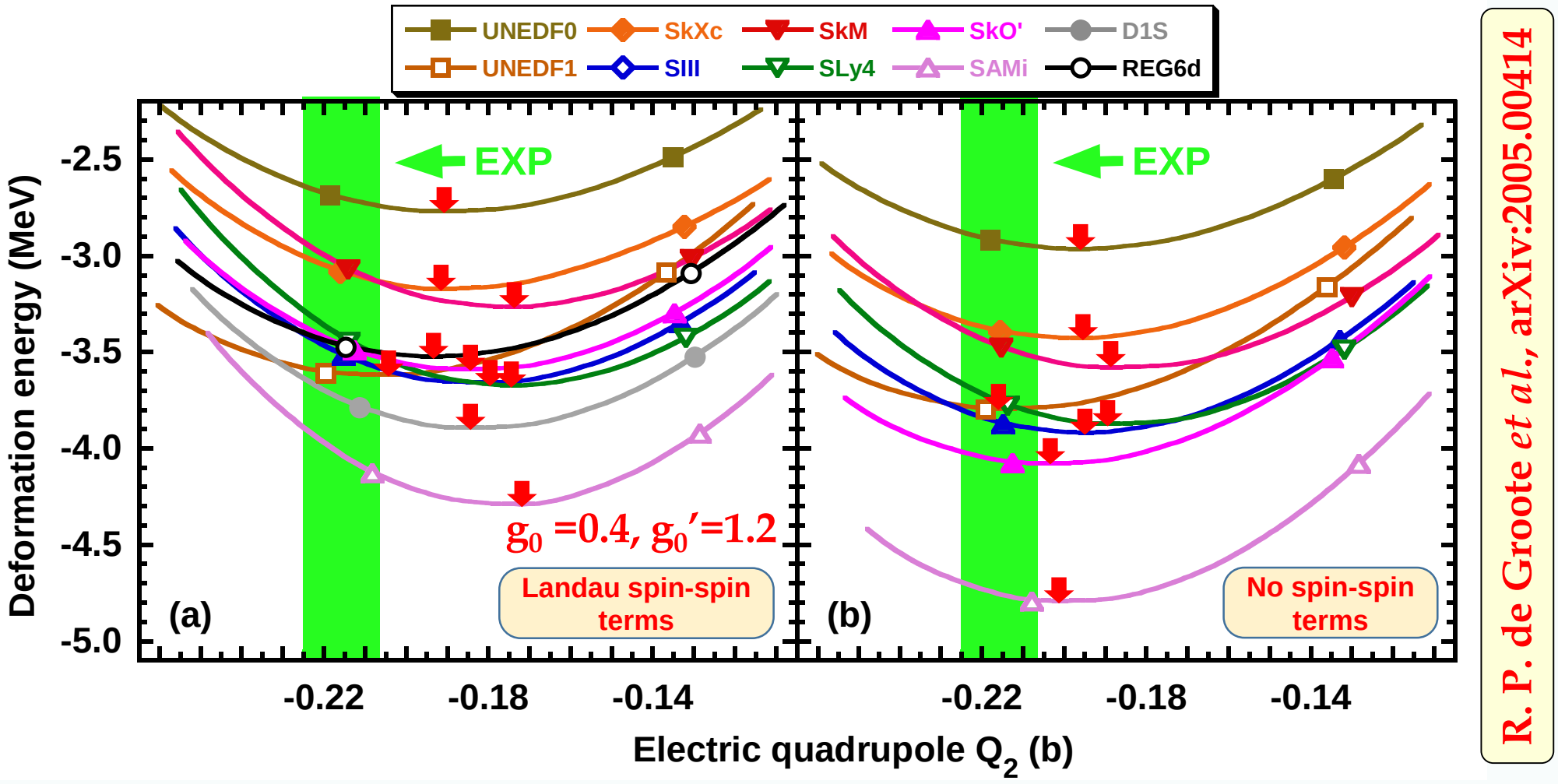


Magnetic moments in ^{45}Sc



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

HF+AMP, deformation energies in ^{45}Sc



isoscalar **isovector** **Landau parameters g_0 & g_0'**

$$V(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4) = N_0\left[g_0(\sigma_1\cdot\sigma_2) + g_0'(\sigma_1\cdot\sigma_2)(\tau_1\cdot\tau_2)\right]\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_1-\vec{r}_3)\delta(\vec{r}_2-\vec{r}_4)$$

HF + angular momentum projection (AMP)

The Hartree-Fock (HF) spin and current intrinsic densities read:

$$\vec{s}(\vec{r}) = \sum_{\sigma\sigma'} \vec{\sigma}_{\sigma'\sigma}\rho(\vec{r}\sigma,\vec{r}\sigma'), \quad \vec{j}(\vec{r}) = \frac{1}{2i}\sum_{\sigma}(\vec{\nabla}-\vec{\nabla}')\rho(\vec{r}\sigma,\vec{r}'\sigma),$$

where the one-body density matrix $\rho(\vec{r}\sigma,\vec{r}'\sigma')$ can be split into the core and odd-particle contributions:

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') = \sum_{i=1}^{A-1}\psi_i(\vec{r}\sigma)\psi_i^*(\vec{r}'\sigma') + \psi_{\rm odd}(\vec{r}\sigma)\psi_{\rm odd}^*(\vec{r}'\sigma'),$$

and where $\psi(\vec{r}\sigma)$ are the self-consistent single-particle wave functions of occupied states. The HF wave function of an odd system $|\Phi\rangle = |\Phi^{\rm core}\rangle \otimes |\psi^{\rm odd}\rangle = \sum_I |\Psi_I\rangle$ has the conserved-angular-momentum components:

$$|\Psi_I\rangle = \sum_{J=0,2,4,\ldots}\ \sum_{j=K,K+2,K+4,\ldots}\left[|\Psi_J^{\rm core}\rangle|\psi_j^{\rm odd}\rangle\right]_I,$$

In ^{45}Sc, the angular-momentum projected ground state can be presented as:

$$\begin{aligned}|\Psi_{7/2}\rangle &= \left[|\Psi_0^{\rm core}\rangle|\psi_{7/2}^{\rm odd}\rangle\right]_{7/2} + \left[|\Psi_2^{\rm core}\rangle|\psi_{7/2}^{\rm odd}\rangle\right]_{7/2} \\ &+ \left[|\Psi_2^{\rm core}\rangle|\psi_{11/2}^{\rm odd}\rangle\right]_{7/2} + \left[|\Psi_4^{\rm core}\rangle|\psi_{7/2}^{\rm odd}\rangle\right]_{7/2} + \cdots\end{aligned}$$

The first term represents a spherical core coupled to the spherical $j = 7/2$ wave function of the odd particle. The second term represents the lowest-order coupling of the odd-particle to the lowest $J = 2$ state of the core.