Electromagnetic moments in nuclei within nuclear DFT

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NucMagMom Collaboration (est. 2017)

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- **Witek Nazarewicz, Mengzhi Chen, MSU**
- **Paolo Sassarini, Jérémy Bonard, York**
- **Ronald Fernando Garcia Ruiz, MIT**

Literature

- **B. Castel and I.S. Towner, *Modern theories of nuclear moments*, (Oxford Studies in Nuclear Physics) vol 12, ed P E Hodgson (Oxford: Clarendon,1990).**
- **Gerda Neyens, Rep. Prog. Phys. 66 (2003) 633–689.**
- **N.J. Stone, At. Data and Nucl. Data Tables 90 (2005) 75–176.**
- **M. Borrajo and J.L. Egido, Phys. Lett. B764 (2017) 328.**
- **L. Bonneau *et al.*,Phys. Rev. C91 (2015) 054307.**
- **O.I. Achakovskiy *et al.*, Eur. Phys. J. A (2014) 50:6.**
- **I. N. Borzov *et al.*, Phys. Atom. Nucl. 71 (2008) 469.**

Outline

1. Recap on nuclear electromagnetic moments
2. Odd near doubly magic nuclei
3. N=83 isotones
4. Magnetic octupole moment in ^{45}Sc
5. Schiff moment in ^{225}Ra
6. ^{229}Th
7. 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:

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

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

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]:

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

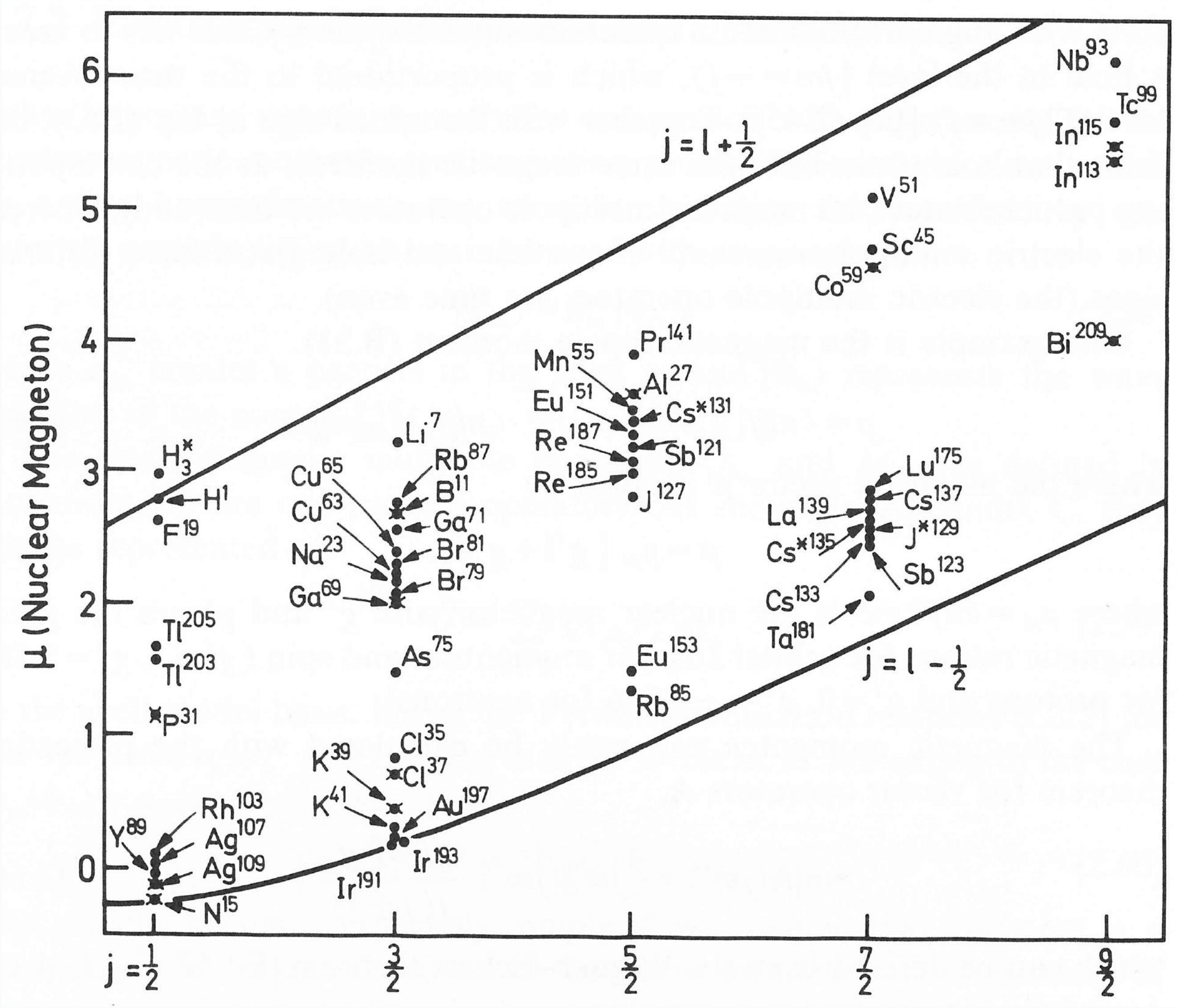
$$\text{for an odd neutron: } \begin{cases} \mu = \mu_\mathrm{n} & \text{for } j = l + \frac{1}{2} \\ \mu = -\dfrac{j}{j+1}\mu_\mathrm{n} & \text{for } j = l - \frac{1}{2} \end{cases} \qquad (2.3)$$

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

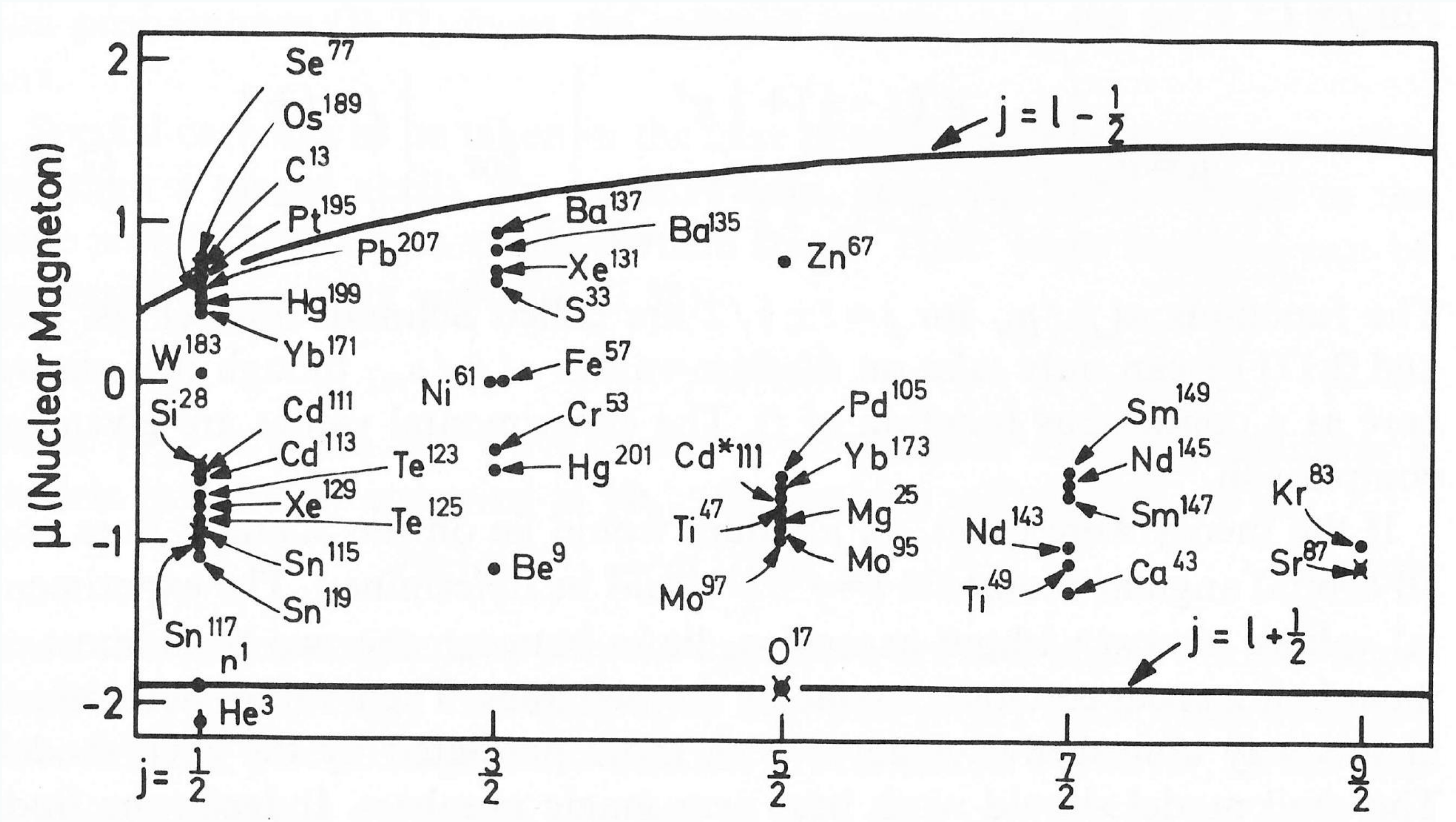
Gerda Neyens, Rep. Prog. Phys. 66 (2003) 633–689

Experiment



M.G. Mayer and J.H.D. Jensen, *Elementary Theory of Nuclear Shell Structure*, (Wiley, New York, 1955)

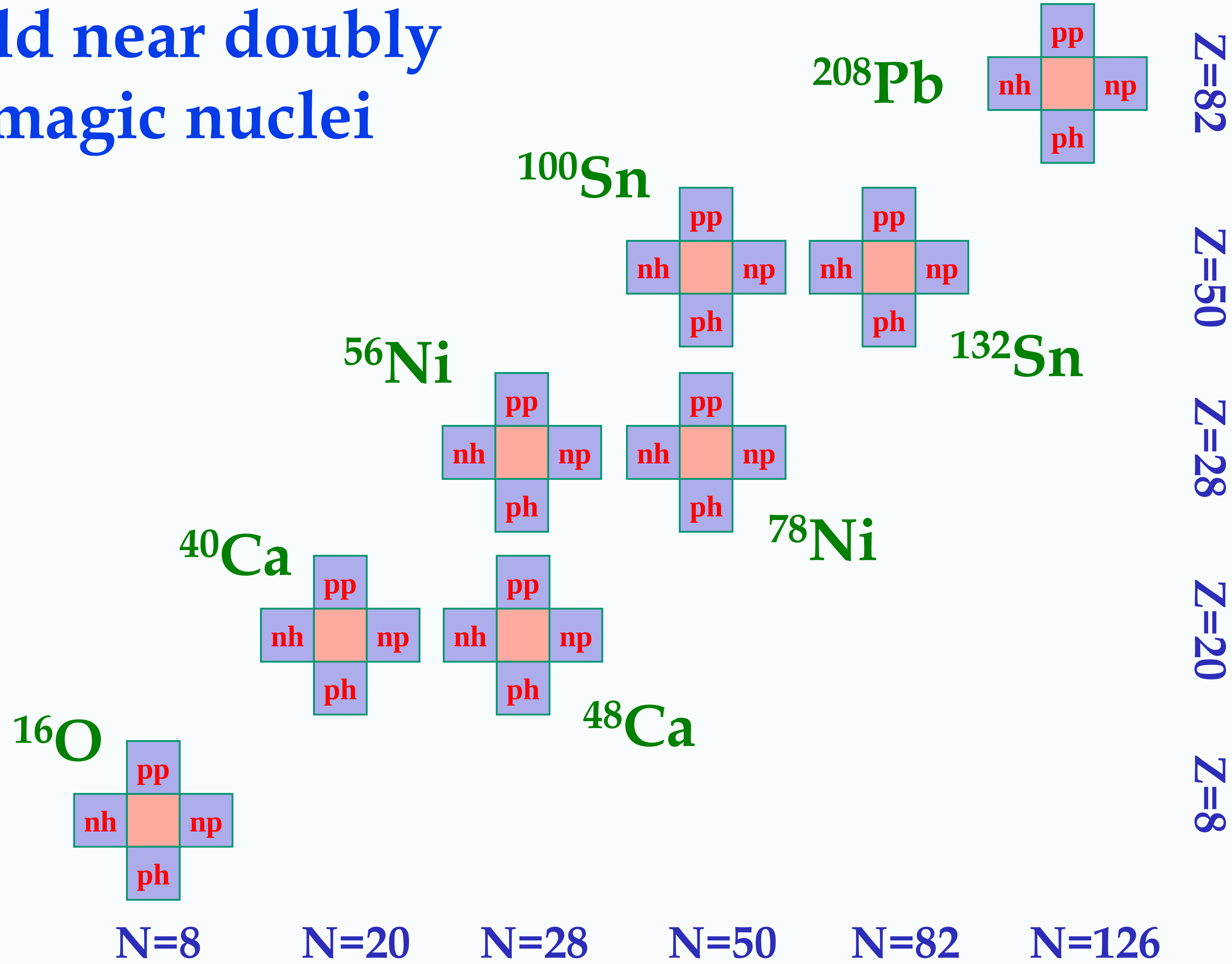
Experiment



M.G. Mayer and J.H.D. Jensen, *Elementary Theory of Nuclear Shell Structure*, (Wiley, New York, 1955)

Odd near doubly magic nuclei

Odd near doubly magic nuclei



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.

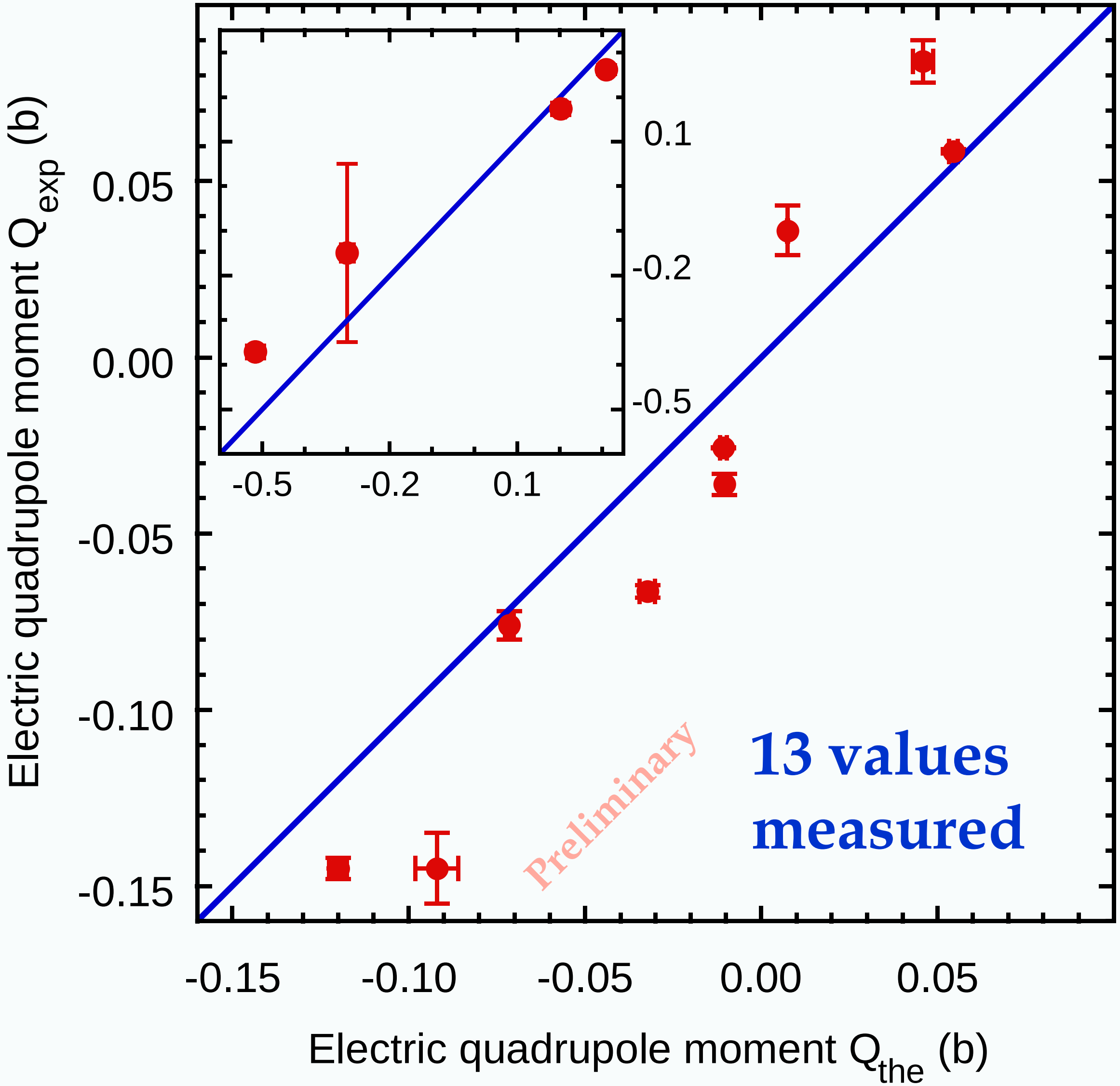
$$V=-\lambda \sigma_1 \sigma_2$$

- 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.

Electric quadrupole moments

Electric quadrupole moments Q

P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published

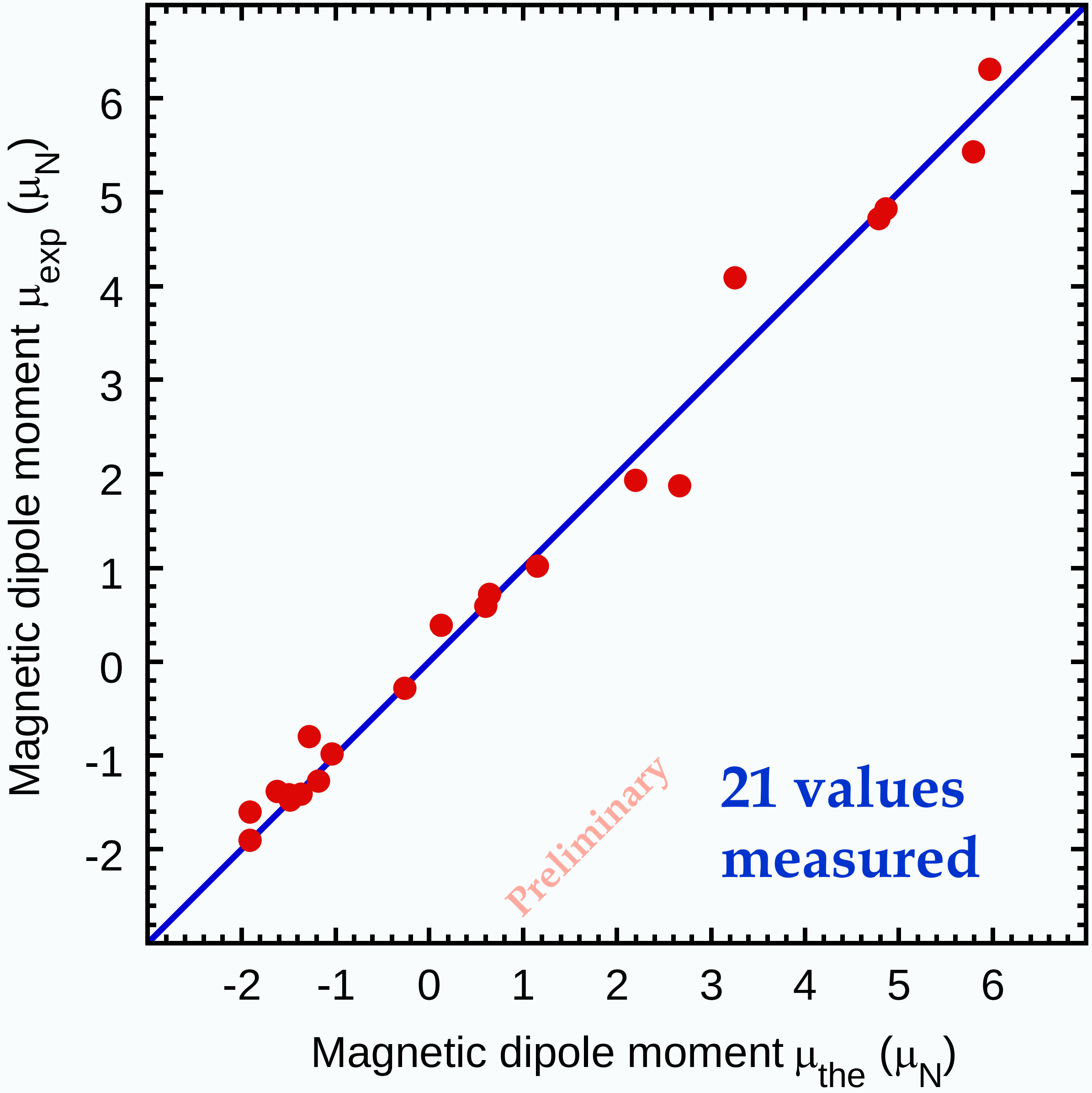


- **Spectroscopic moments**
- **Average values for**
  UNEDF1
  SLy4
  SkO′
  D1S
  N3LO
- **Relative RMS deviations much smaller than the residuals**

Magnetic dipole moments

Magnetic dipole moments μ

P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published



- **UNEDF1 Spectroscopic moments**
- **g'_0=2**

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:

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

  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

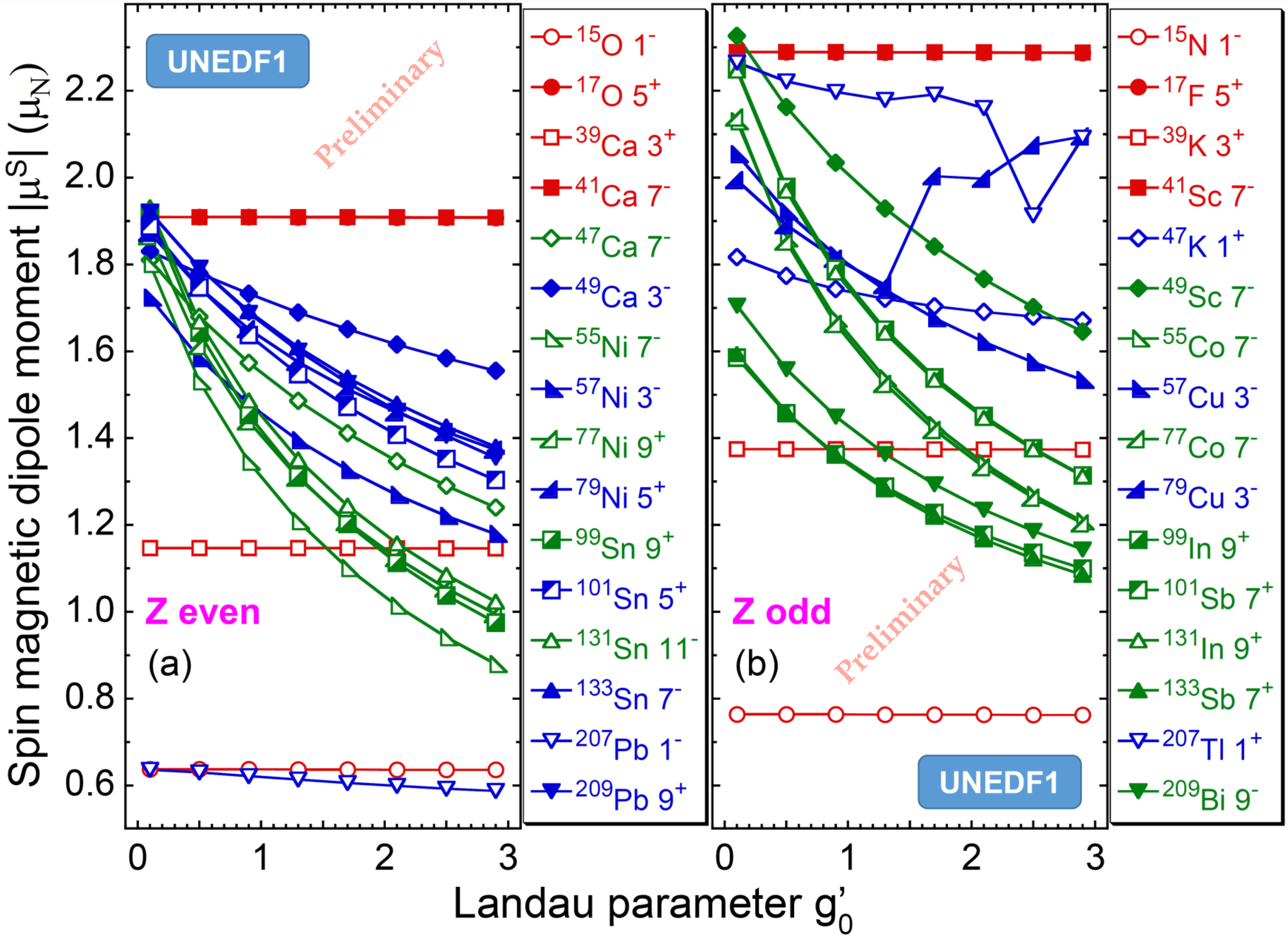
$$g_0' = N_0\left(2C_1^s + 2C_1^T\,(3\pi^2\rho_0/2)^{2/3}\right),$$

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

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

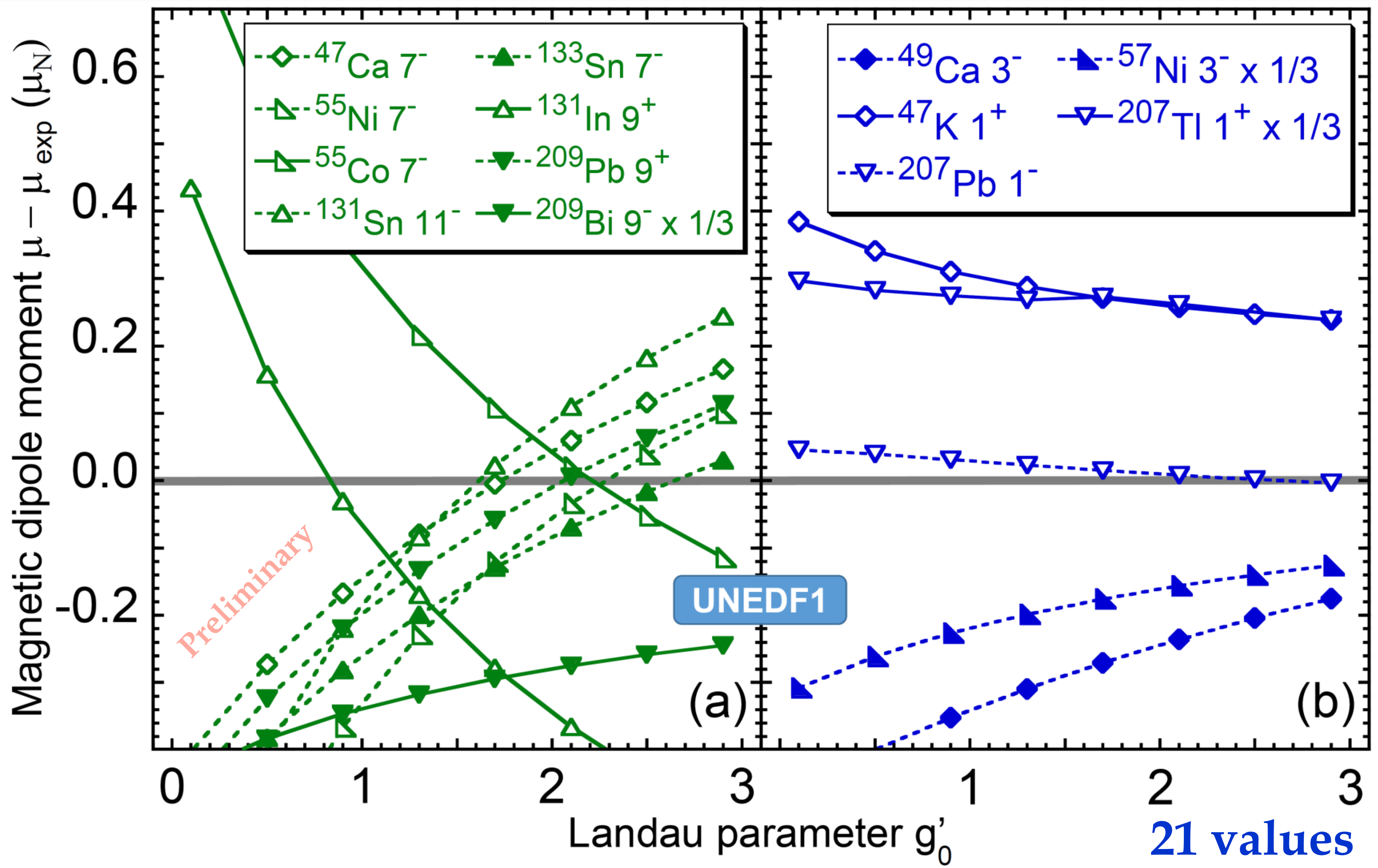
Magnetic dipole moments

P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published



Magnetic dipole moments vs. experiment

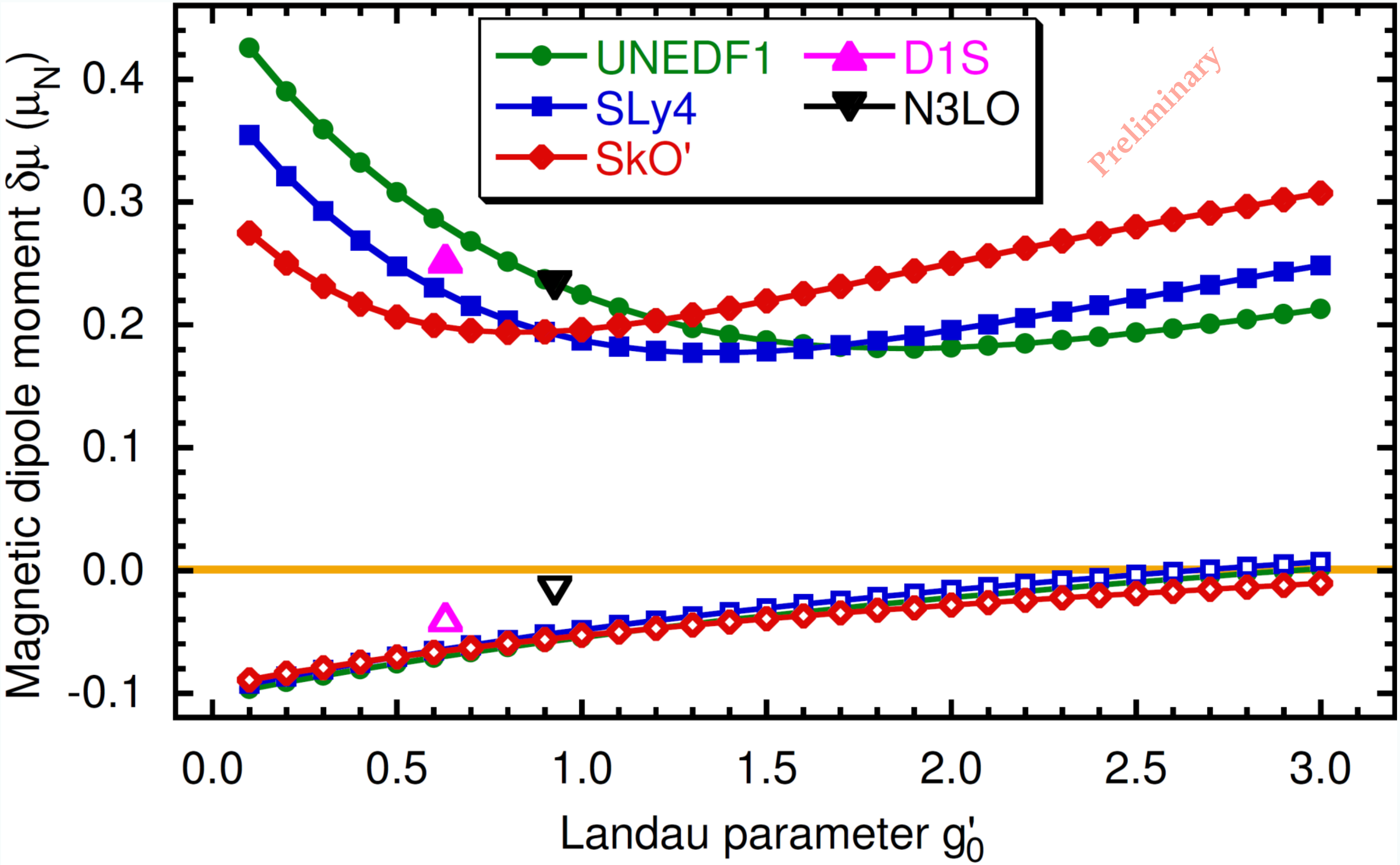
P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published



21 values measured

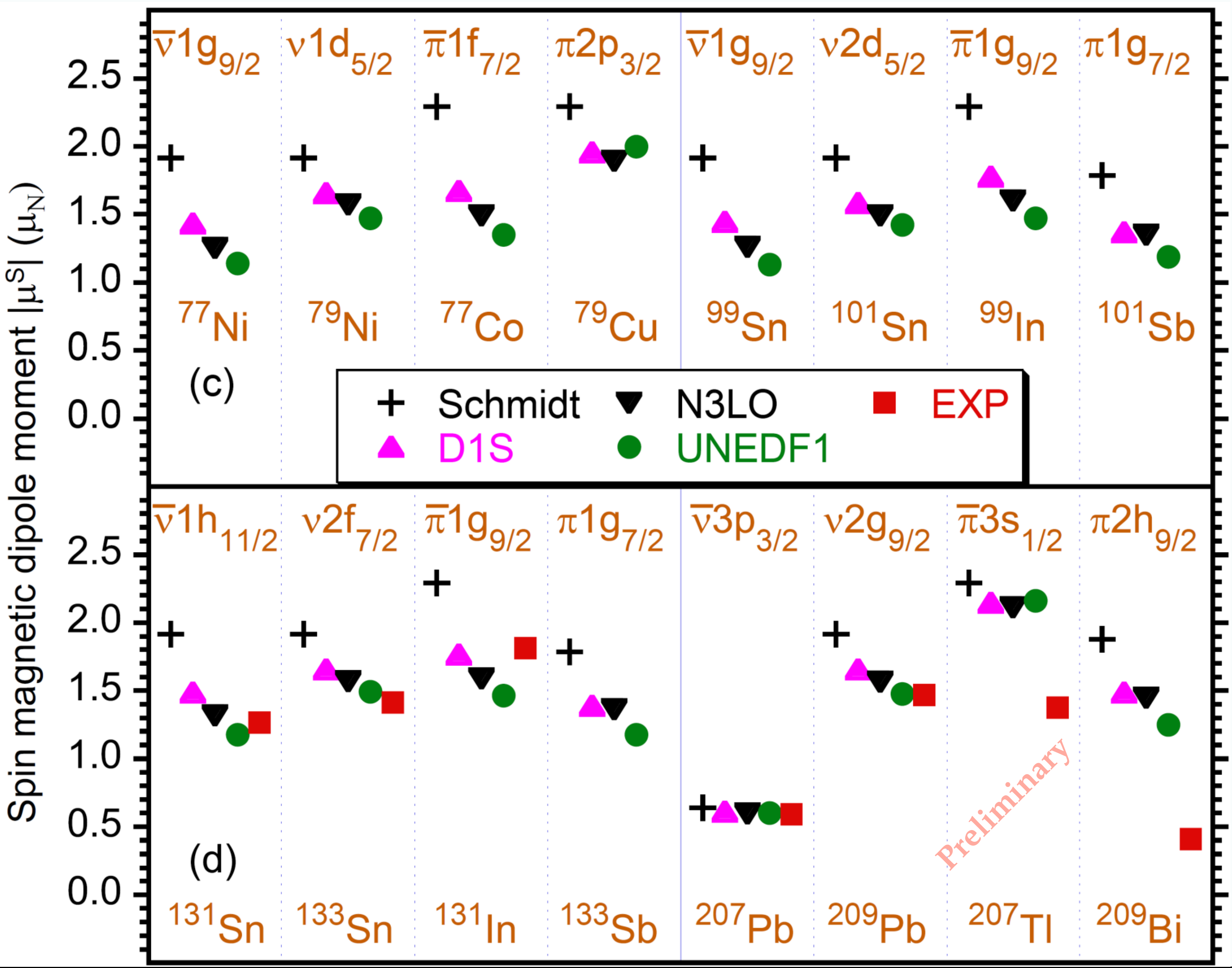
Optimisation of the spin-spin term

P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published



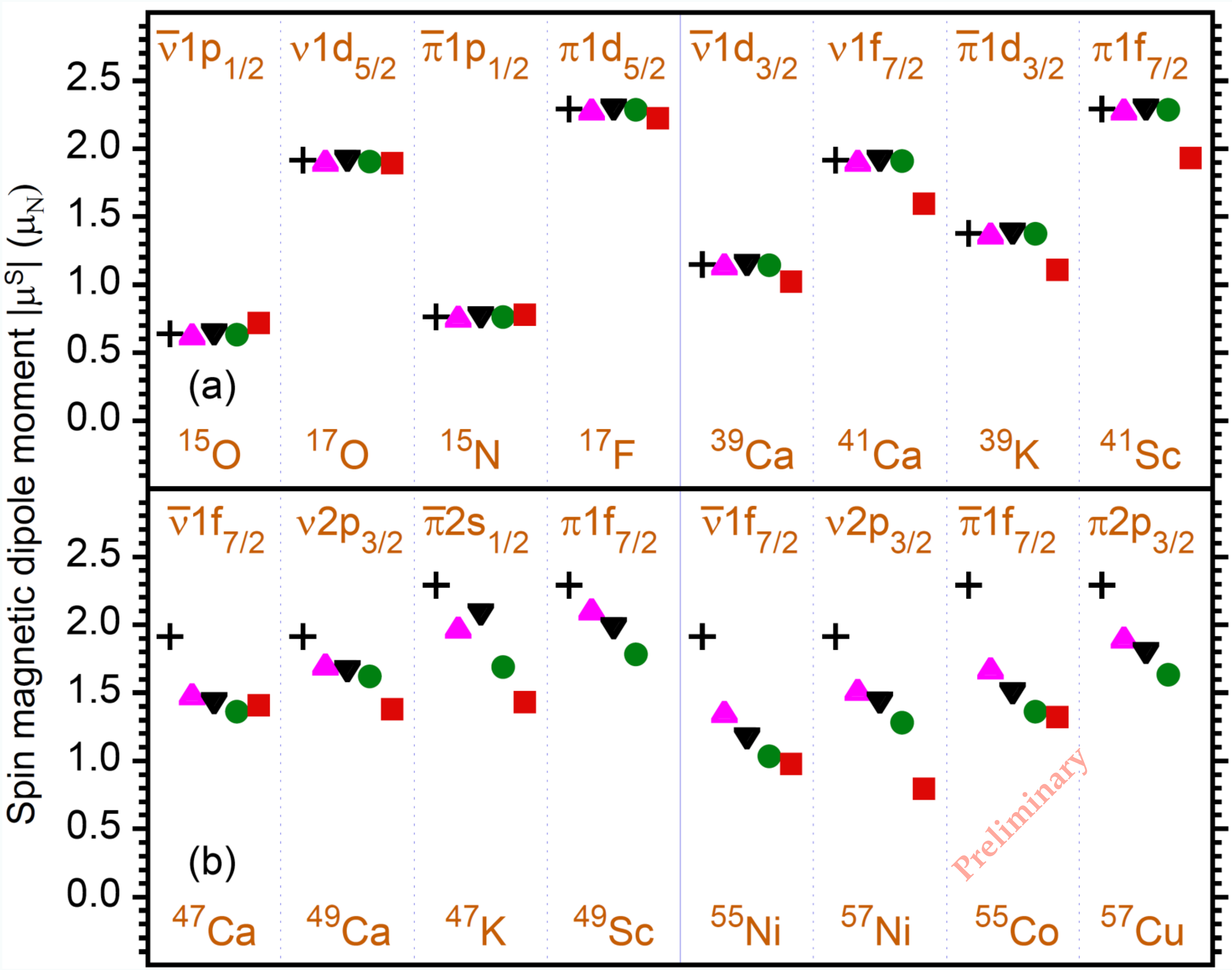
Magnetic dipole moments

P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published

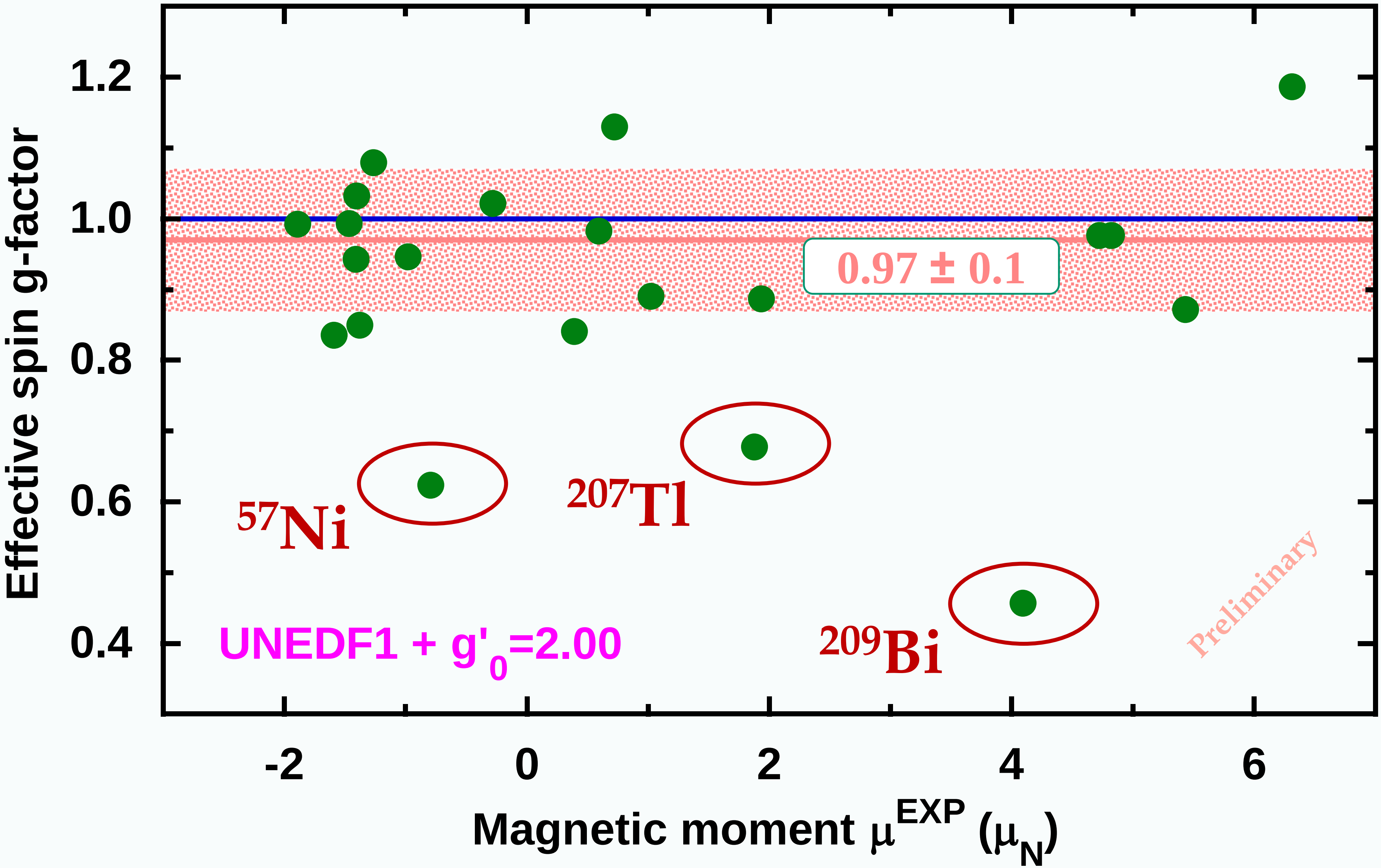


Magnetic dipole moments

P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published



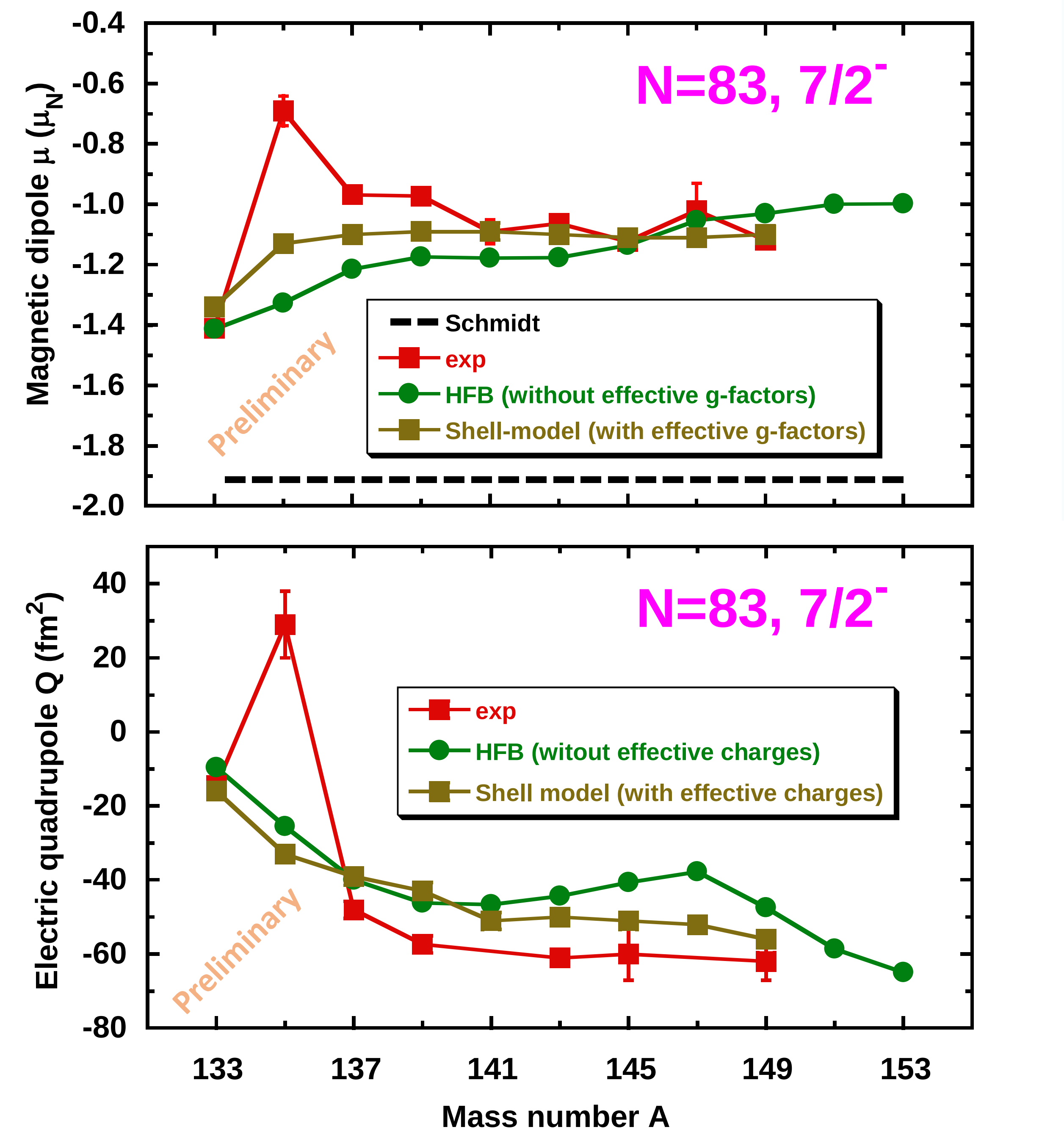
Effective spin g-factor?



P. Sassarini, J.D., J. Bonard, R.F. Garcia Ruiz, to be published

N=83 isotones

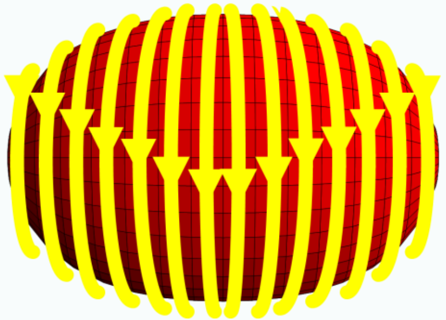
Experiment: & Shell model: L. V. Rodríguez et al. Phys. Rev. C 102, 051301(R) (2020)



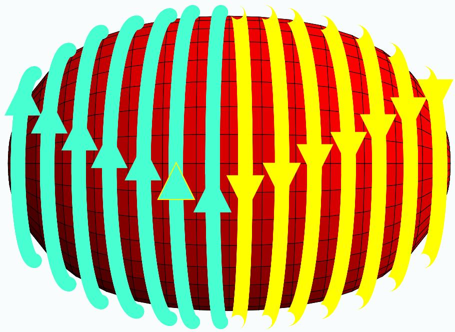
Magnetic octupole moment in ^{45}Sc

Visualisation of the magnetic multipole moments in axial symmetry

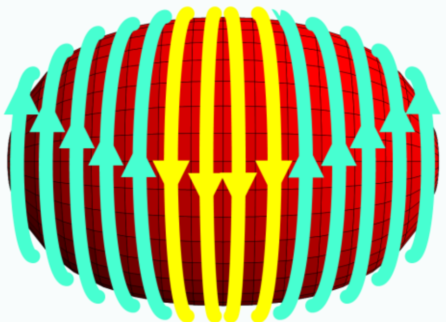
λ=1



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:

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

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

or

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

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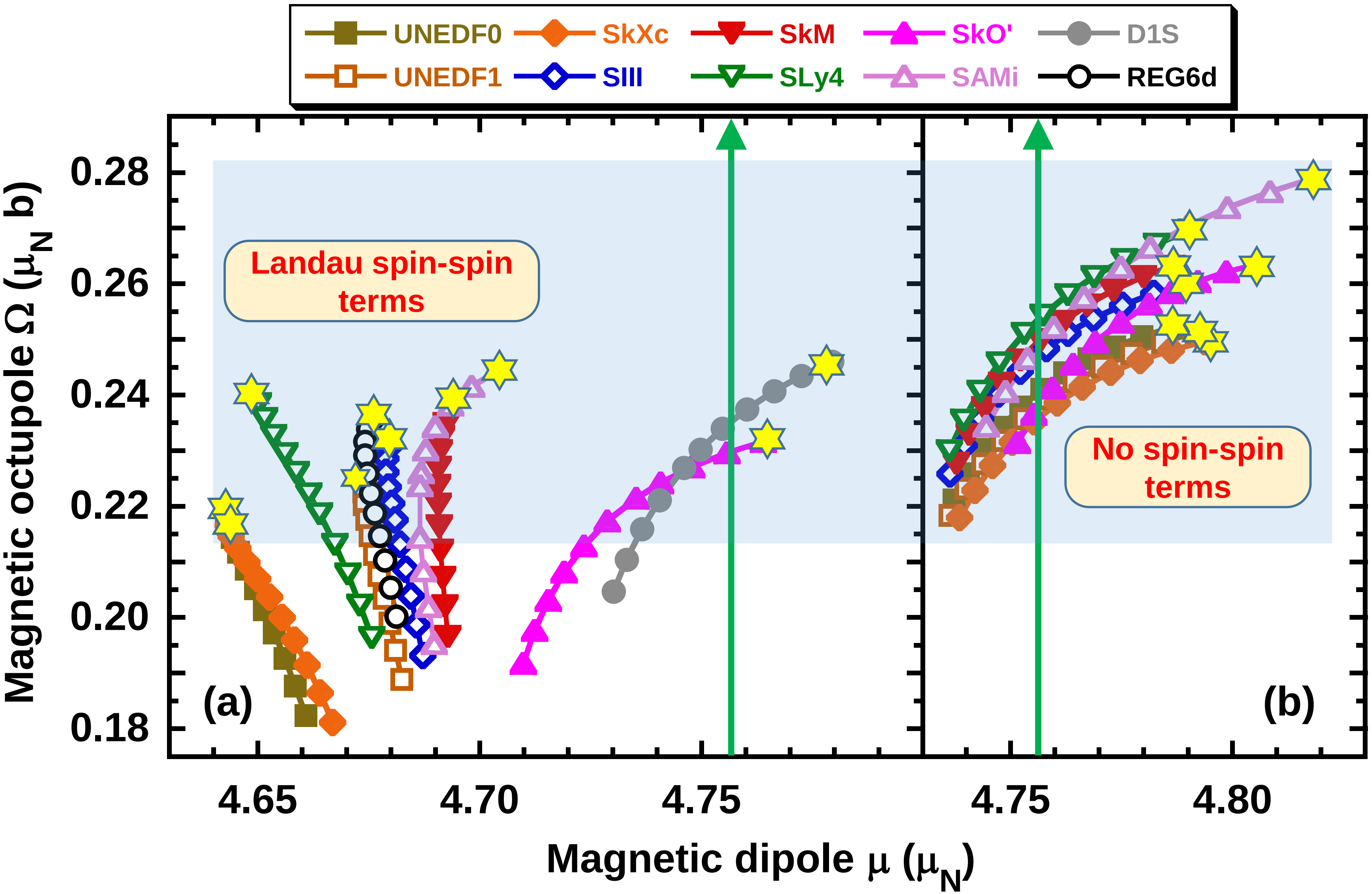
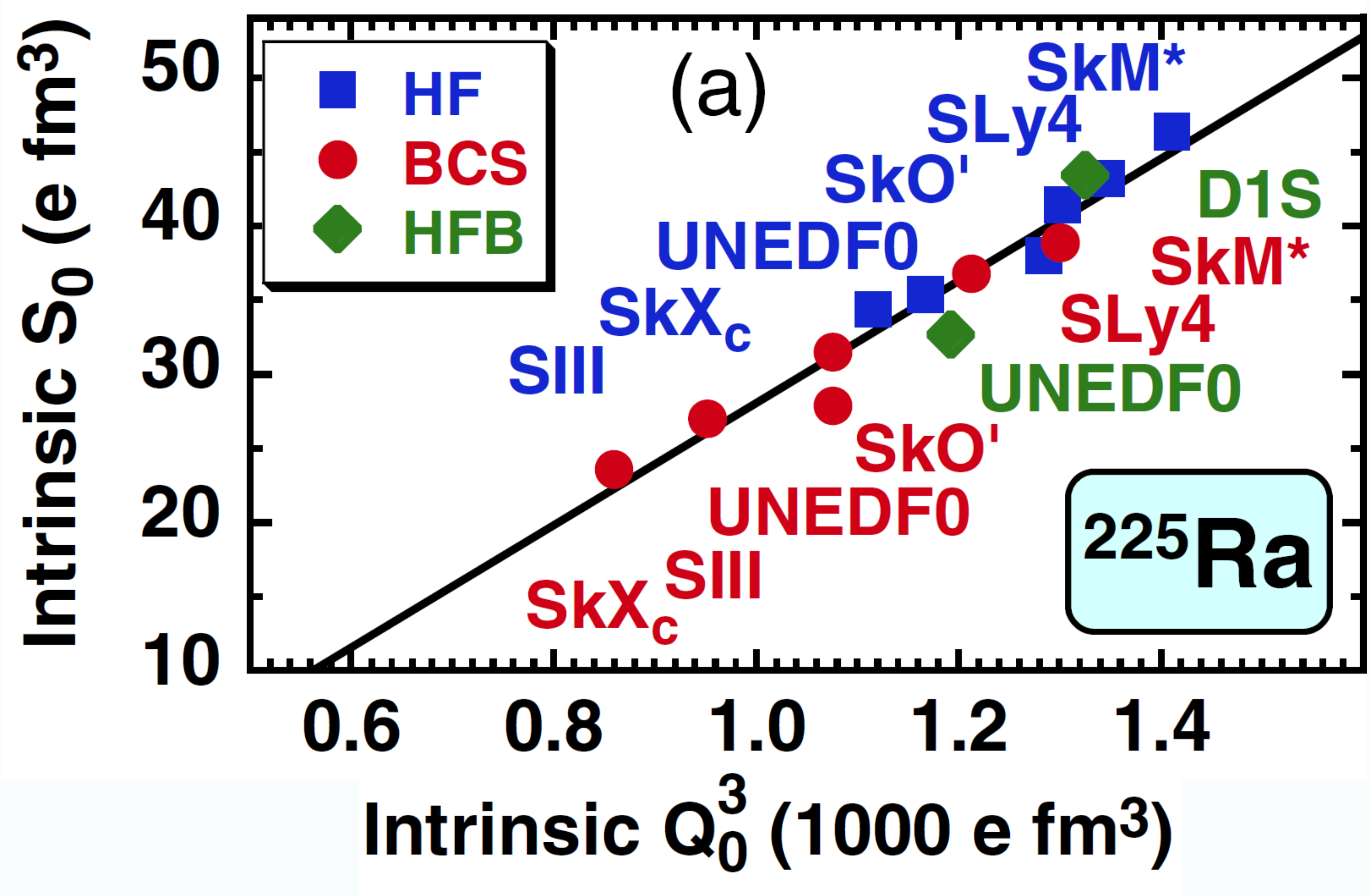
HF+AMP, magnetic moments in ^{45}Sc



R. P. de Groote *et al.*, arXiv:2005.00414

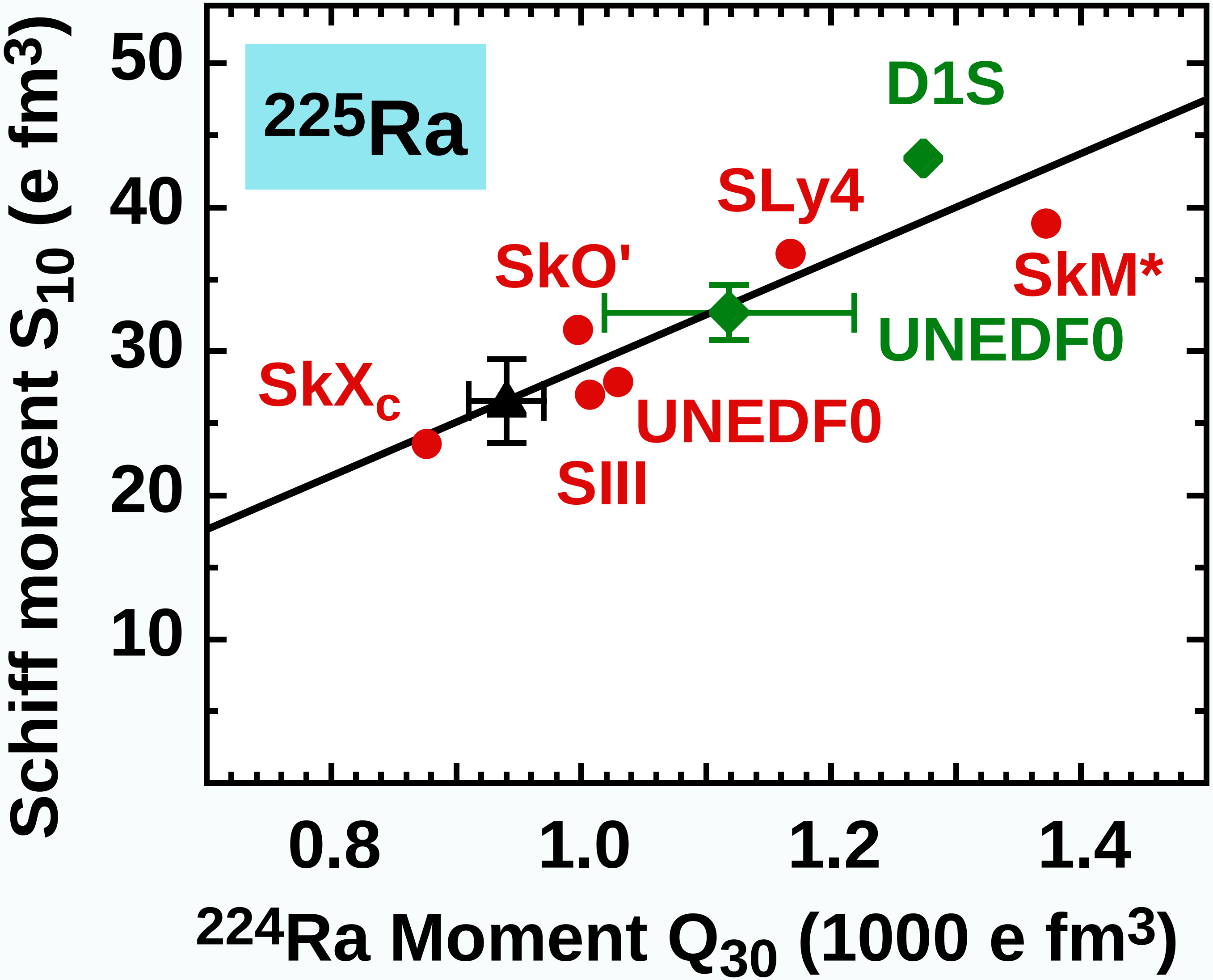
Schiff moment in ^{225}Ra

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



J.D., J. Engel, M. Kortelainen, P. Becker, Phys. Rev. Lett., 121, 232501 (2018)

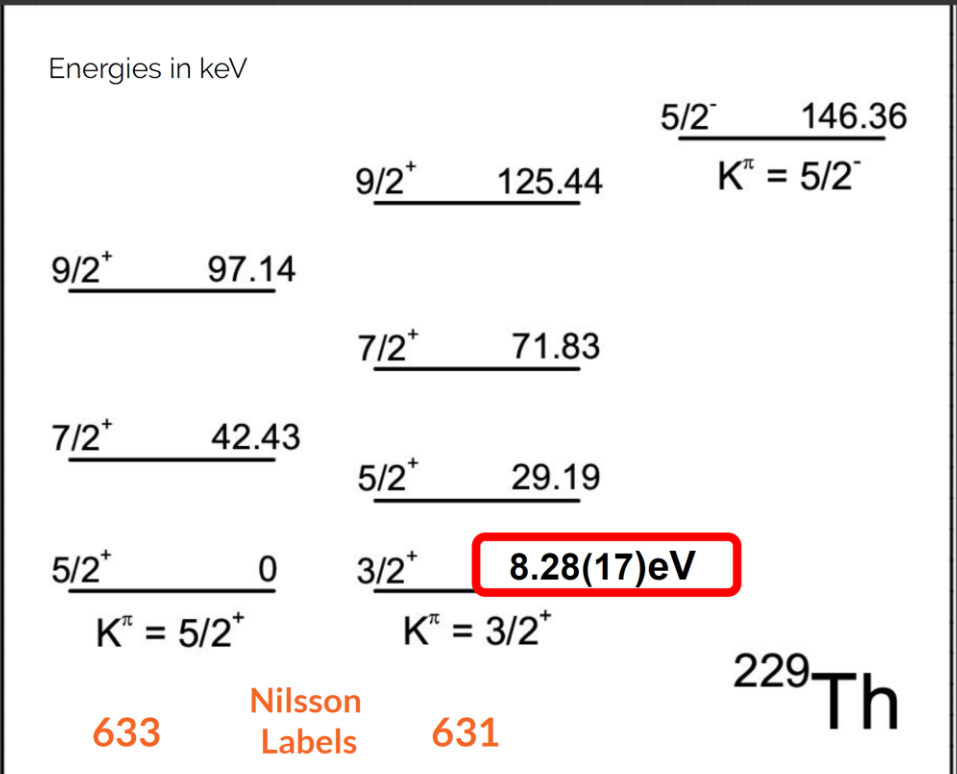
^{225}Ra Schiff moment vs. ^{224}Ra octupole moment



J.D., J. Engel, M. Kortelainen, P. Becker, Phys. Rev. Lett., 121, 232501 (2018)

^{229}Th

What is known about ^{229m}Th?



What we can aim for

1. Binding energies
2. **Odd-Even Mass Staggering**
3. **Axially and octupolly deformed**
4. Half-life
5. **Proton Quadrupole moments**
6. **Magnetic dipole moment**
7. Mean_square radii difference
8. **First few transition rates**

Δ_n = 0.77 MeV

Δ_p = 0.68MeV

Octupole: degree of freedom

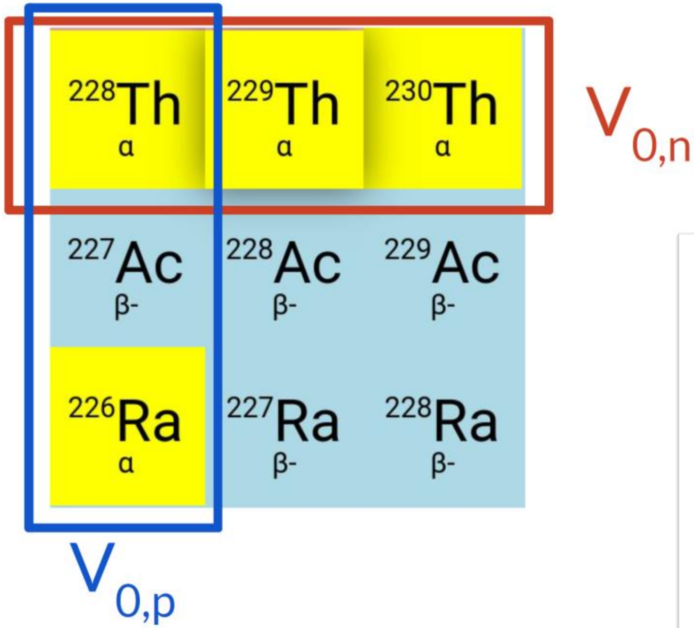
$Q_{5/2}$ = 8.8(1) eb

$Q_{3/2}$ = 8.7(3) eb

$\mu_{5/2}$ = 0.360(7) μ_N

$\mu_{3/2}$ = -0.37(6) μ_N

Reproduction of experimental odd-even mass staggering



Source: https://people.physics.anu.edu.au/~ecs103/chart/

Experimental values to reproduce:

Δ_n = **0.77 MeV**

Δ_p = **0.68MeV**

Adjusted pairing

Interaction	$V_{0,n}$	$V_{0,p}$
SIII	181.15	220.19
SKM*	181.46	216.25
SKO'	163.82	184.34
SKXc	139.02	173.63
SLY4	207.76	231.89
UDF0	130.70	156.45
UDF1	145.35	169.80

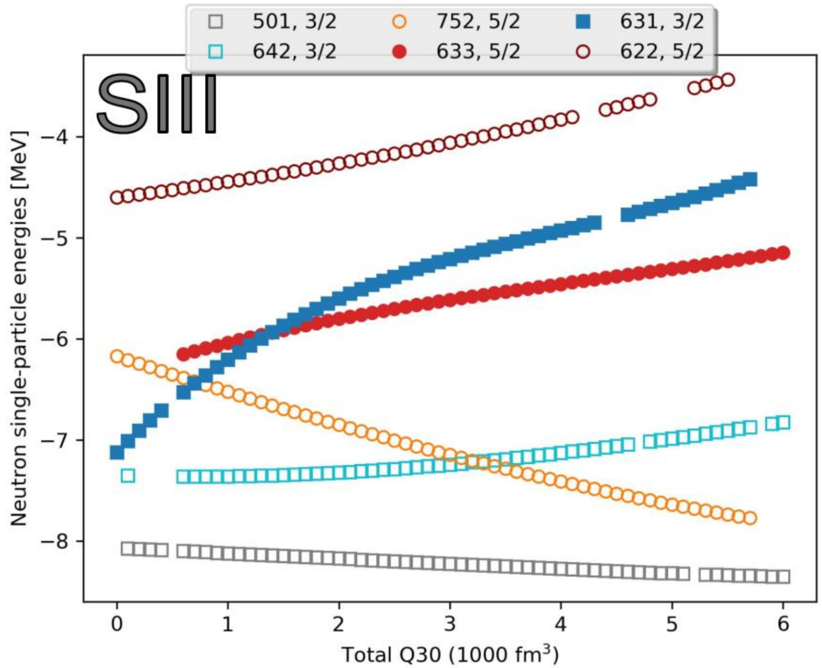
J.D., J. Bonnard, P. Becker, *et al.* to be published

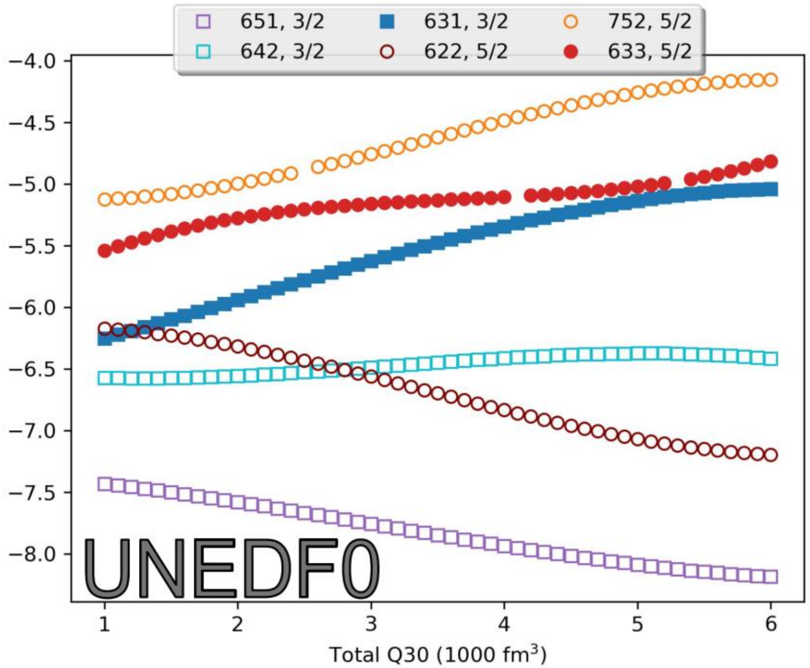
Nilsson levels in ^{229}Th vs. octupole deformation

Let's go crossing hunting

SIII used before for 229Th calculations:
E.Litvinova *et al.*,Phys. Rev.C, 79 064303 (2009)

Preliminary





Evolution of the energy of the blocked state with the octupole deformation in ^{229}Th

J.D., J. Bonnard, P. Becker, *et al.* to be published

Conclusions

1. Ground-state and isomeric electromagnetic moments are known in hundreds of odd and odd-odd nuclei, measured by atomic spectroscopic methods up to a **very high precision**.
2. In the standard shell-model calculations, agreement with data is achieved by using the concept of **effective charges and g-factors**.
3. In the nuclear DFT calculations, magnetic moments have been **rarely considered** so far.
4. Poorly known **time-odd sector** of the nuclear DFT crucially influences the magnetic moments.
5. **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

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

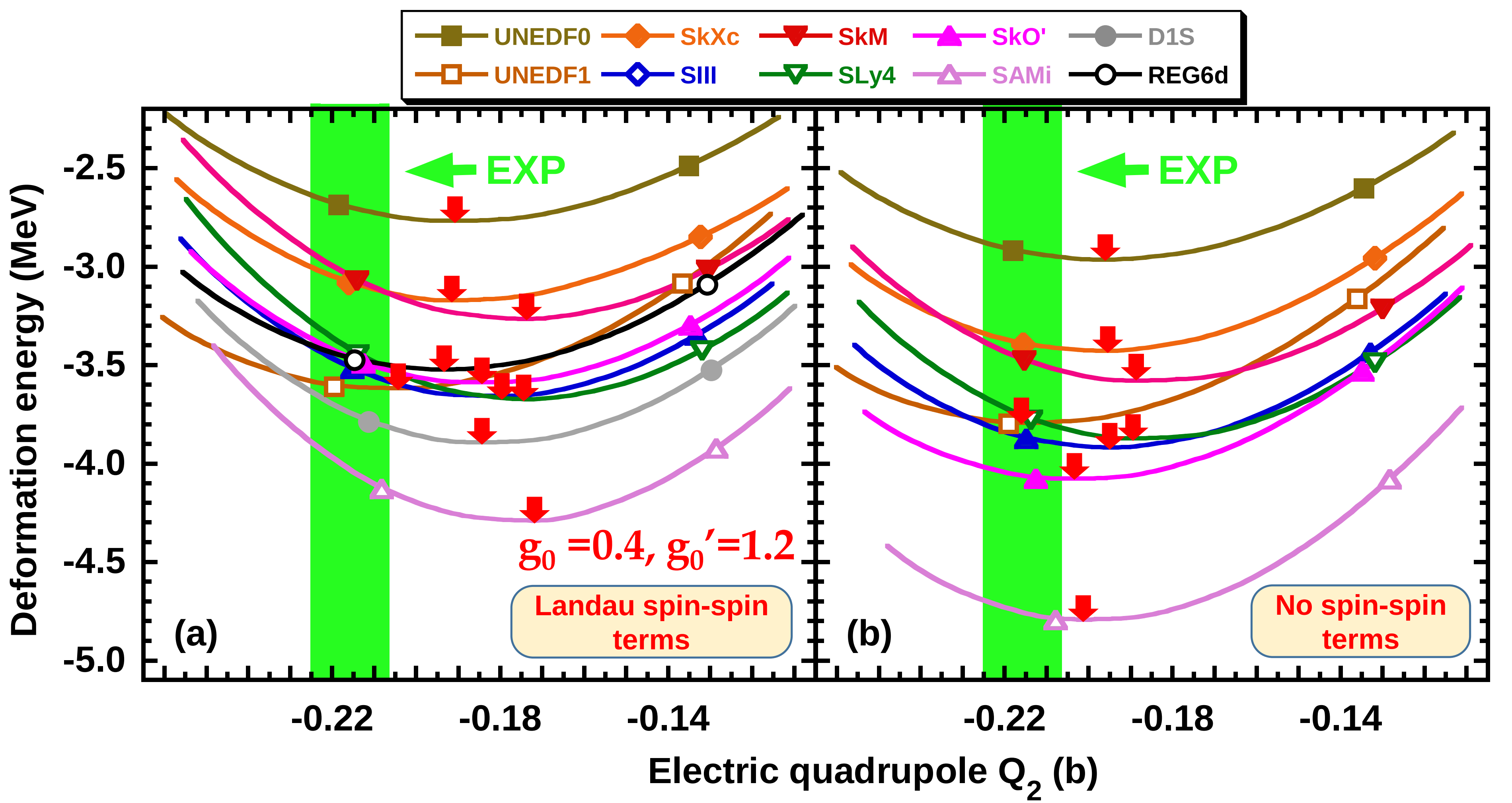
where $\hat{L}_\nu$ and $\hat{S}_\nu$ for $\nu = n,p$ are the operators of orbital and spin angular momenta, respectively. Since the total angular momentum $\hat{J} = \sum_{\nu=n,p}(\hat{L}_\nu + \hat{S}_\nu)$ is conserved, it is convenient to subtract its eigenvalue from the spectroscopic magnetic moments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

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

with

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

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



R. P. de Groote *et al.*, arXiv:2005.00414

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

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

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:

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

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.

Who?

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Gerda Neyens, KU Leuven and CERN, B and CH
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What?

We propose supporting European facilities involved in precision measurements of nuclear moments with novel advanced modelling of these observables within nuclear density-functional-theory (DFT) approaches.

ADVANCING FRONTIER KNOWLEDGE