

Lattice Calculation of Nuclear Magnetic Dipole Moment

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Collaborating with Bing-Nan Lu, Dean Lee, Shuang Zhang and Yuan-Zhuo Ma

Why Study Magnetic Dipole Moment

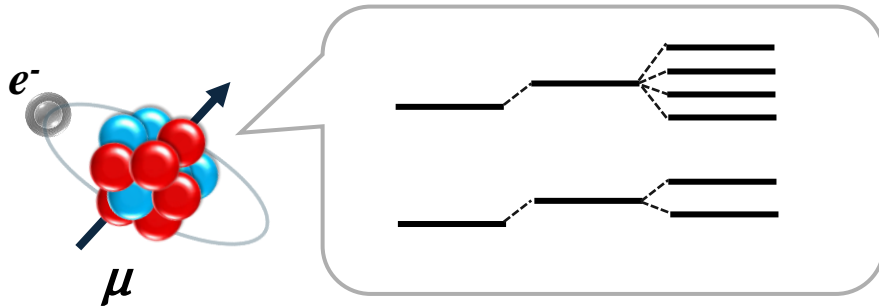
- The calculation of nuclear magnetic dipole moment is important.

➔ From the theoretical side

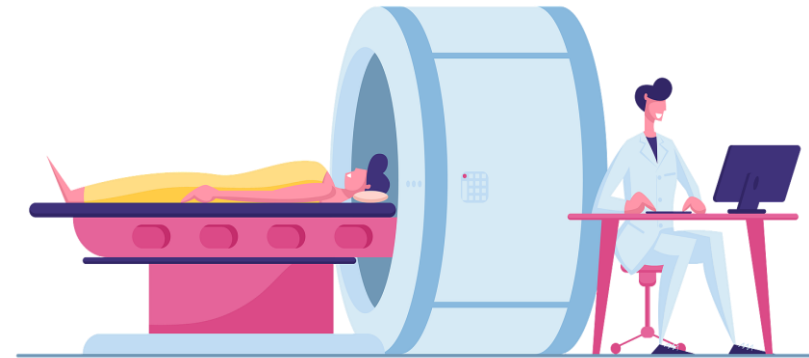
- A key probe to nuclear structures

- A critical test of nuclear models

➔ From the perspective of applications



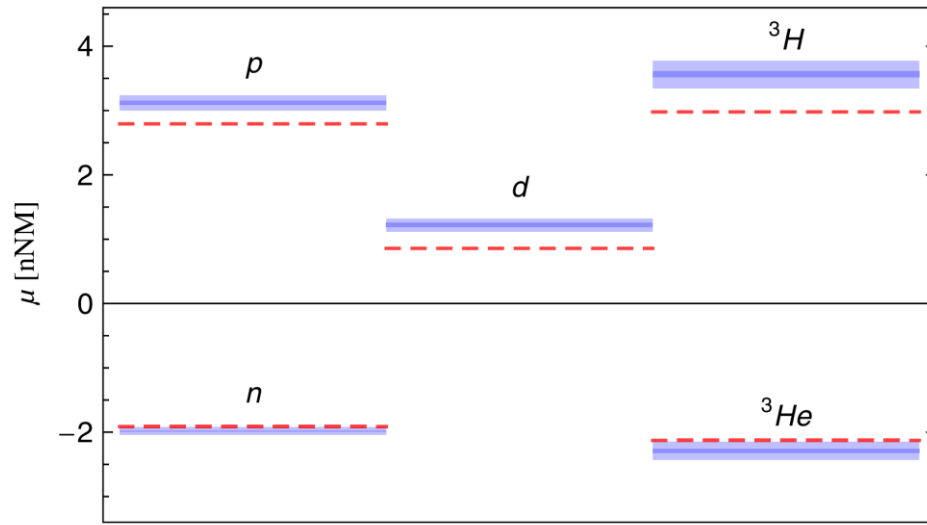
- Hyperfine Splitting



- Magnetic nuclear resonance

Lattice QCD Calculation

- First-principles calculations from Lattice QCD is available at unphysical pion mass. $m_\pi \sim 806 \text{ MeV}$



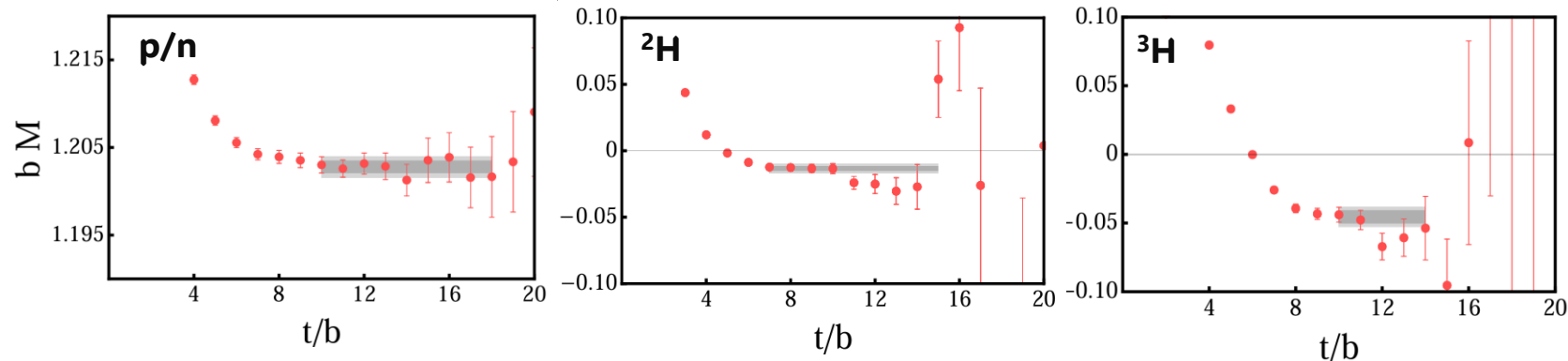
NPLQCD Collaboration, PRL 113, 252001 (2014)

With the growing capability to perform precise LQCD calculations of many quantities of crucial importance to the mission of nuclear physics, including the properties and structure of hadrons and light nuclei and the forces between them, we are truly entering a golden era.



The 2015
LONG RANGE PLAN
for NUCLEAR SCIENCE

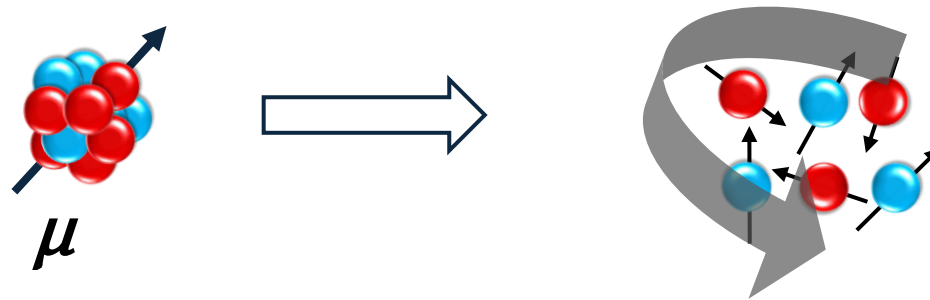
- The application to heavier nuclei is hard due to the exponentially growing computational cost.



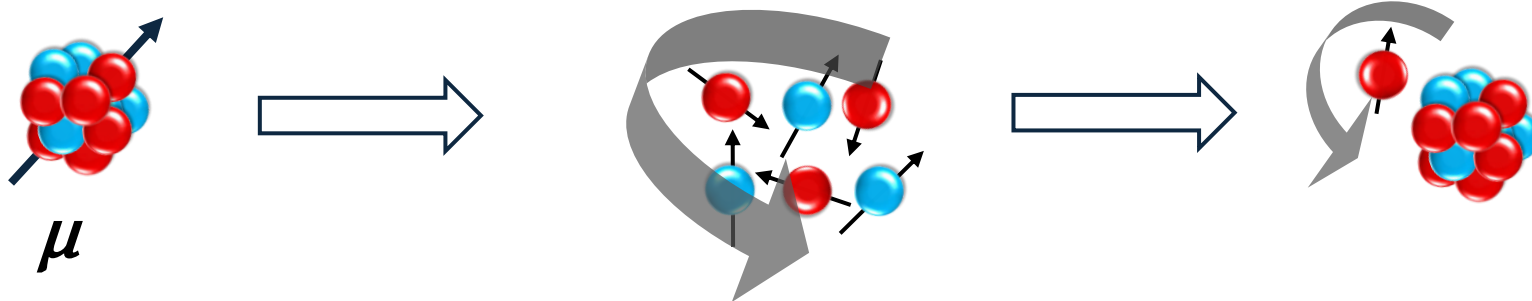
NPLQCD Collaboration,
PRD 87, 034506 (2013)

Interpretation from the Nuclear Shell Model

- In nuclear physics, the dipole moment originates from the orbital motion and intrinsic spin of nucleons.



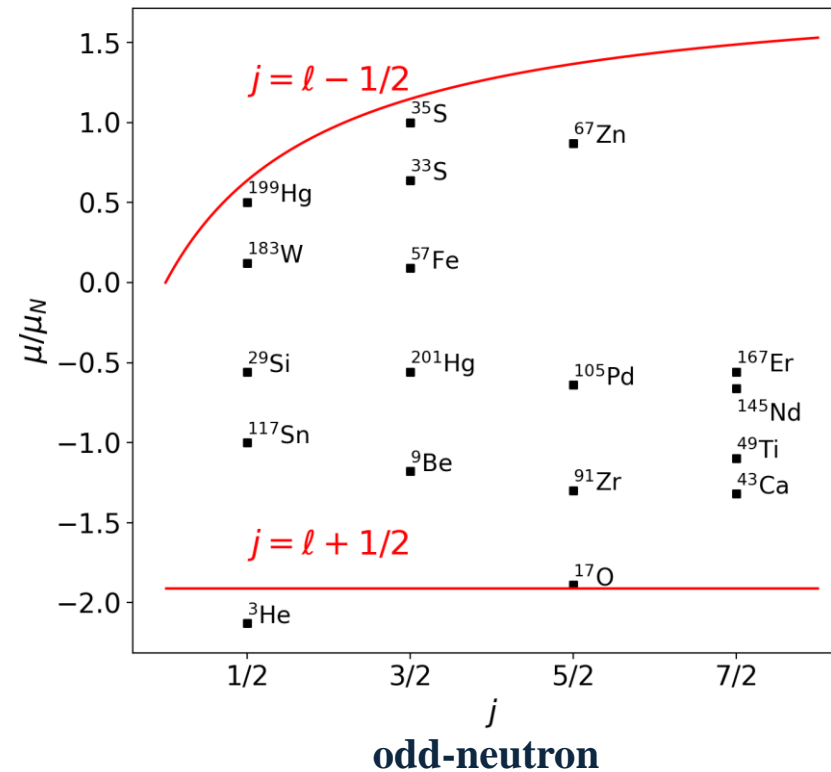
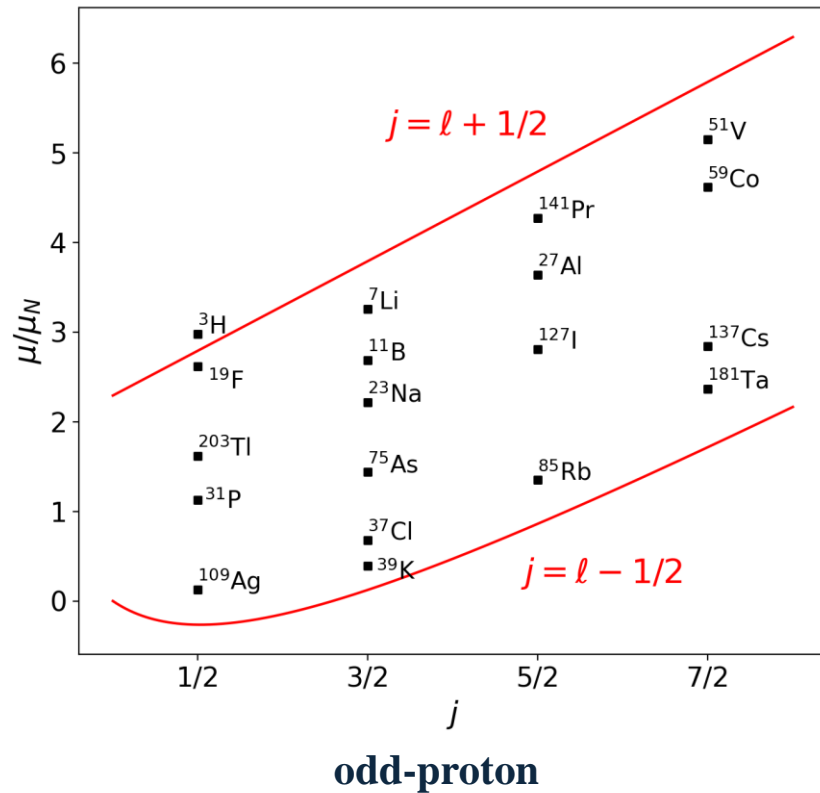
- The nuclear shell model simplifies the dipole moment as the contribution from valence nucleons.



Predictions of the Nuclear Shell Model

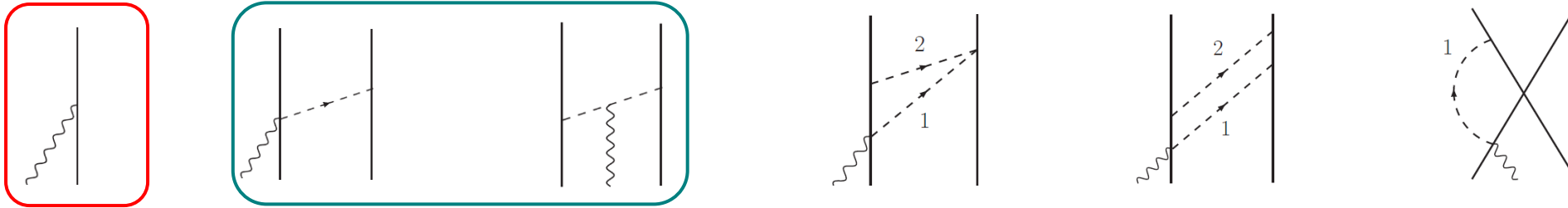
- Almost all experiment values are sandwiched between the two Schmidt lines.

$$\mu = \begin{cases} g_l^{\pi/\nu} l + \frac{1}{2} g_s^{\pi/\nu}, & j = l + \frac{1}{2} \\ \frac{j}{j+1} [g_l^{\pi/\nu} (l+1) - \frac{1}{2} g_s^{\pi/\nu}], & j = l - \frac{1}{2} \end{cases}$$



Interpretation from Chiral EFT

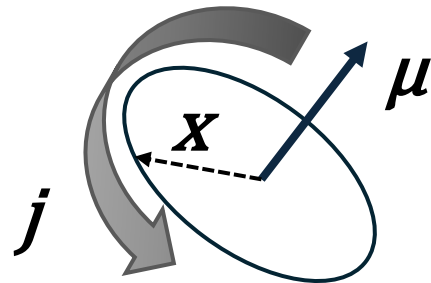
- The nuclear electromagnetic current has been derived up to N³LO in chiral EFT



H. Krebs, E. Epelbaum and U. G. Meißner, *Few-body Syst.* 60, 31(2019)

S. Pastore et al, *PRC* 80, 034004 (2009)

- The dipole moment operator can be constructed from the EM current.



$$\boldsymbol{\mu} = \frac{1}{2} \int d^3\boldsymbol{x} \boldsymbol{x} \times \boldsymbol{j}_{\text{EM}}(\boldsymbol{x})$$

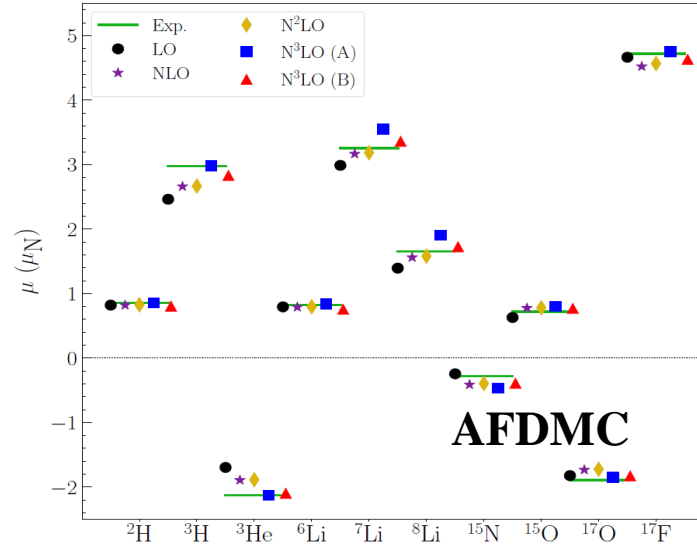
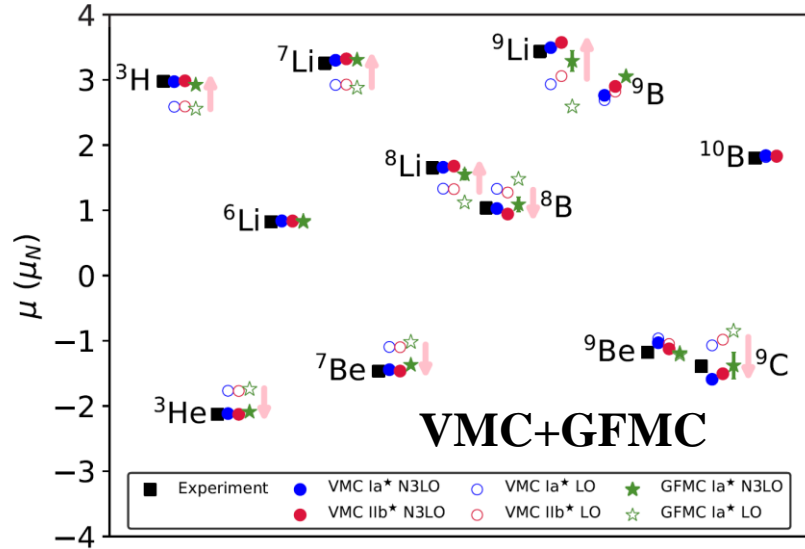
$$\boldsymbol{\mu}_{\text{NLO}}^{1\text{N}} = \mu_N \sum_n \left(\frac{g_S + g_V \tau_n^3}{2} \boldsymbol{\sigma}_n + \frac{1 + \tau_n^3}{2} \boldsymbol{l}_n \right)$$

$$\boldsymbol{\mu}_{\text{NLO}}^{2\text{N}} = \boldsymbol{\mu}_{\text{NLO,cm-dep}}^{2\text{N}} + \boldsymbol{\mu}_{\text{NLO,cm-indep}}^{2\text{N}}$$

S. Pal et al, *PRC* 108, 024001 (2023)

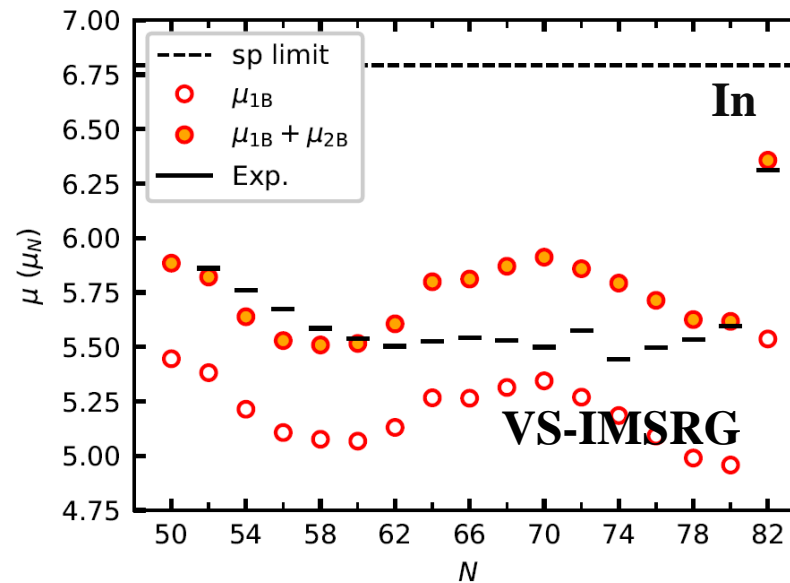
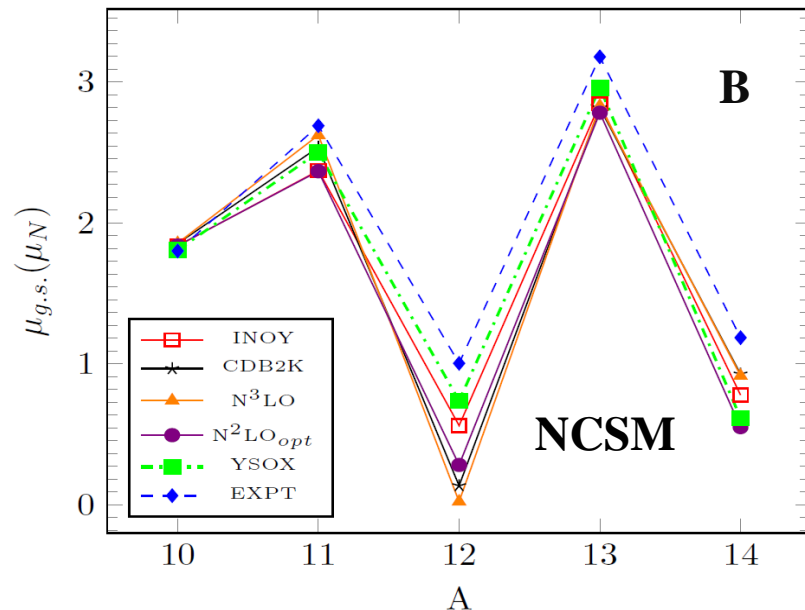
Microscopic Calculations of Chiral Interactions

- Recently, microscopic calculations of magnetic moments based on chiral EFT are emerging.



VMC+GFMC: J. D. Martin et al,
PRC 108, L031304 (2023)

AFDMC: G. Chambers-Wall et al,
PRL 133, 212501 (2024)

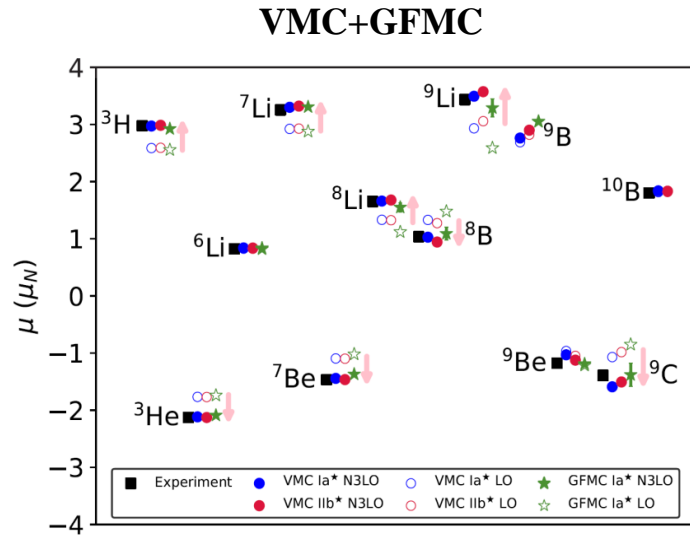


NCSM: P. Choudhary et al,
PRC 102, 044309 (2020)

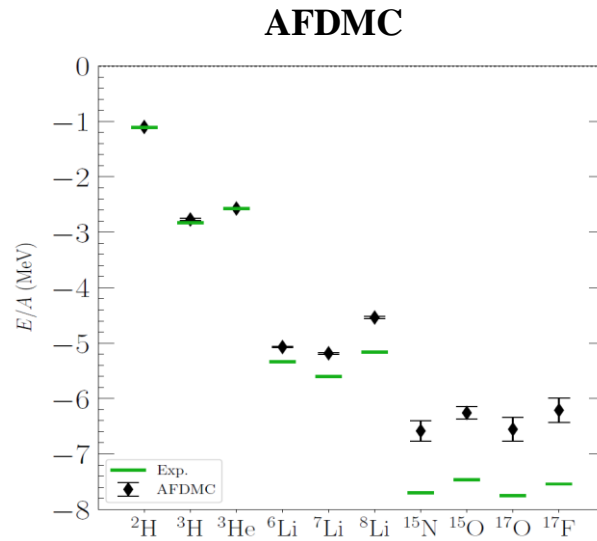
VS-ISMGR: T. Miyagi et al,
PRL 132, 232503 (2024)

Difficulties of Current Methods

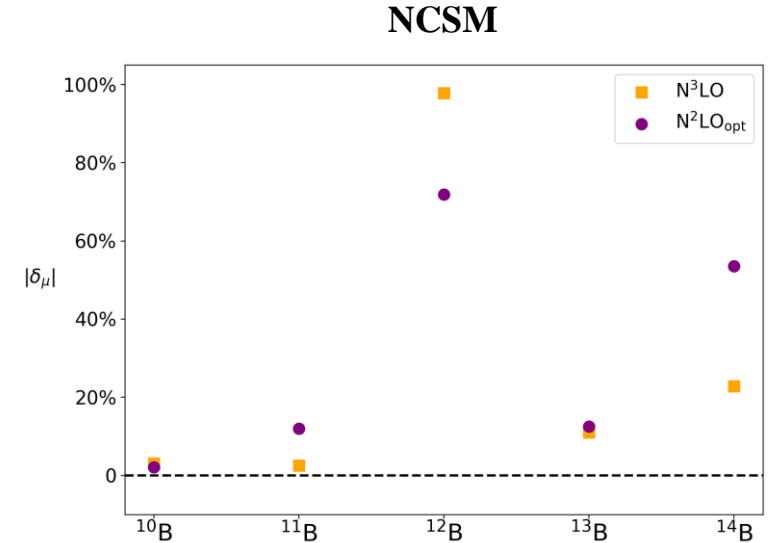
- However, the microscopic approaches above have their own limitations.



limited to nuclei of $A \leq 12$



significant underbinding



large deviations from experiment

- Is there any method which fulfills the following?

- ➔ Can simulate s -, p -shell and even heavier nuclei.
- ➔ Can describe both binding energies and dipole moments.
- ➔ Can provide a reasonable estimation of uncertainties.

Why not try NLEFT?

NLEFT as a Competitive Candidate

- NLEFT is a hopeful candidate to calculating nuclear magnetic moments.

➤ Mild scaling of computational costs as a function of the mass number ($\sim A^2$)

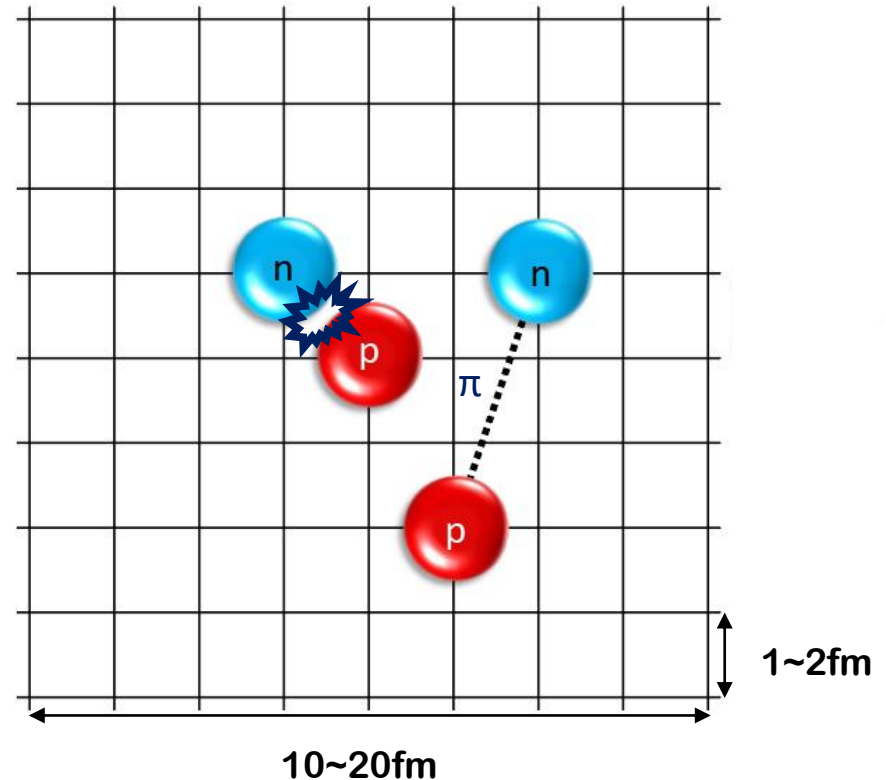
➤ Good predictions on energies, charge radii and properties of nuclear matter.

See Serdar's talk

➤ Statistical errors: SU4 symmetry + perturbation theory.

See Bing-Nan's talk

➤ Systematic errors: full-space calculation + wavefunction matching method.



An Outline

- Master formula

$$\mu = \lim_{L_t \rightarrow \infty} \frac{\langle \Psi_{J,M=J} | \mathcal{M}^{L_t/2} \mu_z \mathcal{M}^{L_t/2} | \Psi_{J,M=J} \rangle}{\langle \Psi_{J,M=J} | \mathcal{M}^{L_t} | \Psi_{J,M=J} \rangle}$$

(J, M) Spin and magnetic quantum numbers

$\mathcal{M} =: e^{-H a_t}$: Transfer matrix

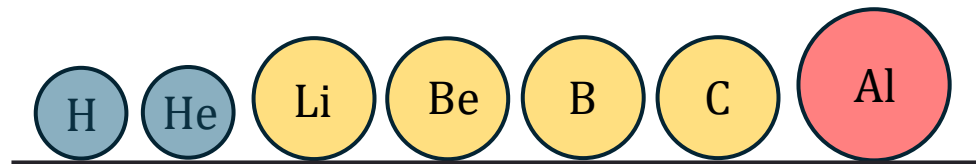
- Key ingredients

- An accurate Hamiltonian H
- A lattice realization of the operator μ_z .
- A trial state Ψ with correct quantum numbers.

- Relevant techniques

- Reduction of lattice artifact
- Perturbation theory
- Wavefunction matching

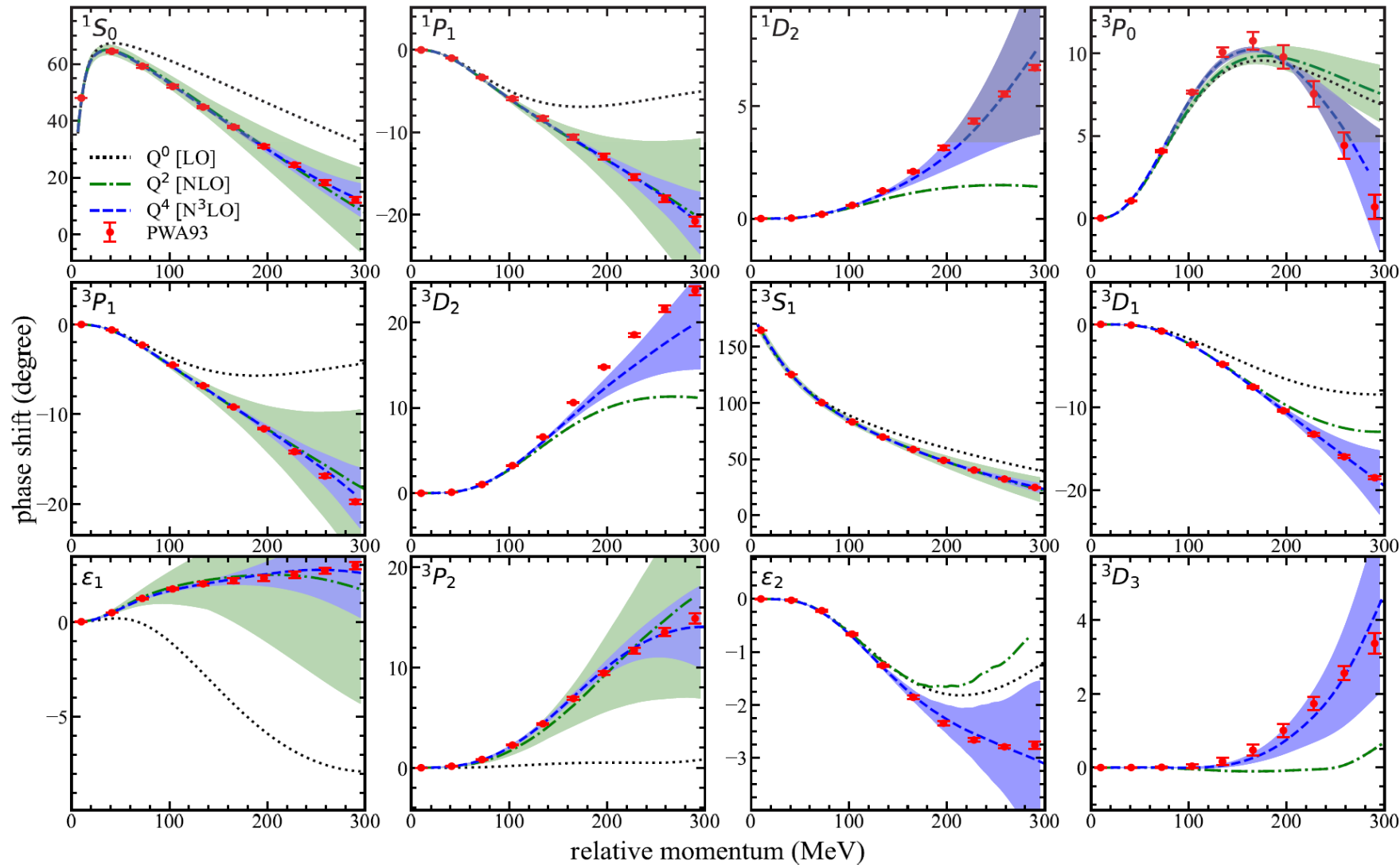
- Target nuclei



Interaction

S. Elhatisa et al, Nature 630(2024)

- We use the high-fidelity $N^3\text{LO}$ lattice chiral interaction at lattice spacing $a=1.32\text{fm}$



Lattice Dipole Moment Operator

- The dipole moment operator μ_z is discretized on the lattice.

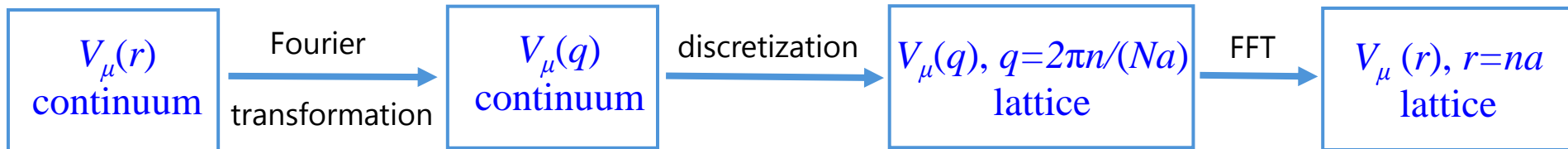
➤ For the 1N term, the orbital part is realized through the lattice derivative operator

$$\mu_{\text{NLO}}^{1\text{N}} = \mu_N \sum_n \left(\frac{g_S + g_V \tau_n^3}{2} \sigma_n + \frac{1 + \tau_n^3}{2} l_n \right)$$

$$\sum_n l_n \Rightarrow \sum_{\mathbf{x}} \mathbf{x} \times \boldsymbol{\theta}(\mathbf{x}) \quad \boldsymbol{\theta}(\mathbf{x}) = -\frac{i}{2} [a^\dagger(\mathbf{x}) \nabla a(\mathbf{x}) - \nabla a^\dagger(\mathbf{x}) a(\mathbf{x})]$$

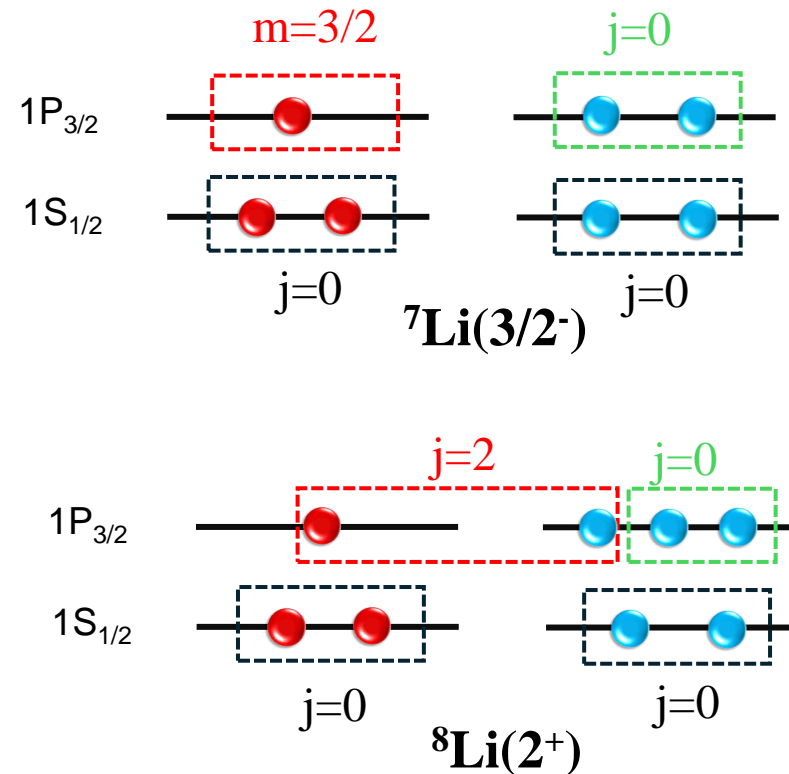
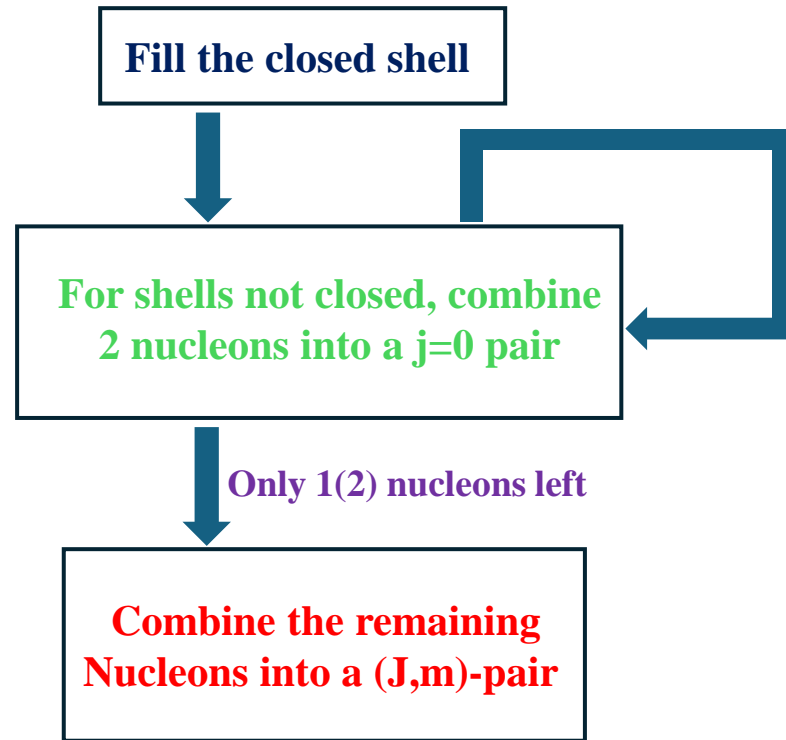
➤ For the 2N term, the singularity of OPE is regularized by the finite lattice spacing.

$$\mu_{\text{NLO}}^{2\text{N}} = \mu_{\text{NLO,cm-dep}}^{2\text{N}} + \mu_{\text{NLO,cm-indep}}^{2\text{N}}$$



Trial State Preparation

- The shell model provides a framework to construct trial states with desired spins.



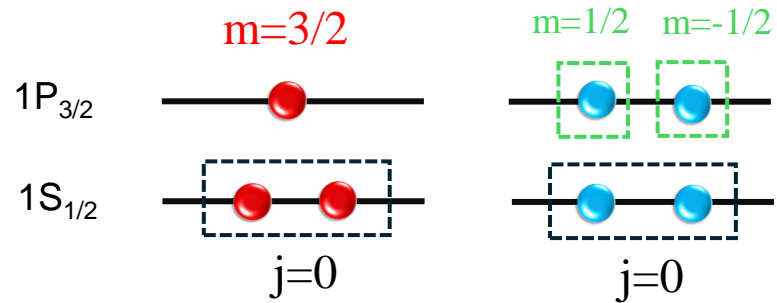
- The resulting trial state is a combination of several Slater determinants, which are sampled through Metropolis Algorithm.

Comparison with Other Works

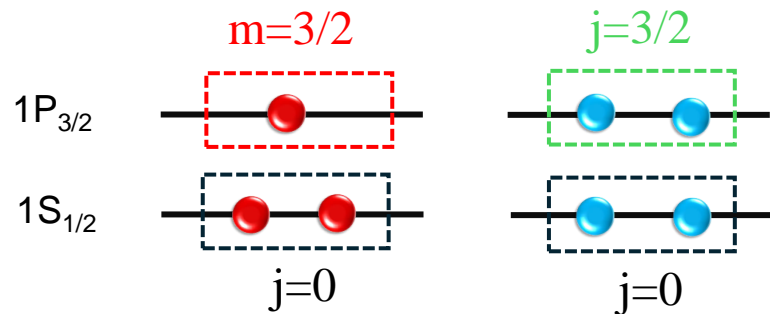
- Our construction of trial state is inspired by previous literature.

➤ M -state: trial state of previous works

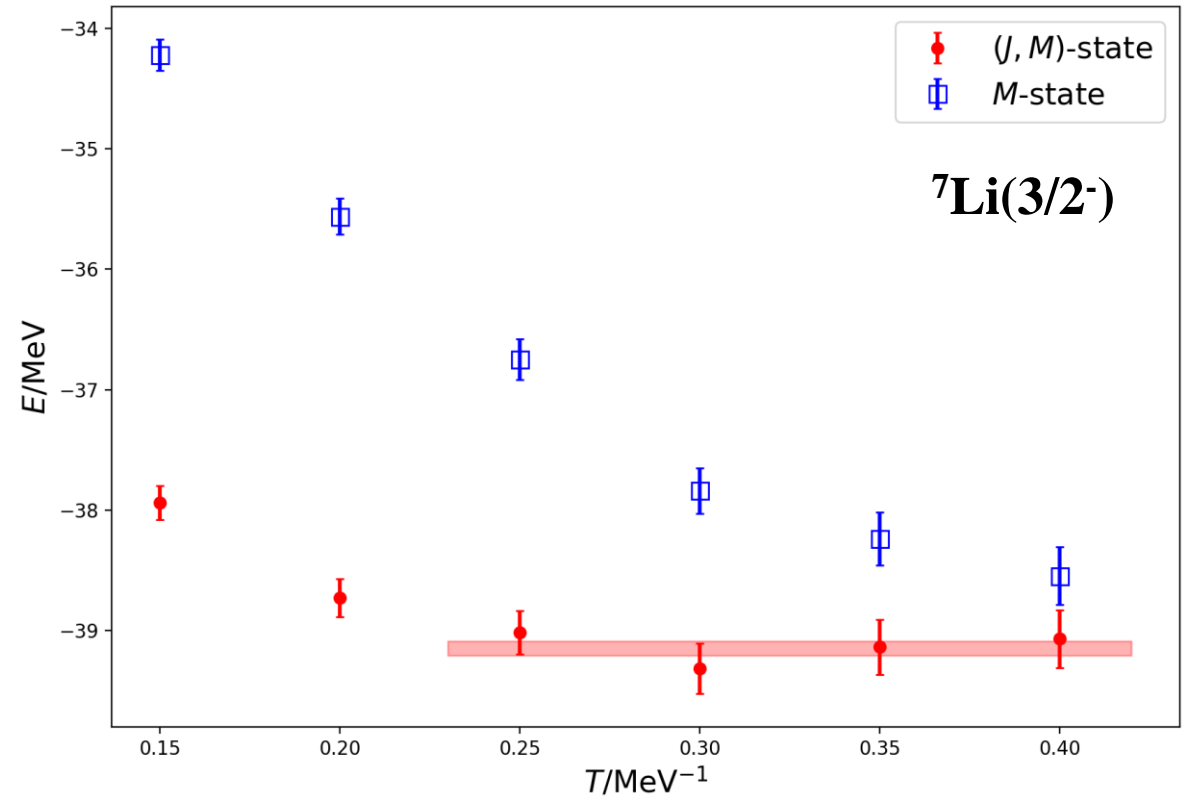
Following S. Shen et al, arXiv:2411.14935



➤ (J,M) -state: trial state of this work



- Our trial state has a larger overlap with the ground state.



Checks on Lattice Spacing Artifact

- The lattice spacing artifact of the dipole moment deserves a check.

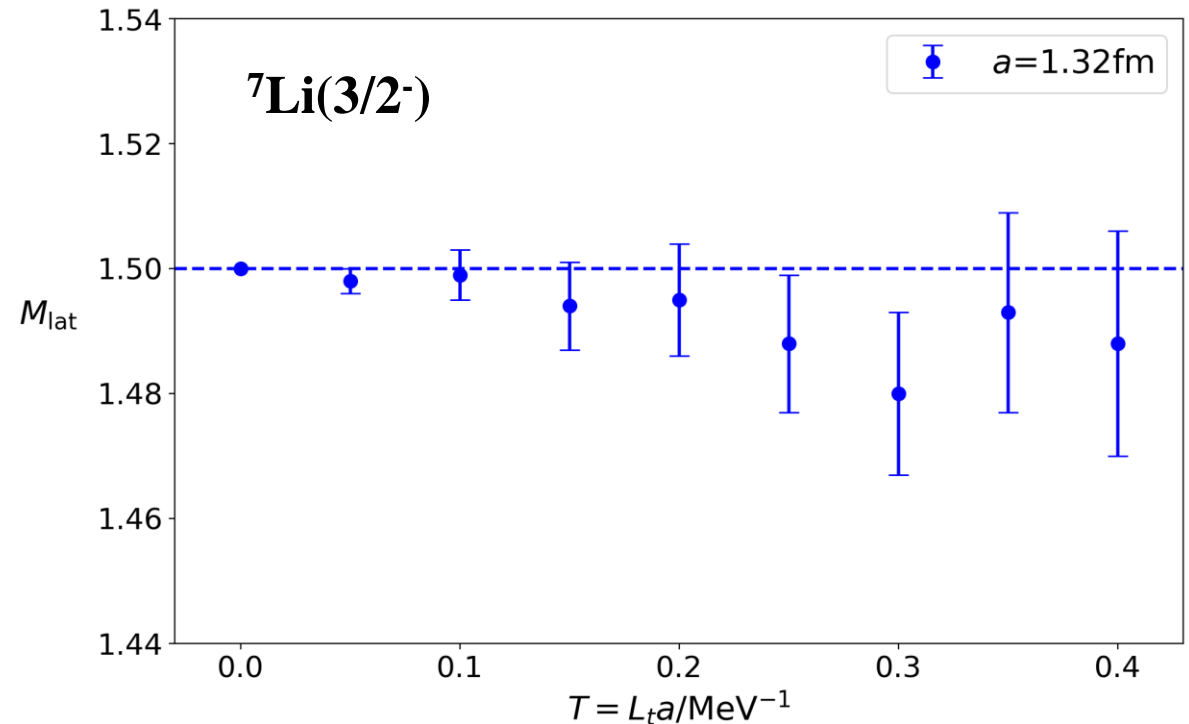
$$\mu_{\text{NLO}}^{1\text{N}} = \mu_N \sum_n \left(\frac{g_S + g_V \tau_n^3}{2} \sigma_n + \frac{1 + \tau_n^3}{2} l_n \right)$$

- Since the lattice spacing is fixed in our interaction ($a=1.32\text{fm}$), check the impact of lattice artifacts on the nucleus spin instead.

$$M_{\text{lat}}(L_t) = \frac{\langle \Psi_{J,M=J} | \mathcal{M}^{L_t/2} J_z \mathcal{M}^{L_t/2} | \Psi_{J,M=J} \rangle}{\langle \Psi_{J,M=J} | \mathcal{M}^{L_t} | \Psi_{J,M=J} \rangle}$$

$$J_z = \sum_n (l_{z,n} + \sigma_{z,n}/2)$$

- A good control of lattice artifact is achieved by using the shell-model trial state at $a=1.32\text{fm}$.



Perturbative Method

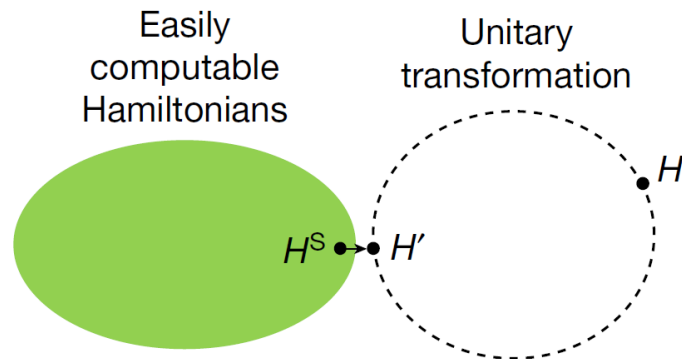
- We mitigate sign problems through perturbation theory.

$$H = H^S + \Delta H$$

➔ H^S : highly SU4 symmetric, locally and non-locally smeared

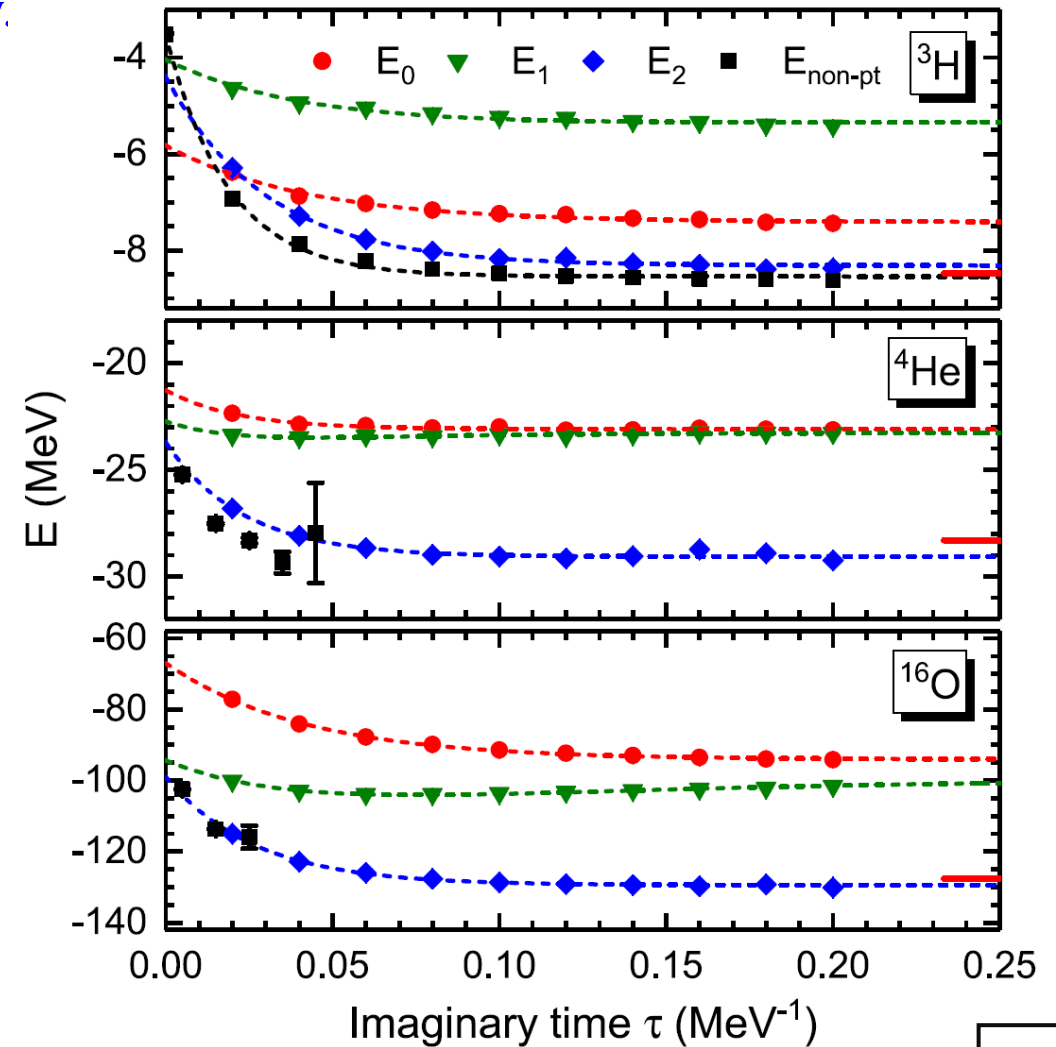
➔ ΔH : treated as a perturbation

- The method of wavefunction matching is used to accelerate the perturbative convergence.



S. Elhatisa et al, Nature 630(2024)

B. N. Lu et al, PRL 128, 242501(2022)

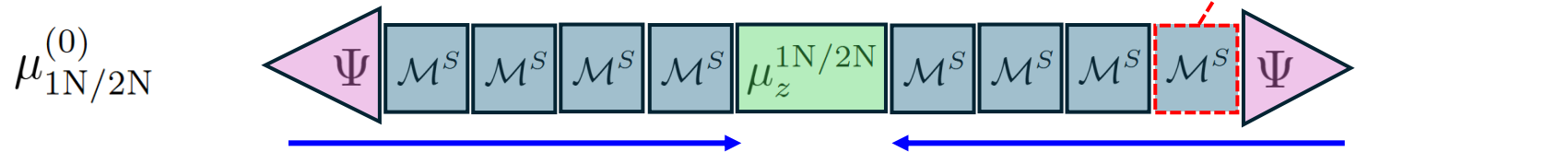


Perturbative Calculation of Dipole Moments

- For the dipole moment, we calculate the 1N and 2N term up to the 1st and 0th order, respectively.
- How to calculate perturbative terms at different orders.

$$\mu \approx \mu_{1N}^{(0)} + \mu_{1N}^{(1)} + \mu_{2N}^{(0)}$$

↪ Numerical realization of the **leading order** perturbative term



auxiliary field transformation

Jacobi formula

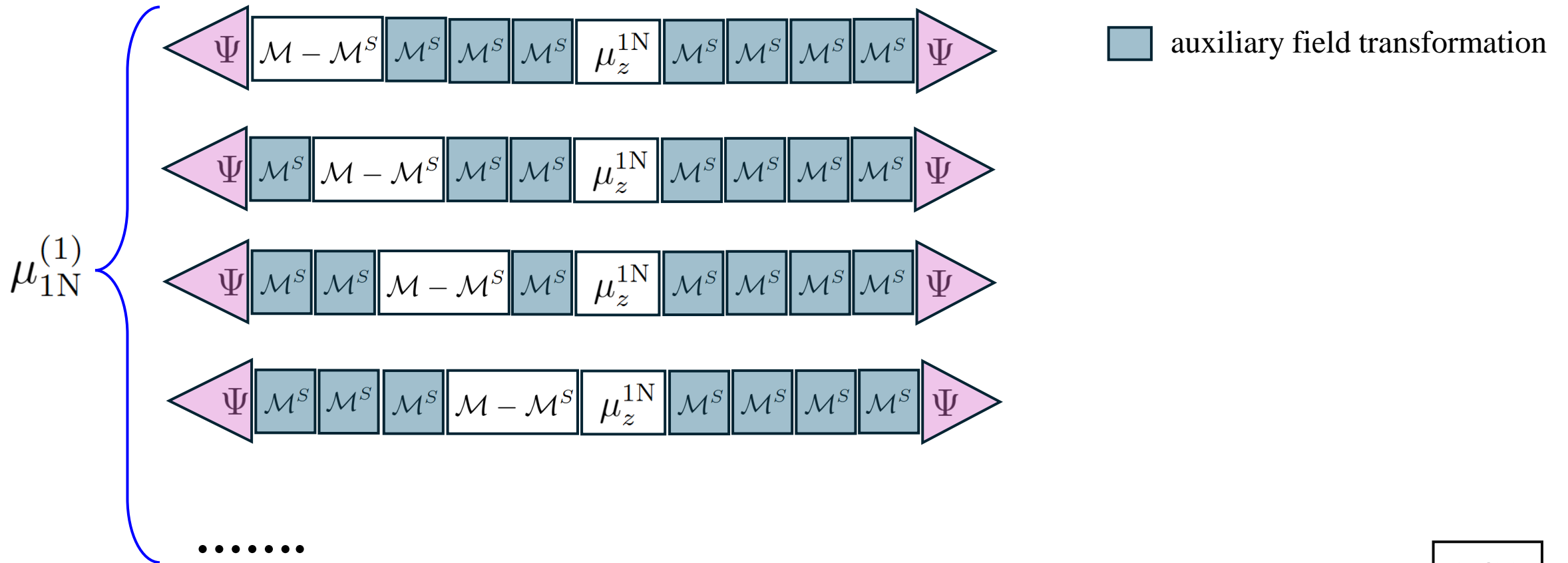
$$e^{-O^2/2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-x^2/2} e^{xO}$$

$$\frac{d}{dt} [\det A(t)] = \det A(t) \cdot \text{tr} [A^{-1}(t) \cdot \frac{d}{dt} A(t)]$$

Perturbative Calculation of Dipole Moments

- How to calculate perturbative terms at different orders.

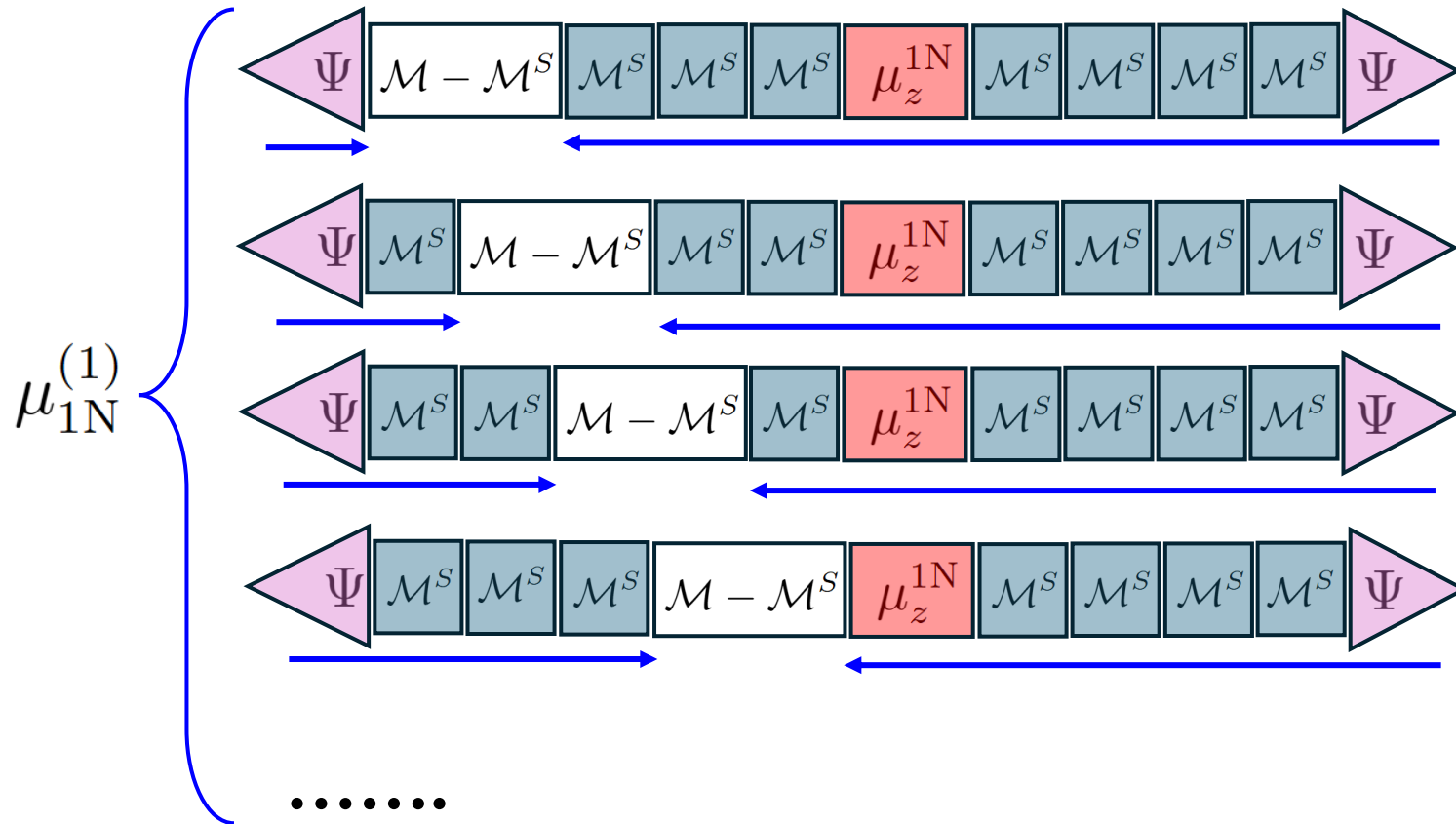
↪ Numerical realization of the **first order** perturbative term



Perturbative Calculation of Dipole Moments

- How to calculate perturbative terms at different orders.

↪ Numerical realization of the **first order** perturbative term



■ auxiliary field transformation

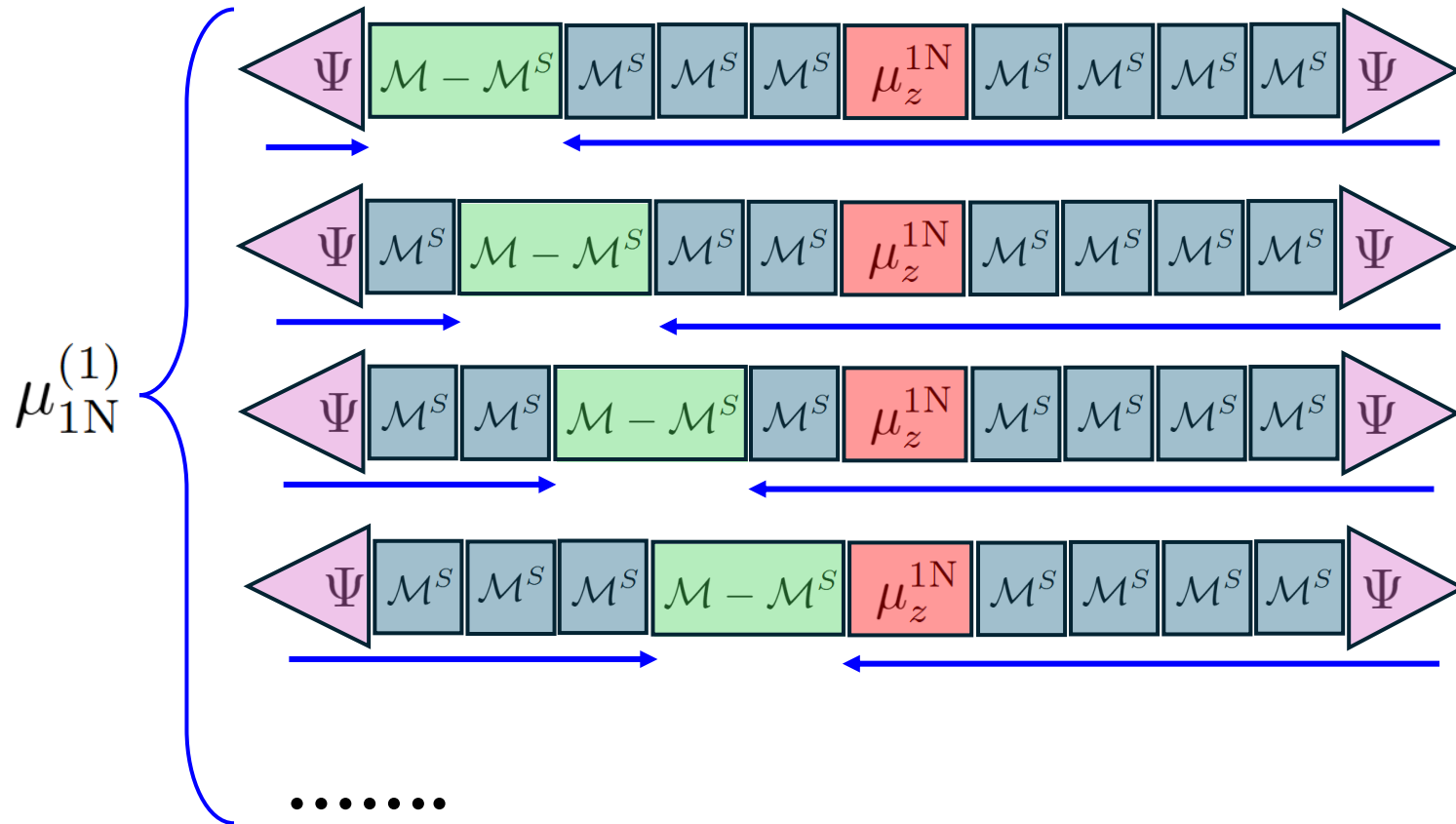
■ derivative method

$$\mu_z^{1N} = \left. \frac{d}{d\epsilon} : e^{\epsilon \mu_z^{1N}} : \right|_{\epsilon=0}$$

Perturbative Calculation of Dipole Moments

- How to calculate perturbative terms at different orders.

↪ Numerical realization of the **first order** perturbative term



■ auxiliary field transformation

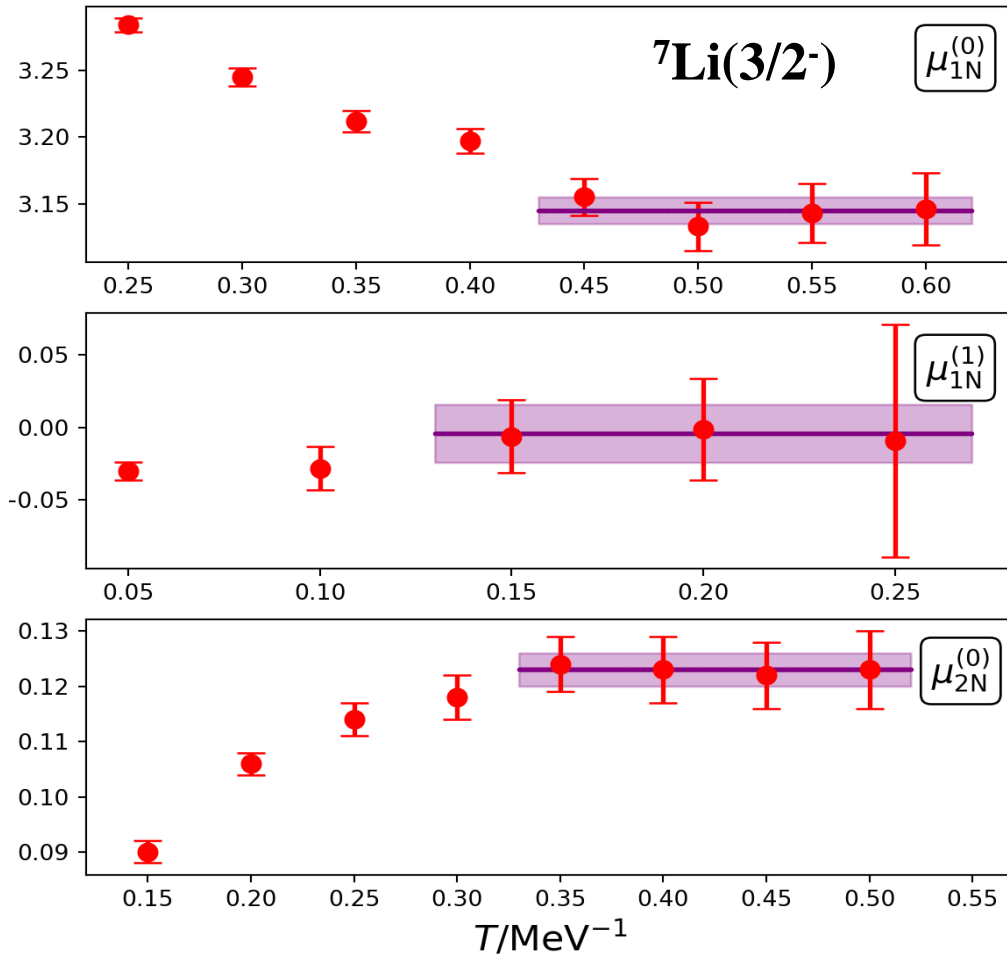
■ derivative method

$$\mu_z^{1N} = \left. \frac{d}{d\epsilon} : e^{\epsilon \mu_z^{1N}} : \right|_{\epsilon=0}$$

■ Jacobi formula

Data Analysis

- The contributions of different perturbative terms are calculated separately.



- Uncertainty analysis.

➔ Statistical uncertainty

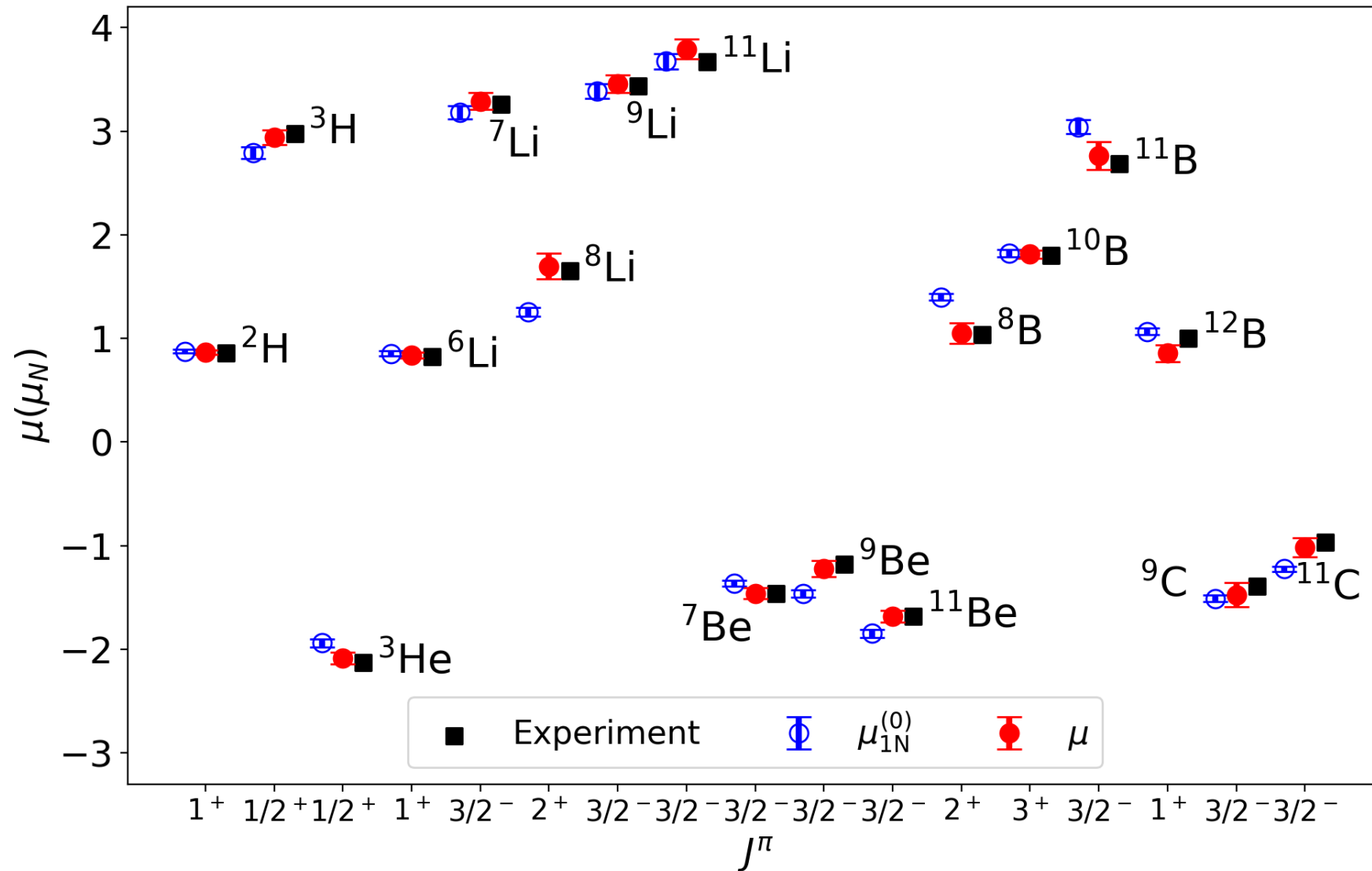
➔ Systematic uncertainties

○ A 2% uncertainty due to lattice artifacts

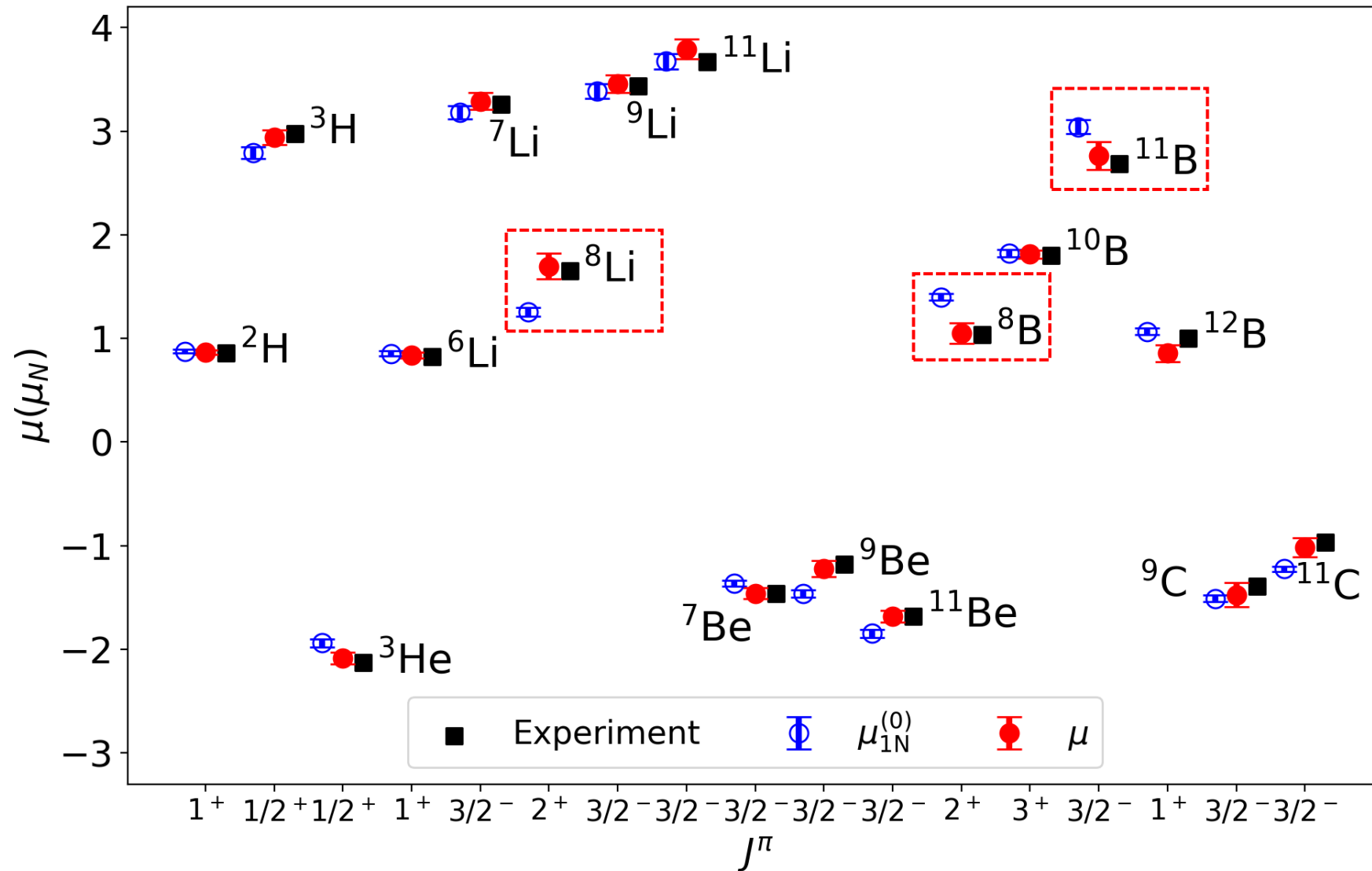
○ An additional 25% uncertainty assigned to $\mu_{1N}^{(1)}$ due to excited states' contamination

○ Model dependence of the nuclear forces and currents(not considered yet)

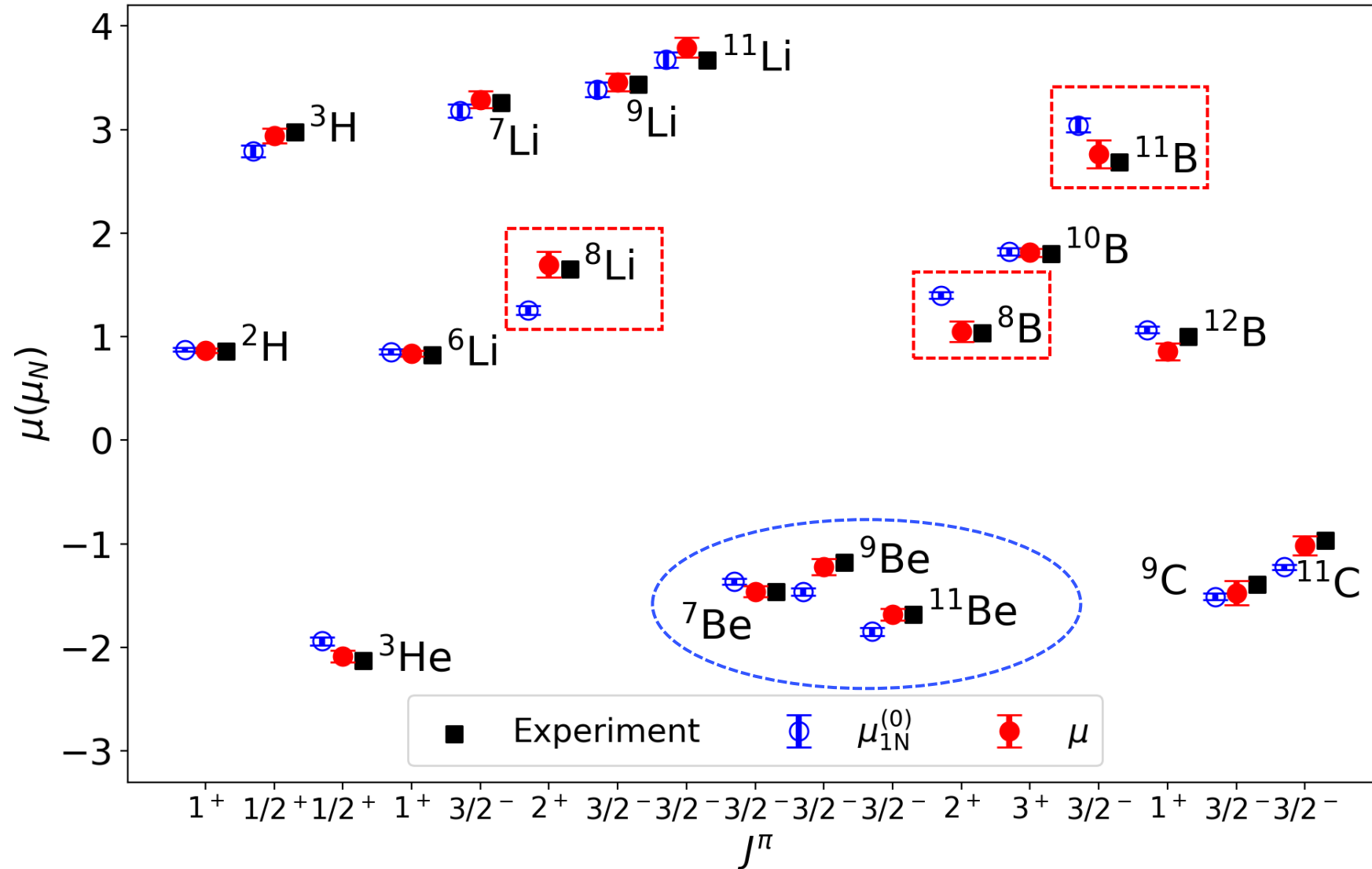
Results of s - and p -shell nuclei



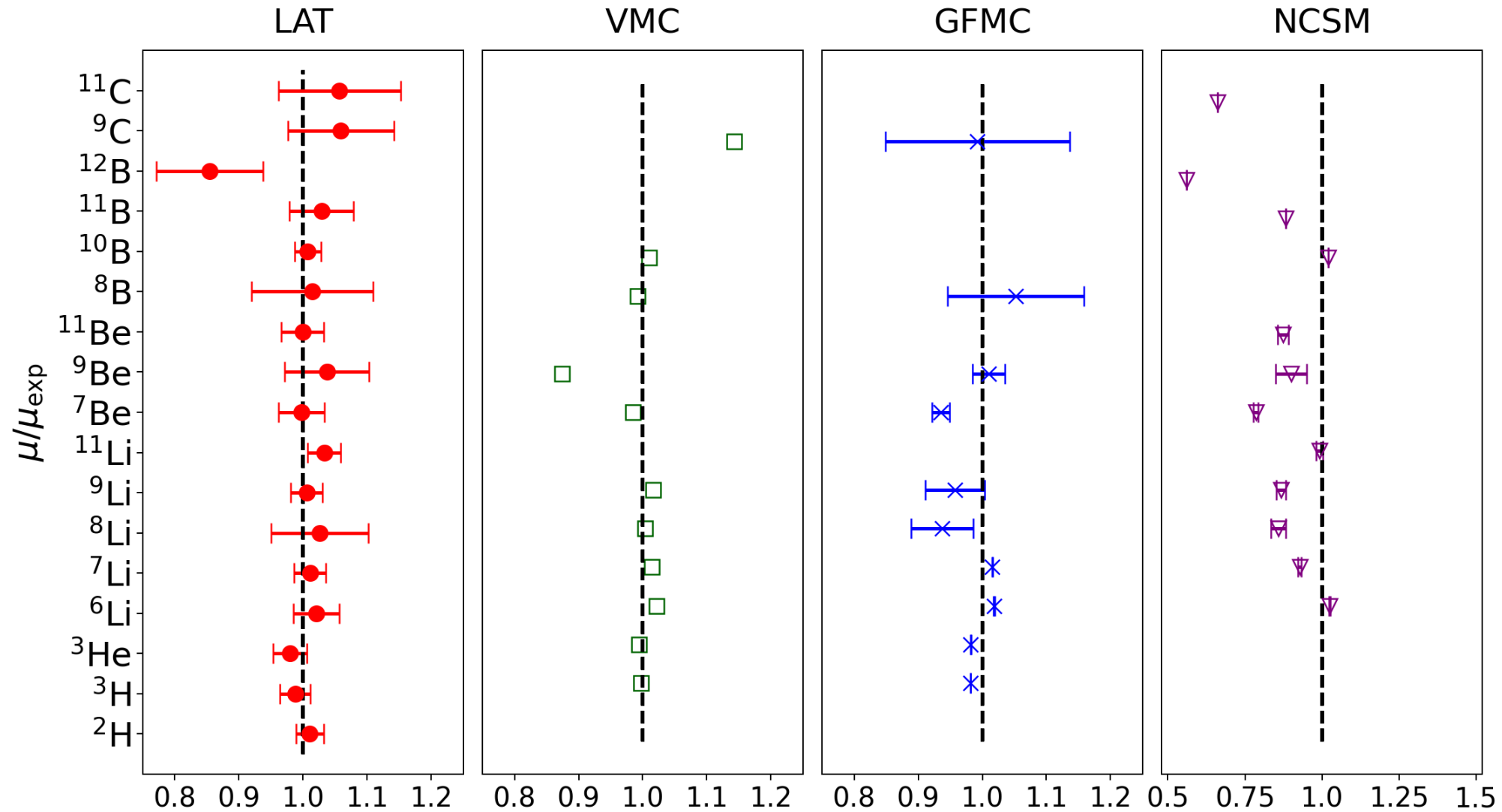
Results of s - and p -shell nuclei



Results of s - and p -shell nuclei

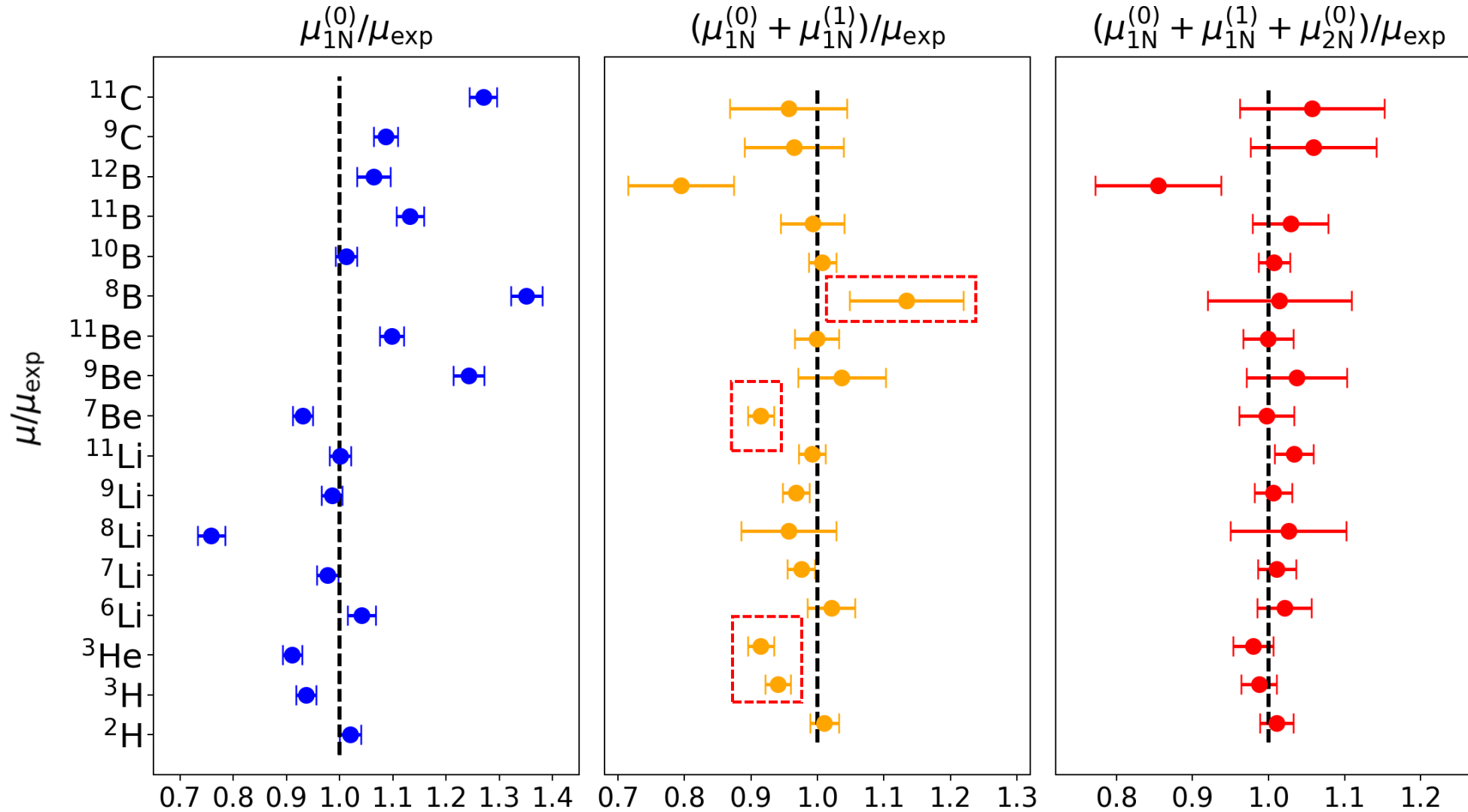


Comparison with Other Methods

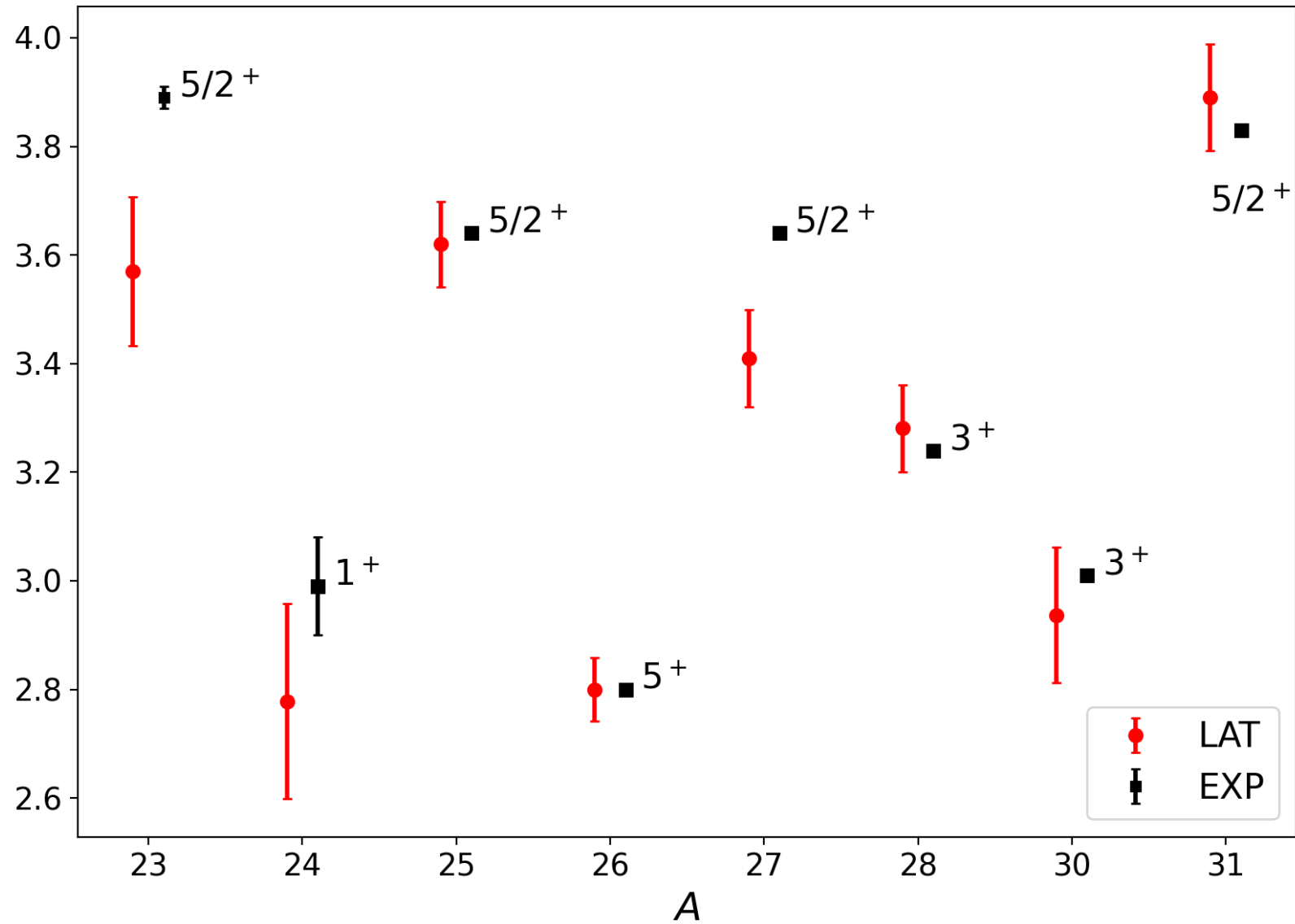


Contributions of Different Terms

$$\mu \approx \mu_{1N}^{(0)} + \mu_{1N}^{(1)} + \mu_{2N}^{(0)}$$



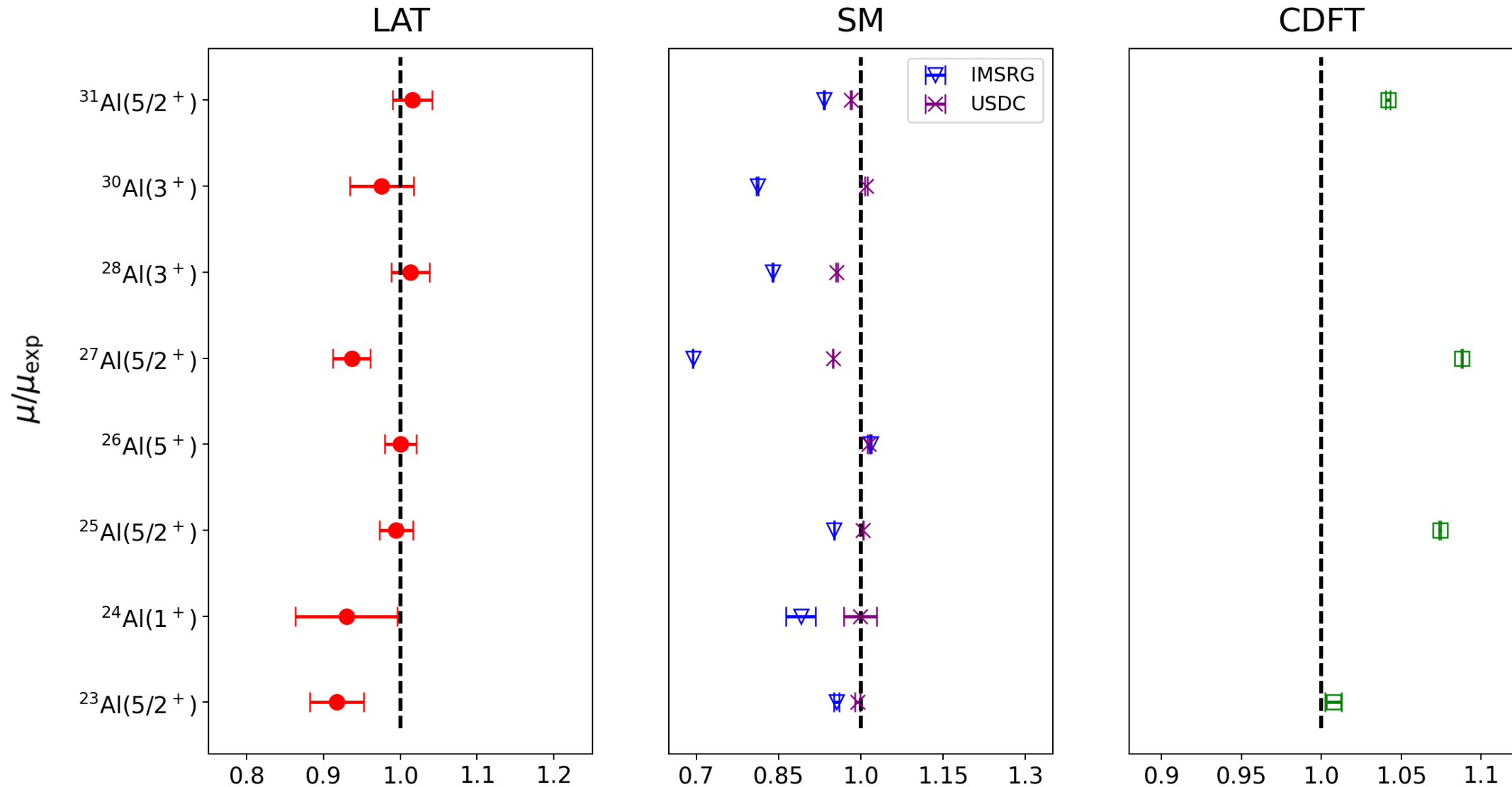
Results of Aluminum Isotopes



Comparison with Other Methods

SM: A. Saxena and P. C. Srivastava, PRC 96, 024316(2017)

CDFT: L. Jian and W. J. Sun, Commun. Theor. Phys. 72, 055301(2020)



Conclusions and Perspectives

- This work is the first NLEFT calculation of nuclear magnetic dipole moments.
 - Our result is in overall agreement with the experiment.
 - Our work gives a critical test on chiral EFT, including the chiral electromagnetic currents and the recently developed N³LO chiral interaction on the lattice.
 - Our work shows that NLEFT is competitive in calculating basic properties of atomic nuclei.
- Perspectives.
 - A further investigation on various uncertainties.
 - A systematic calculation of higher-order moments.
 - A generalization to electromagnetic and electroweak transitions.

Thank You!